A tunable blue light emission of InGaN/GaN quantum well through thermal interdiffusion

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Abstract

In recent years, blue light emitting diodes and lasers of III-nitride semiconductors have been of much interest. This is mainly due to its large bandgap ranging from 1.89 eV (wurtzite InN) to 3.42 eV (wurtzite GaN). InGaN/GaN quantum well (QW) structures have been used to achieve high lumens blue LEDs. In this paper, InGaN/GaN QW intermixing structure is theoretically analyzed and is used to optimize and tune the optical emission. © 1999 Published by Elsevier Science S.A. All rights reserved.

Keywords: Thermal annealing; Quantum well intermixing; Interdiffusion; III-nitride; InGaN/GaN; Light emitting diode

1. Introduction

Wide-bandgap semiconductors such as GaN, AlN, InN and their ternary compounds have been studied so as to realize the semiconductor blue–green laser. As a matter of fact, the demonstration of high-brightness blue–green light-emitting diodes from the wurtzite GaN semiconductor has stimulated a lot of research on the fabrication of blue–green laser diodes using nitride-based semiconductors [1]. InGaN/GaN single-quantum-well (QW) structures have been used to achieve high-power blue and green light-emitting diodes [2]. Also, room temperature pulsed lasing of a strained InGaN/GaN multiquantum-well laser diode has recently been demonstrated [3]. In 1995, Nakamura discovered that the efficiency could be further improved by doping InGaN with both Zn and Si, which probably involve Si–Zn DA pairs.

The nature crystal structure of most of the group III nitrides is wurtzite. Strain is also present in most of the group III nitrides because of the lack of substrate materials with a matched lattice constant and a thermal expansion coefficient. Indeed, fundamental studies of the effects of strain on wurtzite band structure play an important role in understanding the electronic and optical properties of GaN-based optoelectronic materials and devices.

2. Thermal annealing

This paper presents a theoretical study of the effects of interdiffusion on a 50 Å well width of an In$_{0.16}$Ga$_{0.84}$N/GaN single QW structure, whose properties leads to the shift in spontaneous emission rate. The effects of interdiffusion on the strains, the splitting of the heavy-hole (HH), the light-hole (LH), the crystal-field split-hole (CH) subbands, the conduction band (CB) and their dispersions, are calculated theoretically, based on the Hamiltonian derived using the multi-band k·p model by Chuang and Chang [4].

The QW composition intermixing refer to the thermal induced interdiffusion of the constituent atoms through the hetero-interface. In fact, the interdiffused QW (DFQW) structures created by both impurity induced and impurity-free vacancy promoted processes have recently attracted much attention [5–7]. The interdiffusion mechanism can be a single-phase diffusion for two constituent atoms or it can be a two-phase or multiple-phase one and/or for multiple species. In InGaN/GaN DFQW structures, only the interdiffusion of group-III atoms, i.e. In and Ga atoms, occurs as there is no N concentration gradient across the interface. The diffusion of group III atoms in the QW structure is usually described by Fick’s law with constant diffusion coefficients in both the well and the barrier layers. The composition profile after the interdiffusion is characterized by a diffusion length $L_d$ defined as $L_d = \sqrt{(Dt)}$, where $D$ is the diffusion coefficient and $t$ is the anneal-
ing time of thermal processing. The In mole fraction across the InGaN/GaN DFQW structure after the interdiffusion is given by:

\[ x_{\text{In}}(z) = \frac{x_0}{2} \left[ \text{erf} \left( \frac{L_w + 2z}{4L_d} \right) + \text{erf} \left( \frac{L_w - 2z}{4L_d} \right) \right], \]

where \( z \) denotes the co-ordinate along the crystal growth direction, \( L_w \) is the as-grown well width and \( x_0 \) is the as-grown In mole fraction. In the case of group-III interdiffusion, In atoms diffuse into the GaN barrier and Ga atoms diffuse into the QW, thus forming an InGaN/InGaN interface. The distribution of the In and Ga atoms is described by the error function distribution, while the N concentration profiles do not change. At the initial stage of diffusion, the In atoms start to move away from the well center and decrease with the degree of interdiffusion. The diffusion of In and Ga atoms results in such changes of structural properties as the bandgap of each layer, the effective mass of carriers and the in-plane strain induced by lattice mismatches. The as-grown square well structure resulting from the intermixing of atoms will gradually change from the abrupt interface to continuous profiles. As-grown square well profiles such as atomic concentration, in-plane strain and the bandgap of layers are changed to non-square continuous profiles.

3. Subband energy

The strain of InGaN/GaN DFQW is compressive in nature. The strain which exists pushes the valence subbands downwards and further increases the bandgap. As seen from the Schrödinger equation (Eq. (2)), \( U(r) \)
is the confinement potential term, which depends on the strain presence. The built-in electric field as a result of the interdiffusion is not considered here. The Schrödinger equation is as follows:

\[
\left[ -\frac{\hbar^2}{2m_0} \nabla^2 + U(r) \right] \Psi(r) = E \Psi(r),
\]

(2)

where \( \Psi(r) \) is the envelope wavefunction and \( m_0 \) is the carrier effective mass. In fact, Eq. (2) is solved numerically using a finite difference method with the confinement profile shown in Fig. 1. For \( L_d = 10 \) and 50 Å, the potential profiles are determined by error function distribution. The effective barrier heights of all confinement potentials decrease as a consequence of interdiffusion, resulting in a reduction of carriers in the wells.

