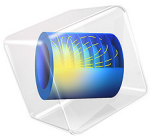
Created in COMSOL Multiphysics 5.6



InGaN/AlGaN Double Heterostructure LED

This model simulates a GaN-based light emitting diode (LED). It demonstrates how the Semiconductor interface can be used to evaluate optical emission from electrically driven optoelectronic devices using the Optical Transition feature. It also gives an example of how current-driven problems can be solved by first generating suitable initial conditions from voltage-driven studies. The emission spectrum, intensity, and quantum efficiency are calculated as a function of the driving current in order to evaluate the optimum operating conditions. Note that quantum confinement effects within the thin active region are not included in the model.

Introduction

LEDs are revolutionizing the lighting industry, as they are often much more efficient and durable than traditional incandescent light technologies. For example, typical consumer LED light bulbs operate at 10–20% of the power needed to run an incandescent bulb of comparable brightness and have lifetimes of over 25,000 hours, compared to only 1000 hours for incandescent bulbs. LEDs are so much more efficient than incandescent bulbs because they function in a very different way. LEDs are semiconductor devices that emit light when electrons in the conduction band transition across the band gap via radiative recombination with holes in the valence band. Incandescent bulbs rely on resistive heating of a filament, which emits light when it has become hot enough to glow. This uses lots of energy just to heat the filament, and only a smaller fraction of output energy goes into light production. The high temperatures involved also lead to shorter lifetimes, as burnt out filaments are nearly always the cause of incandescent bulb failures.

Unlike incandescent bulbs, LEDs emit light over a very narrow range of wavelengths. Initially, red, green, and yellow LEDs were developed in the 1950s–1960s; however, it was the invention of the blue LED that led to the creation of new efficient white light sources. Blue light emitted from such LEDs can be used to stimulate a wider spectrum of emission from a phosphor layer around the LED casing or can be directly combined with red and green LEDs to create white light.

The blue LEDs were more challenging to develop in part because they require a larger band-gap material. The first high efficiency blue LED was created in 1994, and the 2014 Noble Prize in Physics was awarded to Isamu Akasaki, Hiroshi Amano, and Shuji Nakamura for their work toward this achievement. A summary of the history of LED development can be found in Ref. 1.

Although LEDs are much more efficient than previous lighting technology, there are still some science and engineering challenges to overcome to further improve their design. In particular, the efficiency of LEDs decreases at larger driving currents. This phenomenon

is known as LED droop and causes the total emitted light to increase sublinearly with increased current bias, restricting the intensity that can be achieved whilst maintaining high efficiency. Consequently, to increase the total brightness it is often necessary to increase the area of the device, or add additional LEDs to a bulb, rather than simply applying more current. This adds to the expense of the bulb and increases the cost of LED products.

In this model, the active light-emitting region of a GaN-based blue LED is modeled. The emission properties are investigated as a function of driving current, and the efficiency is calculated.

Model Definition

The materials and geometry of this model are based on the device described by Nakamura et al. in Ref. 2. Only the active double heterojunction region, from which the desired wavelength of light is emitted, is modeled. This region consists of a 50 nm thick layer of $In_{0.06}Ga_{0.94}N$, sandwiched between 0.15 µm thick layers of $Al_{0.15}Ga_{0.85}N$. As the device is laterally invariant, it can be modeled using a 1D line cut in the z direction, as shown in Figure 1. The cross sectional area of the device is calculated assuming the active region has lateral dimensions of 200-by-200 µm, which is a typical LED mesa size.

The lower AlGaN layer is n-doped and the upper AlGaN layer is p-doped. The InGaN layer is undoped. This creates a PIN diode structure, with the light emitting InGaN layer in the central intrinsic (undoped) region. The material properties are based on the GaN material from the semiconductor module material library. However, the band-gap energy and electron affinity values have been changed to reflect the In and Al alloy compositions. Note that the band gap of the InGaN material has been selected to match the spectral range of the emission from the device in Ref. 2. As well as amending these properties, Auger recombination factors and carrier lifetimes for Trap-Assisted recombination have been added to the materials. Values for these properties were found in Ref. 3 and Ref. 4. Note that quantum confinement effect are not included in this model.

Although the polarization charge effect is not included in this model, it is straightforward to add it by first computing the surface and/or space charge densities from the polarization field, then enter them into the **Surface Charge Density** boundary condition and/or the **Space Charge Density** domain condition.

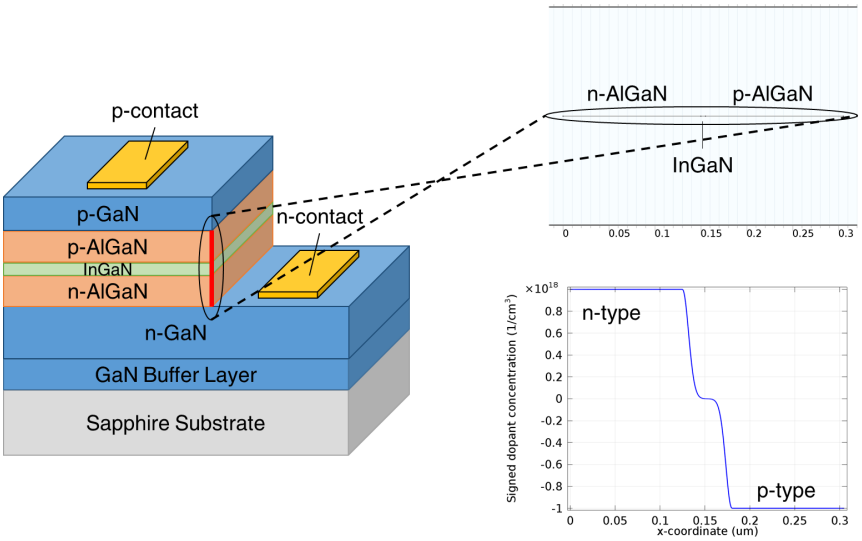


Figure 1: Geometry and doping of the LED device. Left: Structure of the LED on which this model is based. The section which is modeled is highlighted with a red bar. Top right: The geometry models the double heterostructure region of the full device. Lower-right: The doping profile is a PIN diode with the InGaN layer forming the intrinsic region.

