Modelling of GaN/InGaN Tricolour Multiple Quantum Well Light Emitting Diodes

Since lighting is estimated to account for 20% of the world’s electricity consumption, the search for reliable and efficient lighting technologies to replace incandescent and fluorescent modules is intense.

GaN/InGaN quantum well based light emitting diodes (LED) produce light in the ultra violet to the green range. This material plays a vital role in the production of white light through the use of phosphorus layers to obtain other wavelengths. This article focuses on the simulation of a triple quantum well GaN/InGaN structure with three emission peaks from wells of different thickness and molar fractions. This structure was published in Applied Physics Letters by Charash et. al. in 2009[1].

LED Structure Details

In the reported study by Charash et. al., four combinations of InGaN quantum wells were grown using metal organic vapour phase deposition epitaxy (MOVPE) on sapphire substrates. Following a layer of n-GaN three 2nm – 1.2nm InGaN wells were grown with 6nm GaN barrier layers in between. A top 130nm magnesium (Mg) doped p-GaN layer was grown to complete the structure.

In this article we have reproduced the results from one of the QW combinations that is shown in table 1. This device produced the highest light output.

The room temperature behaviour of this device was simulated using ATLAS BLAZE and reasonable agreement with observed measurements was obtained. To prepare this structure for ATLAS simulation, we used the AUTO parameter on the MESH statement. This will allow the user to build the structure layer by layer so that the input deck syntax will appear similar to the structure grown by MOVPE technique used to create these LEDs. Once the x.mesh statements were defined the user can then select the material, molar fraction, number of y mesh points and doping on each REGION statement. The BOTTOM logical parameter adds each layer below the previous one. This way the top layer appears at the top. This simplifies building and modifying the structure. When a layer is modified, the location and doping of all other layers are automatically adjusted. Here is a segment of the used syntax:

```
mesh AUTO
#
x.mesh loc=0.0 spac=0.5
x.mesh loc=1.0 spac=0.5
#
region num=1 material=GaN thickness=0.13
   ny=50 acceptors=1e17 bottom

# Top barrier
#~~~~~~~~~~~~
region num=2 material=GaN thickness=0.006
   ny=10 bottom acceptors=1e17

# Top Well QW – 3
#~~~~~~~~~~~~
region num=3 material=InGaN thickness=0.002
   ny=20 x.comp=0.25 name=well1 \ qwell led calc.strain polarization
   polar.scale=2.2 strain=0 bottom
```

There are useful facilities in defining the quantum well regions. Here we used the QWELL logical parameter for radiative and gain calculations for the optoelectronic models. The LED logical parameter signifies a region to be a light emitting region for subsequent post process analysis.

Since this material set is a Wurtzite material, both the polarisation and the strain have to be accounted for. A number of models have been implemented recently for these materials. The POLARIZATION logical parameter

<table>
<thead>
<tr>
<th>Structure</th>
<th>QW 1 Molar fraction, thickness and emission wavelength</th>
<th>QW 2 Molar fraction, thickness and emission wavelength</th>
<th>QW 3 Molar fraction, thickness and emission wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>5% In, 1.2nm, 380nm</td>
<td>15% In, 1.6nm, 430nm</td>
<td>25% In, 2.0nm, 490nm</td>
</tr>
</tbody>
</table>

Table 1. Quantum Well molar fractions and thicknesses used for structure B.
will enable the calculation of the interfacial charge due to the spontaneous and piezoelectric polarisation. The CALC.STRAIN will calculate the inbuilt strain in this region based on the lattice mismatch with the adjacent regions. An option to override this calculation is available to the user via the STRAIN parameter, which will assign a tensile or compressive strain depending on the sign of the value used.

ATLAS supports four sets of spontaneous polarisation and piezoelectric constants combinations for InN, GaN and AlN. The user can select any of these sets via the POL.SET parameter on the material statement. In this paper we used the default POL.SET=1. However, ATLAS supports a nonlinear polarisation model for AlInGaN and its ternary and binary compounds. Here the spontaneous and piezoelectric polarisation will have a quadratic dependence on composition and strain of the material identified. This model is selected by using the parameter POL.SET=4 [2-3].

The gain broadening, due to intra-band scattering, can be simulated by specifying the LORENTZ parameter on the models statement. To control the Lorenzian shape function the WELL.GAMMA0 parameter is defined on the material statement. This is used in this work to fit the measured data from this LED structure. Setting this parameter to zero by using WELL.GAMMA0=0 will force a zero broadening.

To account for the optical transitions between the conduction band and the heavy/light hole bands, we used the WZ.KP model. This is the same as the WZ.THREE model. This strained wurtzite model uses the k.p method for three valence bands. Using it on the models statement will use the WZ.THREE band structure parameter for the drift-diffusion equations. Finally to include the radiative recombination rate into the drift diffusion calculations, we use the SPONTANEOUS parameter on the models statement.

LED Behaviour Analysis

This structure produces three nominal emission peaks of 490nm, 430nm and 380nm. Here the simulation produced peaks shown in Figure 2.

At low bias conditions the electroluminescence (EL) obtained from this structure is dominated by the top well. Figure 2 shows that there are three orders of magnitude difference between the top and middle well emission. At higher bias conditions the middle well begins to contribute to the EL emission as can be seen in Figure 3. Under a current density flow of 2550 A/cm² the middle well shows a luminescence emission peak at 430nm that is just under a tenth of the principle peak at 500nm.

In order to obtain the spectral response in ATLAS use the SAVE statement with the SPECTRUM=myfile.SPC parameter. Here ATLAS will automatically find the spectral range. This is convenient when the lower and upper photon energies shift due to changing bias. However, the user can fix these bounds by using LMIN and LMAX parameters to limit the wavelength range used.

To explain this behaviour, the authors argue that given sufficient excitation power, all wells will emit using photoluminescence when carrier transport is not limited by the heterostructure bandgap profile. During electroluminescence, the electrons will be injected efficiently into all the three quantum wells from the n doped substrate. However, this process is limited by the hole transport and since QW 3 is closest to the p-doped contact, most of the EL emission is obtained from there. Under higher bias conditions contribution from the middle well will be noticed.

The simulation results bear this analysis out. We have generated device structure files at low and high bias conditions then obtained the band gap profile and the electron and hole density profiles.

![Figure 2. Three different luminescence emission peaks are obtained depending on the indium molar fraction, well thickness and proximity to the carrier injection source region.](image)

![Figure 3. Electroluminescence emission peaks at a current density of 2550 A/cm².](image)
Figure 4. Band structure at low and high bias conditions. QW band gap reflects the indium content. Sub-bands are not shown in this figure.

Figure 5. Electron and hole concentration profiles under low and high bias conditions.

Figure 5 shows that indeed the electron concentration is high for both low and high bias condition, while the hole concentration is reduced further away from the p-doped region. However at high bias conditions the concentration becomes significant in the middle well but remains low in the bottom well.

The carrier transport through the heterostructure is enhanced through thermionic emission and tunnelling. These two models were included in the simulation by adding THERMIONIC, TUNNEL and S.S parameters on the INTERFACE statement.

The IV and LI curves show similar behaviour to the reported data as can be seen in Figure 6.

Conclusions

We have demonstrated the simulation of tricolour InGaN/GaN multiple quantum well structure. The simulation captures the observed luminescence peaks and electroluminescence behaviour with increased bias. The electron and hole distribution confirms the authors explanation for the lack of luminescence from the bottom quantum well.

References