Metal contact boundary conditions are applied to the bounds of the geometry in order to apply voltage and current biases to the device. In addition, a second Continuity/ Heterojunction boundary condition is added to enable toggling between the continuous quasi-Fermi levels and thermionic emission heterojunction continuity models. An Optical Transitions feature is used to calculate the spontaneous emission from the device. Non-radiative recombination mechanisms are included via Auger Recombination and Trap-Assisted Recombination features, which are added to all domains.

Three studies are used to solve the current driven model. The first study is a preliminary study, which uses the **Semiconductor Equilibrium** study step to obtain the equilibrium solution as the initial condition for the following study.

The equation system for heterojunctions is highly nonlinear and numerically challenging. In this tutorial we uses the **Semiconductor Equilibrium** study step to achieve better convergence. See the verification model example `heterojunction_1d` for more ways to overcome the numerical challenge.

The second study is a voltage biased study, which sweeps the applied voltage across the device from 0 to 3.3 V. From this study, the energy level diagram for the device is created, along with the carrier concentration distribution and a current-voltage curve.

The final study is a current biased study, which sweeps the applied current driven through the device over several orders of magnitude from 1 μA to 700 mA. This study uses a solution from the voltage driven study as the initial conditions in order to converge. The data from this study is added to the current-voltage curve to ensure agreement with the voltage driven case. The emission rate throughout the device, emission spectrum from the InGaN material, total emission rate integrated over the InGaN layer, and internal quantum efficiency, are then plotted as a function of the current bias.

Results and Discussion

The energy level diagram for the device is shown at two different voltage biases in Figure 2 and Figure 3. The conduction and valence band are labeled `semi.Ec` and `semi.Ev`, respectively, and the electron and hole quasi-Fermi levels are labeled `semi.Efn` and `semi.Efp`, respectively. In both cases the PIN doping is apparent, as it causes a potential barrier between the left hand n-doped region and the right hand p-doped region. The lower band gap InGaN layer causes a potential well in both the conduction and valence bands. For a fully accurate simulation quantum confinement effects of this 50 nm thick well should be accounted for. These effects are not included in this model. The main consequence of this is that the calculated emission spectrum will not include contributions from bound exciton states or transitions between quantum confined energy levels in the two potential wells. In the zero bias case (Figure 2) the quasi-Fermi levels are far from the band edges in the InGaN layer. This is expected when the device is in equilibrium and no light is being emitted. When a voltage of 3.3 V is applied to the p-side of the device (Figure 3) the forward bias has reduced the height of the potential barrier between the n-type and p-type regions as expected. The electron quasi-Fermi energy level is now above the conduction band edge in the InGaN layer, so we expect the conduction band to be populated with electrons in this region. The hole quasi-Fermi energy level is very close to the valence band edge, so we expect the valence band to be populated with holes.

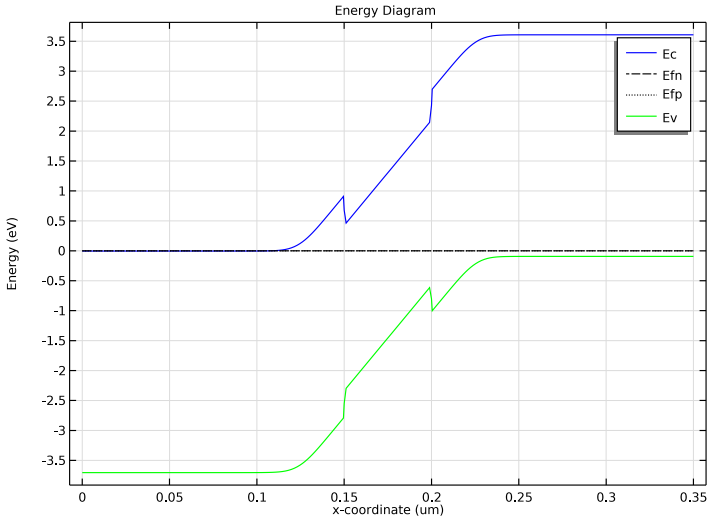


Figure 2: Energy level diagram for the case of zero bias. The conduction band (semi.Ec) and valence band (semi.Ev) show a potential barrier between the left hand n-doped and right hand p-doped regions. The InGaN layer creates a potential well in both bands.

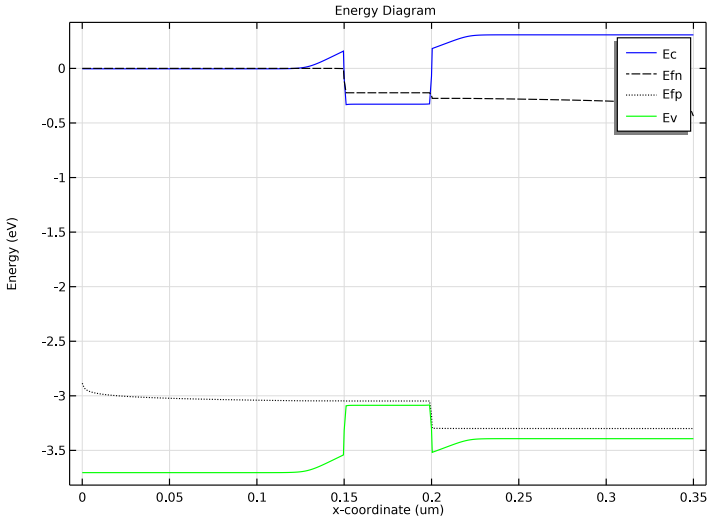


Figure 3: Energy level diagram for a forward voltage bias of 3.3 V. The height of the potential barrier has been reduced by the forward bias.

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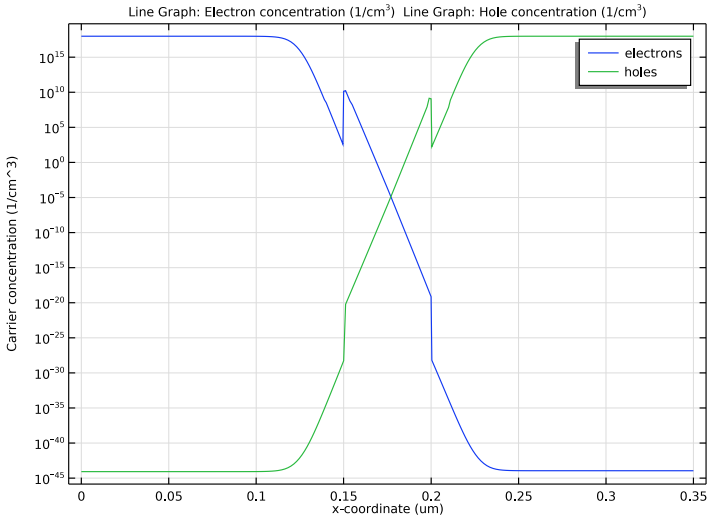

Figure 4: Carrier concentration at zero bias. The n-type and p-type regions have large concentrations of electron and holes, respectively. The depleted region has a small increase in carrier concentration in the InGaN layer due to the potential well, however the concentration is orders of magnitude smaller than the surrounding material.

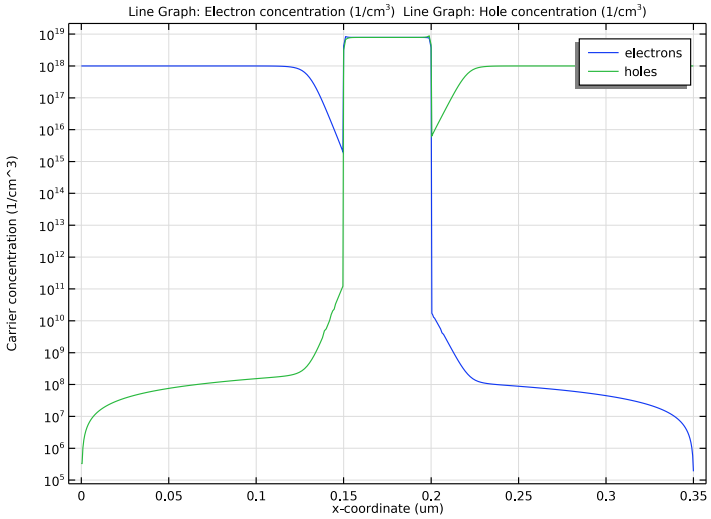

Figure 5: Carrier concentration at a 3.3 V forward bias. The InGaN layer is heavily populated with both electrons in the conduction band and holes in the valence band.

Figure 4 and Figure 5 show the carrier concentration throughout the device at zero and 3.3 V forward bias, respectively. As expected, the InGaN region is not populated with carriers in the equilibrium case, but the application of a forward bias causes carriers to collect in the potential well created by the InGaN layer. Importantly, the concentration of electrons in the conduction band is of similar magnitude to the concentration of holes in the valence band. This allows for efficient light output, as each photon that is emitted requires an electron to recombine across the band gap with a hole.

Figure 6 shows the emission rate throughout the device for the range of current biases. In all cases the emission from the InGaN layer is significantly larger than in the cladding material. This is because the InGaN layer is the only region of the device which has a high concentration of both electrons and holes. As the current bias increases so does the rate of emission, due to the increased carrier injection rate.

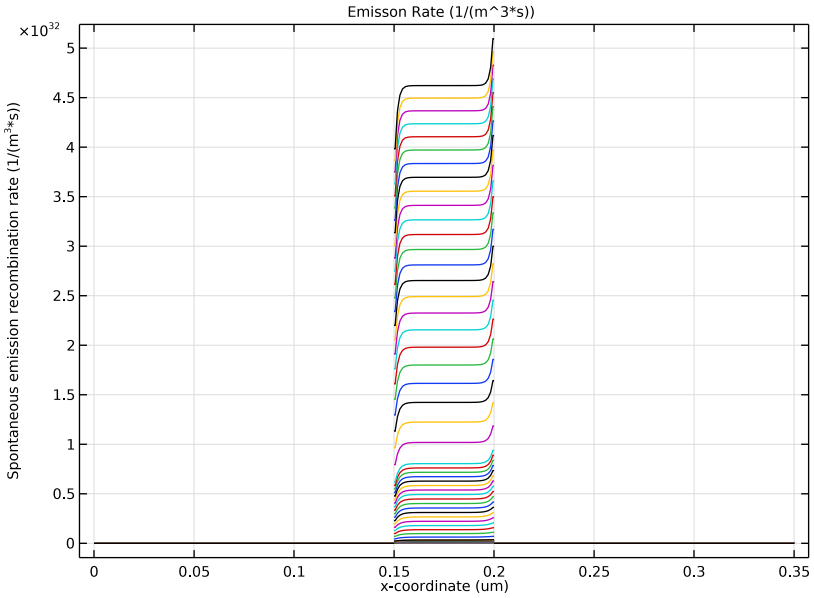

Figure 6: Emission rate throughout the device for a range of current biases. The emission rate is largest in the InGaN layer, as this region has a plentiful supply of both electrons in the conduction band and holes in the valence band.

The emission spectrum from the center of the InGaN layer is shown in Figure 7. The peak emission occurs around photon energies of 2.8–2.9 eV, which corresponds to a wavelength range of ~430–445 nm. This falls inside the target blue range of the spectrum, as expected since the band gap for the InGaN layer was calculated to match the emission

spectrum from the device described in Ref. 2. Again it is clear that with increased current the total emission intensity increases.

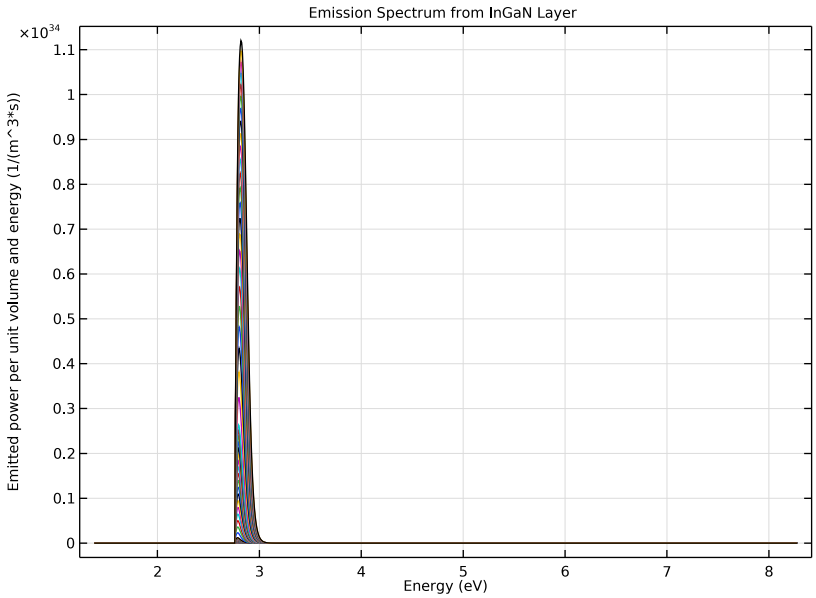

Figure 7: Emission spectrum from the center of the InGaN layer.

Although the total light emitted increases with current bias, it is not always favorable to simply operate at larger currents to increase the device brightness. This is because the efficiency of the device decreases with increased current density, resulting in a sublinear increase in the total emission rate with current bias. Figure 8 shows the total emission rate from the InGaN layer as a function of the applied current bias, and this effect is clearly visible. This phenomenon is known as LED droop, and is a subject of ongoing research within the solid-state lighting community. One metric by which the efficiency can be assessed is the Internal Quantum Efficiency (IQE). This is the fraction of injected carriers that radiatively recombine in the InGaN layer. Figure 9 shows the IQE as a function of the current density. There is a peak in the IQE at current densities around 30 A cm^{-2} and for densities in excess of ~100 A cm^{-2} there is a rapid drop off in the IQE. The peak efficiency

is achieved with applied currents in the 10–30 mA range, which is typical for LED devices of this size.

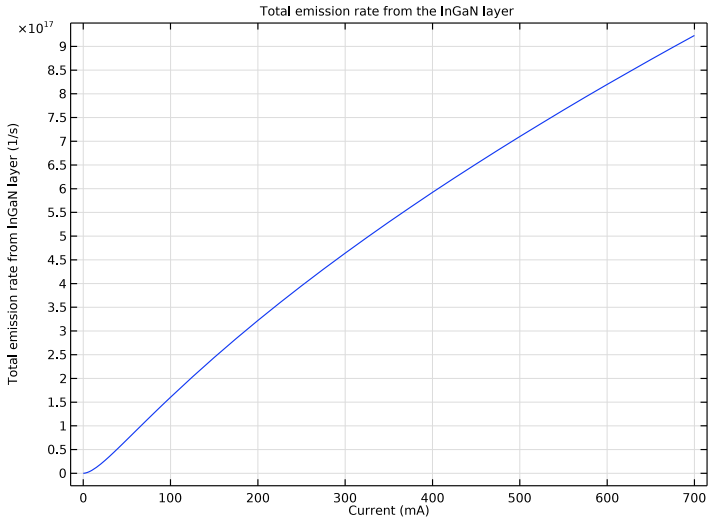

Figure 8: Total emission rate from the InGaN layer as a function of current bias. The sublinear increase is characteristic of LED droop and is common to LED devices.

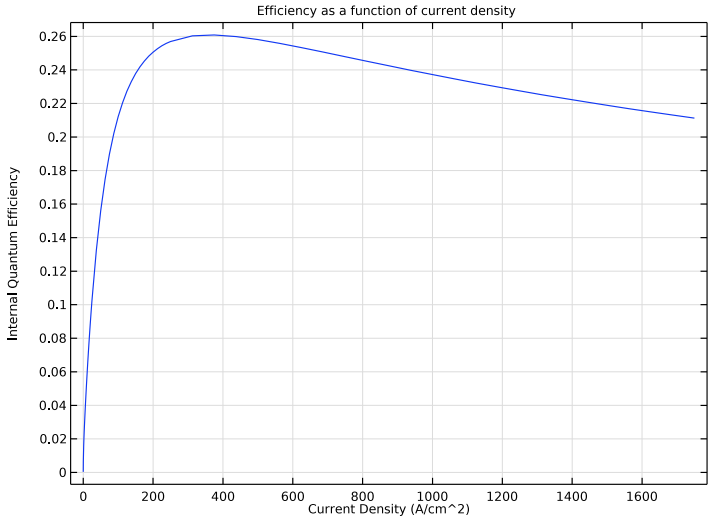

Figure 9: Internal Quantum Efficiency as a function of current density. The rapid decrease for densities above ~100 A cm^{-2} limits the current bias which can be applied whilst maintaining acceptable efficiency.

The current-voltage curve in Figure 10 highlights the significance of the LED droop problem. The optimum efficiency occurs at currents which are only slightly above the turn-on threshold. The device could function at much larger currents without any electrical issues, however the drop in IQE limits the current to a small fraction of its potential maximum value if high efficiency is desired.

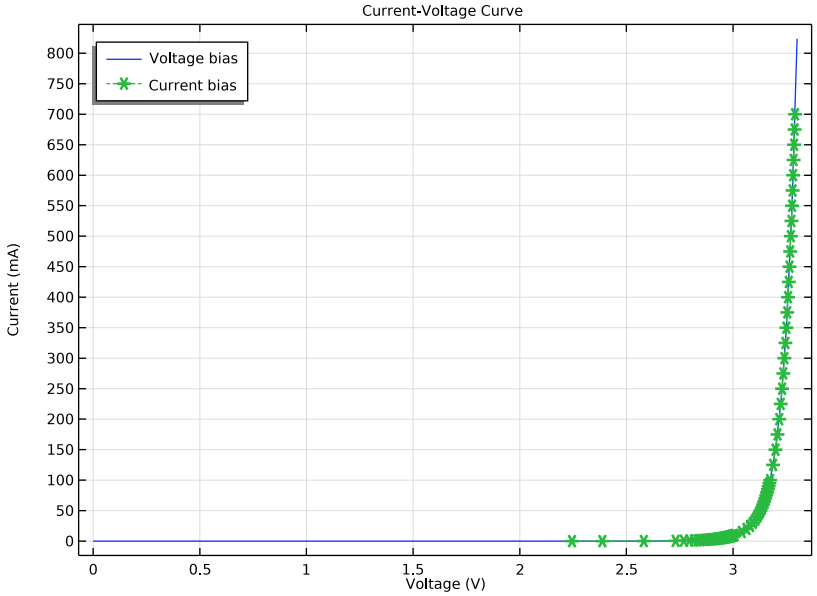

Figure 10: The current-voltage curve for the device under both voltage and current bias. The two studies are in agreement. The optimum efficiency is achieved with currents in the 10-30 mA range, which occur at voltage slightly above the turn-on threshold.

The cause of LED droop is yet to be fully understood. In this model, the drop in IQE is due to the nonradiative recombination mechanisms which are included. The rate of Auger recombination is proportional to the cube of the carrier density, whilst the rate of direct radiative recombination is proportional to only the square of the carrier density. This causes the fraction of recombination events which occur via the radiative mechanism to greatly reduce as the carrier density is increased. Hence the drop in efficiency for increased current densities.

References

1. *The Nobel Prize in Physics 2014 - Advanced Information. Nobelprize.org.,* Nobel Media AB 2014. Web. 29 Oct 2014. http://www.nobelprize.org/nobel_prizes/physics/laureates/2014/advanced.html

2. S. Nakamura,T. Mukia, and M. Senoh, "Candelaclass highbrightness InGaN/AlGaN doubleheterostructure bluelight emitting diodes," *Appl. Phys. Lett.*, vol. 64, p. 1687, 1994.

3. Y.C. Shen, G.O. Mueller, S. Watanabe, N.F. Gardner, A. Munkholm, and M.R. Krames, "Auger recombination in InGaN measured by photoluminescence," *Appl. Phys. Lett.*, vol. 91, p. 141101, 2007.

4. Q. Dai and others, "Internal quantum efficiency and nonradiative recombination coefficient of GaInN/GaN multiple quantum wells with different dislocation densities," *Appl. Phys. Lett.*, vol. 94, p. 111109, 2009.

Application Library path: `Semiconductor_Module/Photonic_Devices_and_Sensors/gan_double_heterostructure_led`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

2 In the **Select Physics** tree, select **Semiconductor>Semiconductor (semi)**.

3 Click **Add**.

The first study will be a preliminary study that is used to create initial conditions for the subsequent voltage biased study. This is needed due to the nonlinear nature of the equations involved in modeling recombination effects and heterojunctions.

There are several different ways to overcome the numerical challenge posted by the nonlinearity in the equation system. Here we use the **Semiconductor Equilibrium** study step to obtain the equilibrium solution as the initial condition for the following study.

For other alternative ways to achieve convergence, see the verification model example heterojunction_1d.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Semiconductor Equilibrium**.

6 Click **Done**.

Add some global parameters to the model.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
V_n	0[V]	0 V	n-contact voltage
V_p	0[V]	0 V	p-contact voltage
InGaN_bg	((h_const*c_const)/450[nm])/(1.6e-19[C])	2.759 V	Band gap energy of InGaN layer
I_p	1e-6[A]	1E-6 A	p-contact current
A_cross	200[um]*200[um]	4E-8 m^2	Cross sectional area

Create the model geometry.

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **µm**.

Interval 1 (i1)

1 Right-click **Component 1 (comp1)>Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (μm)
0
0.15[um]

Interval 2 (i2)

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (μm)
0.15[um]
0.2[um]

Interval 3 (i3)

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (μm)
0.2[um]
0.35[um]

Add materials to the geometry domains. The two cladding layers are $Al_{0.15}Ga_{0.85}N$, which has a band gap energy of 3.7 eV. The central layer is $In_{0.06}Ga_{0.94}N$. The band gap energy of the InGaN has been estimated from the emission spectra in the reference paper. The electron affinity of the InGaN has been set such that the central layer creates a potential well for both electrons in the conduction band and holes in the valence band.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Semiconductors>GaN (Zinc Blende) - Gallium Nitride**.

4 Click **Add to Component** in the window toolbar.

5 Click **Add to Component** in the window toolbar.

MATERIALS

Al_0.15_Ga_0.85_N

1 In the **Settings** window for **Material**, type `Al_0.15_Ga_0.85_N` in the **Label** text field.

2 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Band gap	Eg0	`3.7[V]`	V	Semiconductor material

In_0.06_Ga_0.94_N

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **GaN (Zinc Blende) - Gallium Nitride 1 (mat2)**.

2 In the **Settings** window for **Material**, type `In_0.06_Ga_0.94_N` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `2` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Material**, locate the **Material Contents** section.

7 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Band gap	Eg0	`InGaN_bg`	V	Semiconductor material
Electron affinity	chi0	`4.6[V]`	V	Semiconductor material

8 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

Create a nonlocal integration coupling in the component definitions node. This will allow the emission rate to be integrated over the entire InGaN layer when creating graphs later.

DEFINITIONS

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `2` in the **Selection** text field.

5 Click **OK**.

Next configure the physics in the Semiconductor interface.

SEMICONDUCTOR (SEMI)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.

2 In the **Settings** window for **Semiconductor**, locate the **Cross-Section Area** section.

3 In the A text field, type `A_cross`.

4 Locate the **Model Properties** section. From the **Carrier statistics** list, choose **Fermi-Dirac**.

n Doping

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `n Doping` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Distribution** section. From the list, choose **Box**.

5 Locate the **Impurity** section. From the **Impurity type** list, choose **Donor doping (n-type)**.

6 In the N_{D0} text field, type `1e18[1/cm^3]`.

7 Locate the **Uniform Region** section. In the W text field, type `0.125[um]`.

8 Locate the **Profile** section. In the d_j text field, type `0.025[um]`.

p Doping

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `p Doping` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Distribution** section. From the list, choose **Box**.

5 Locate the **Impurity** section. In the N_{A0} text field, type `1e18[1/cm^3]`.

6 Locate the **Uniform Region** section. Specify the r_0 vector as

`0.225[um]`	X

7 In the W text field, type `0.125[um]`.

8 Locate the **Profile** section. In the d_j text field, type `0.025[um]`.

n Contact

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 In the **Settings** window for **Metal Contact**, type `n Contact` in the **Label** text field.

3 Select Boundary 1 only.

4 Locate the **Terminal** section. In the V_0 text field, type `V_n`.

p Contact

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 In the **Settings** window for **Metal Contact**, type `p Contact` in the **Label** text field.

3 Select Boundary 4 only.

4 Locate the **Terminal** section. In the V_0 text field, type `V_p`.

Continuity/Heterojunction - Thermionic Emission

1 In the **Physics** toolbar, click **Boundaries** and choose **Continuity/Heterojunction**.

2 In the **Settings** window for **Continuity/Heterojunction**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

4 In the **Label** text field, type `Continuity/Heterojunction - Thermionic Emission`.

5 Locate the **Heterojunction** section. From the **Continuity model** list, choose **Thermionic emission**.

Optical Transitions 1

1 In the **Physics** toolbar, click **Domains** and choose **Optical Transitions**.

2 In the **Settings** window for **Optical Transitions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Optical Transitions** section. Clear the **Stimulated absorption and emission** check box.

p Contact - Current

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 In the **Settings** window for **Metal Contact**, type `p Contact - Current` in the **Label** text field.

3 Select Boundary 4 only.

4 Locate the **Terminal** section. From the **Terminal type** list, choose **Current**.

5 In the I_0 text field, type `I_p`.

Auger Recombination 1

1 In the **Physics** toolbar, click **Domains** and choose **Auger Recombination**.

2 In the **Settings** window for **Auger Recombination**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

Trap-Assisted Recombination 1

1 In the **Physics** toolbar, click **Domains** and choose **Trap-Assisted Recombination**.

2 In the **Settings** window for **Trap-Assisted Recombination**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

The two nonradiative recombination mechanisms require extra material properties to be added. Auger recombination factors and Shockley-Read-Hall (SHR) carrier lifetimes have been looked up in recent literature, however these parameters are highly dependent on the material growth conditions so there is a rather wide range of plausible values.

MATERIALS

Al_0.15_Ga_0.85_N (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Al_0.15_Ga_0.85_N (mat1)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Auger recombination factor, electrons	Cn	`1.7e-30[cm^6/s]`	m^6/s	Auger recombination
Auger recombination factor, holes	Cp	`1.7e-30[cm^6/s]`	m^6/s	Auger recombination
Electron lifetime, SRH	taun	`1e-8`	s	Shockley-Read-Hall recombination
Hole lifetime, SRH	taup	`1e-8`	s	Shockley-Read-Hall recombination

In_0.06_Ga_0.94_N (mat2)

1 In the **Model Builder** window, click **In_0.06_Ga_0.94_N (mat2)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Auger recombination factor, electrons	Cn	`1.7e-30[cm^6/s]`	m^6/s	Auger recombination
Auger recombination factor, holes	Cp	`1.7e-30[cm^6/s]`	m^6/s	Auger recombination
Electron lifetime, SRH	taun	`1e-8`	s	Shockley-Read-Hall recombination
Hole lifetime, SRH	taup	`1e-8`	s	Shockley-Read-Hall recombination

Configure a suitable mesh.

MESH 1

Edge 1

1 In the **Mesh** toolbar, click **Edge**.

2 In the **Settings** window for **Edge**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Entire geometry**.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

2 Select Domains 1 and 3 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type `100`.

6 In the **Element ratio** text field, type `6`.

7 Select the **Symmetric distribution** check box.

Distribution 2

1 In the **Model Builder** window, right-click **Edge 1** and choose **Distribution**.

2 Select Domain 2 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type `30`.

6 In the **Element ratio** text field, type 2.

7 Select the **Symmetric distribution** check box.

8 Click **Build All**.

Configure the first study, which is a preliminary study that is used to create initial conditions for the subsequent voltage biased study. This is needed due to the nonlinear nature of the equations involved in modeling recombination effects and heterojunctions.

There are several different ways to overcome the numerical challenge posted by the nonlinearity in the equation system. Here we use the **Semiconductor Equilibrium** study step to obtain the equilibrium solution as the initial condition for the following study. For other alternative ways to achieve convergence, see the verification model example heterojunction_1d.

STUDY 1: PRELIMINARY STUDY

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1: Preliminary study` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

4 In the **Home** toolbar, click **Compute**.

Next configure the second study to perform a voltage bias sweep. The voltage across the device will be varied from 0 to 3.5 V by sweeping the value of the parameter `V_p`. The solution from the preliminary study is used for the initial values of the dependent variables.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2: VOLTAGE BIAS

1 In the **Model Builder** window, click **Study 2**.

2 In the **Settings** window for **Study**, type `Study 2: Voltage bias` in the **Label** text field.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 2: Voltage bias** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>p Contact - Current**.

5 Click **Disable**.

6 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

7 From the **Method** list, choose **Solution**.

8 From the **Study** list, choose **Study 1: Preliminary study, Semiconductor Equilibrium**.

9 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

10 Click **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V_p (p-contact voltage)	`range(0,0.1,3) range(3.025, 0.025,3.3)`	V

12 In the **Home** toolbar, click **Compute**.

RESULTS

Energy Levels (semi)

The default plot groups show the energy level diagram, carrier concentrations, and electric potential for the device. Plotting only the data at one bias voltage allows the results to be viewed with more clarity.

1 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

2 Select the **x-axis label** check box.

3 In the associated text field, type `x-coordinate (um)`.

4 Locate the **Data** section. From the **Parameter selection (V_p)** list, choose **From list**.

5 In the **Parameter values (V_p (V))** list, select **0**.

6 In the **Energy Levels (semi)** toolbar, click **Plot**.

The response of the energy levels as the bias is increased can be observed by varying the value of V_p for which the data is plotted. This is done by selecting values from the **Parameter values (V_p)** selection box.

7 In the **Parameter values (V_p (V))** list, select **3.3**.

8 In the **Energy Levels (semi)** toolbar, click **Plot**.

As the forward bias is increased the height of the potential barrier between the n and p-type regions is reduced as the bands "flatten out". The quasi-Fermi levels also move closer to the band edges, reflecting the fact that more carriers are flowing through the device, leading to an increased probability that carriers are in the quantum well region formed by the lower band gap InGaN layer.

The Carrier Concentration plot shows that the population of carriers in the InGaN layer increases drastically with the increased bias. Again, this can be seen more clearly by selecting to plot data for one value of V_p at a time and switching through different values.

Carrier Concentrations (semi)

1 In the **Model Builder** window, click **Carrier Concentrations (semi)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **x-axis label** check box.

4 In the associated text field, type `x-coordinate (um)`.

5 Locate the **Data** section. From the **Parameter selection (V_p)** list, choose **From list**.

6 In the **Parameter values (V_p (V))** list, select **0**.

7 In the **Carrier Concentrations (semi)** toolbar, click **Plot**.

8 In the **Parameter values (V_p (V))** list, select **3.3**.

9 In the **Carrier Concentrations (semi)** toolbar, click **Plot**.

This is the expected behavior, as the bias is increased more current flows through the device and the carrier concentration in the InGaN layer is increased. Importantly, the concentration of both electrons and holes peaks in the InGaN layer, which causes the radiative recombination to be localized to this region. This will be seen when the rate of spontaneous emission throughout the devices is plotted after the next study.

The I-V curve for the device can be created by plotting the current as a function of the applied bias. This shows that the device displays typical diode behavior as expected.

Current vs. Voltage

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Current vs. Voltage` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Voltage bias/ Solution 2 (sol2)**.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Current-Voltage Curve`.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `Voltage (V)`.

8 Select the **y-axis label** check box.

9 In the associated text field, type `Current (mA)`.

10 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 Right-click **Current vs. Voltage** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`abs(semi.IO_1)`	`mA`	`Voltage bias`

4 In the **Current vs. Voltage** toolbar, click **Plot**.

Next configure a final study to perform a current bias sweep. This study will use the **p contact - current** boundary condition to apply a range of currents to the device. It uses a solution from the previous voltage driven study as an initial condition. In order to find which value of V_p gives the best initial solution for the current bias study, a global evaluation can be used to view the current as a function of `V_p` from the Voltage bias study.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2: Voltage bias/Solution 2 (sol2)**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`semi.IO_2`	`A`	`Terminal current`

5 Click **Evaluate**.

The current bias study will begin with an applied bias of 1 uA, from the table we can see that this magnitude of current flows when a voltage of `V_p`=2.2 V is applied. Therefore we will choose the corresponding solution for the initial condition in the current bias study, and set the **Initial voltage** input field of the current-driven metal contact boundary condition to the same value. Note that the range of applied currents is chosen to resolve

nonlinear features in the Current versus Voltage plot and a subsequent plot of the efficiency.

SEMICONDUCTOR (SEMI)

p Contact - Current

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)** click **p Contact - Current**.

2 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

3 In the V_{init} text field, type `2.2[V]`.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3: CURRENT BIAS

1 In the **Model Builder** window, click **Study 3**.

2 In the **Settings** window for **Study**, type `Study 3: Current bias` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 3: Current bias** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Values of Dependent Variables** section.

3 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 2: Voltage bias, Stationary**.

6 From the **Parameter value (V_p (V))** list, choose **2.2 V**.

7 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

8 Click **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
I_p (p-contact current)	`1e-6 1e-5 1e-4 range(5e-4,2.5e-4,10e-3) range(15e-3,5e-3,100e-3) range(125e-3,25e-3,700e-3)`	A

10 In the **Home** toolbar, click **Compute**.

Add the data from the current driven study to the Current vs. Voltage plot group.

RESULTS

Global 2

1 In the **Model Builder** window, under **Results>Current vs. Voltage** right-click **Global 1** and choose **Duplicate**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 3: Current bias/Solution 3 (sol3)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`abs(semi.IO_3)`	`mA`	`Current bias`

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `semi.VO_3`.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

9 From the **Positioning** list, choose **In data points**.

10 In the **Current vs. Voltage** toolbar, click **Plot**.

Plot the rate of radiative transitions throughout the device from the current bias dataset. Notice how the emission is concentrated in the active InGaN layer as expected, and that increasing the current increases the rate of emission.

Emission Rate

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Emission Rate` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Current bias/ Solution 3 (sol3)**.

4 Locate the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Emisson Rate (1/(m^3*s))`.

6 Locate the **Plot Settings** section. Select the **x-axis label** check box.

7 In the associated text field, type `x-coordinate (um)`.

Line Graph 1

1 Right-click **Emission Rate** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `semi.ot1.R_spon`.

5 In the **Emission Rate** toolbar, click **Plot**.

Create a solution dataset to hold the extra dimension data, which allows quantities to be plotted in the frequency domain. The emission spectrum from the InGaN layer can then be plotted.

Current bias study - frequency domain

1 In the **Results** toolbar, click **More Datasets** and choose **Solution**.

2 In the **Settings** window for **Solution**, locate the **Solution** section.

3 From the **Solution** list, choose **Solution 3 (sol3)**.

4 From the **Component** list, choose **Extra Dimension from Optical Transitions 1 (semi_ot1_xdim)**.

5 In the **Label** text field, type `Current bias study - frequency domain`.

The emission spectrum can be plotted using the expression `comp1.atxd1(0.1525e-6, semi.ot1.dP_dE)`. The variable `semi.ot1.dP_dE` is the emitted power per unit volume and energy. The command `comp1.atxd1(coord,var)` gets the variable `var`, which is calculated in an extra dimension attached to component 1, from coordinate `coord` in the model geometry.

In this case, coordinate 0.1525e-6 corresponds to the center of the InGaN layer, so this command gets `semi.ot1.dP_dE` as a function of frequency (the extra dimension) at this spatial point.

The default x-axis for the plot is a normalized variable which is proportional to the angular frequency, with $x = 1$ corresponding to the angular frequency of the band gap energy. In order to plot the data as a function of energy the expression `hbar_const*`

`comp1.atxd1(0.1525e-6,semi.ot1.omega)/e_const` is used. The variable `semi.ot1.omega` returns the angular frequency, which is then converted into energy in eV via multiplication by `hbar_const` and division by `e_const`.

Emission Spectrum

1. In the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Emission Spectrum` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Current bias study - frequency domain (sol3)**.
4. Locate the **Title** section. From the **Title type** list, choose **Manual**.
5. In the **Title** text area, type `Emission Spectrum from InGaN Layer`.
6. Locate the **Plot Settings** section. Select the **x-axis label** check box.
7. In the associated text field, type `Energy (eV)`.
8. Select the **y-axis label** check box.
9. In the associated text field, type `Emitted power per unit volume and energy (1/(m^3*s))`.

Line Graph 1

1. Right-click **Emission Spectrum** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. From the **Selection** list, choose **All domains**.
4. Locate the **y-Axis Data** section. In the **Expression** text field, type `comp1.atxd1(0.1525e-6,semi.ot1.dP_dE)`.
5. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
6. In the **Expression** text field, type `hbar_const*comp1.atxd1(0.1525e-6,semi.ot1.omega)/e_const`.
7. In the **Emission Spectrum** toolbar, click **Plot**.

From the emission rate and spectra it can be seen that as the current is increased the emission intensity of the LED increases. This can be seen more clearly by plotting the total emitted intensity integrated over the InGaN layer as a function of current bias.

Total Emission Rate from InGaN Layer vs. Current

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Total Emission Rate from InGaN Layer vs. Current` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Current bias/ Solution 3 (sol3)**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Current (mA)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Total emission rate from InGaN layer (1/s)`.

8 Locate the **Title** section. From the **Title type** list, choose **Manual**.

9 In the **Title** text area, type `Total emission rate from the InGaN layer`.

Global 1

1 Right-click **Total Emission Rate from InGaN Layer vs. Current** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit
`intop1(semi.ot1.R_spon)*A_cross`	

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `I_p`.

6 From the **Unit** list, choose **mA**.

7 Click to expand the **Legends** section. Clear the **Show legends** check box.

8 In the **Total Emission Rate from InGaN Layer vs. Current** toolbar, click **Plot**.

The emission intensity does not increase linearly with current. This is a phenomenon known as LED droop, which limits the emission intensity that can be obtained whilst maintaining reasonable efficiency.

The efficiency can be assessed by calculating the internal quantum efficiency (IQE) of the device, which is the fraction of injected carriers which radiatively recombine within the InGaN layer.

Efficiency

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Efficiency` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Current bias/ Solution 3 (sol3)**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Current Density (A/cm^2)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Internal Quantum Efficiency`.

8 Locate the **Title** section. From the **Title type** list, choose **Manual**.

9 In the **Title** text area, type `Efficiency as a function of current density`.

Global 1

1 Right-click **Efficiency** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit
`intop1(semi.ot1.R_spon)*A_cross/(semi.I0_3/e_const)`	1

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `semi.I0_3/(A_cross*10000)`.

6 Locate the **Legends** section. Clear the **Show legends** check box.

7 In the **Efficiency** toolbar, click **Plot**.

It is clear that the maximum efficiency is obtained for current densities around 30 A/cm^2 and that there is a sharp drop-off in efficiency for current densities in excess of around 100 A/cm^2, which is typical for LEDs fabricated in GaN based materials. This corresponds to an optimal operating current of 10 ~ 30 mA, which is typical for LEDs of this size. From the Current versus Voltage plot it can be seen that this current range occurs just above the turn-on voltage for the device, and that the electrical properties of the device would allow it to function at much larger currents. The rapid reduction in efficiency with increased current, which limits the operation current to a small fraction of its potential maximum, is thus a major hindrance to the development of LED lighting technologies.

The mechanisms responsible for this efficiency drop are the subject of active research. In this model the drop in efficiency is mainly due to Auger recombination, which occurs with a rate that is proportional to the cube of the carrier density. The rate of direct radiative transitions is proportional to the square of the carrier density. Thus, as the carrier density in the InGaN layer is increased with larger current densities the fraction of carriers which undergo Auger recombination increases. This leads to a reduction of the efficiency.