For the long diffusion length, i.e. \( L_d = 50 \) Å, it contributes to the shallow potential well for the confinement of carriers which decrease the efficiency of radiation.

For the valence band structure, it is necessary to diagonalize the Luttinger–Kohn Hamiltonian with appropriate confinement potentials for heavy hole, light hole and split hole. In this paper, the effective-mass Hamiltonian approach described in the work of Chuang and Chang [4] is used to calculate the valence subband structure. The in-plane valence band dispersion of the InGaN/GaN SQW is calculated using the parameters of Ga and InN as listed in Table 1. Meanwhile, alloy properties of In\(_{x}\)Ga\(_{1-x}\)N are obtained by linear interpolation, except for the gap energy, in which a bowing parameter of \( b = 1.75 \) eV for InGaN/GaN is taken. The partition ratio for the band edge discontinuity at the heterojunction for the valence and conduction bands is assumed to be 33:67 for both QW systems.

The properties of the interdiffused QW are considered to be different from those of the square QW. The valence subband edge energy levels of the as-grown square QW are shifted down while the conduction subband edge energy levels are shifted up in the interdiffused QW, and this initially increases the transition energy. Seen from Fig. 2, as \( L_d \) increases from zero, the subband energies increase, reaching a maximum at \( L_d = 20 \) Å for both energy subbands and then decreasing to bulk InGaN bandgap energy as \( L_d \to \infty \), which resembles a bulk material. The reduction of transition energy is due to the release of compressive strain in the well. Although QW intermixing will cause the shifting up of transition energy, the release of compressive strain will cause a decrease in the QW bandgap.

### 4. Light emission

We assume that the injected carrier density is \( 1 \times 10^{-13} \) cm\(^{-2} \) in the InGaN/GaN DFQW. The spontaneous emission rate is calculated by integrating the emission rate over all the electrons and holes recombination processes. The spontaneous emission is given by the following equation:

\[
\begin{align*}
    r_{sp}(E) &= \frac{q^2 \hbar \omega}{\pi \hbar^3 \varepsilon_0 m_0 L_w} \int dk |P_{pq}(k)|^2 \\
    &\times f^e(E_p(k)) [1 - f^h(E_p(k))] \\
    \end{align*}
\]

(3)

where \( q \) is the electric charge, \( n_r \) is the refractive index, \( \varepsilon_0 \) is the dielectric constant of the vacuum, \( c \) is the speed of light, \( L_w \) is the width of the quantum well, \( E \) is the photon energy, \( P_{pq} \) is the optical matrix element, and \( f^e \) and \( f^h \) are the Fermi distribution functions for electrons in the conduction subband and holes in the

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**Table 1**

Material parameters used in calculating the band structure of InGaN/GaN QW

<table>
<thead>
<tr>
<th>Parameters</th>
<th>GaN</th>
<th>InN</th>
</tr>
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<tbody>
<tr>
<td>( a (\text{Å}) )</td>
<td>3.189878</td>
<td>3.544</td>
</tr>
<tr>
<td>( E_g ) at 300 K (eV)</td>
<td>3.44</td>
<td>1.89</td>
</tr>
<tr>
<td>( \Delta_1 ) (meV)</td>
<td>10</td>
<td>27.8</td>
</tr>
<tr>
<td>( \Delta_2 ) (meV)</td>
<td>5.170204</td>
<td>3.9</td>
</tr>
<tr>
<td>( m_e^* (m_0) )</td>
<td>0.2</td>
<td>0.11</td>
</tr>
<tr>
<td>( m_h^* (m_0) )</td>
<td>0.18</td>
<td>0.1</td>
</tr>
<tr>
<td>( A_1 )</td>
<td>-6.56</td>
<td>-9.28</td>
</tr>
<tr>
<td>( A_2 )</td>
<td>-0.91</td>
<td>-0.6</td>
</tr>
<tr>
<td>( A_3 )</td>
<td>5.65</td>
<td>8.68</td>
</tr>
<tr>
<td>( A_4 )</td>
<td>-2.83</td>
<td>-4.34</td>
</tr>
<tr>
<td>( A_5 )</td>
<td>-3.13</td>
<td>-4.32</td>
</tr>
<tr>
<td>( A_6 )</td>
<td>-4.86</td>
<td>-6.08</td>
</tr>
<tr>
<td>( a_y (\text{eV}) )</td>
<td>-11.8</td>
<td>-1.2</td>
</tr>
<tr>
<td>( D_1 (\text{eV}) )</td>
<td>0.7</td>
<td>0.35</td>
</tr>
<tr>
<td>( D_2 (\text{eV}) )</td>
<td>2.1</td>
<td>1.05</td>
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<tr>
<td>( D_3 (\text{eV}) )</td>
<td>1.4</td>
<td>1.31768</td>
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<tr>
<td>( D_4 (\text{eV}) )</td>
<td>-0.7</td>
<td>-0.7412</td>
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<tr>
<td>( C_{13} (10^{11} \text{ dyn cm}^{-2}) )</td>
<td>10</td>
<td>9.4</td>
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<tr>
<td>( C_{33} (10^{11} \text{ dyn cm}^{-2}) )</td>
<td>39.2</td>
<td>20</td>
</tr>
</tbody>
</table>

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Fig. 2. The transition energy between the valence and conduction subbands for various diffusion length.
DFQW can be applied to blue LEDs, which can adjust the wavelength of the emitted photons.

5. Conclusion

In this paper, the InGaN/GaN QW intermixing structure is theoretically analyzed, and it is used to tune the operation wavelength of light emission devices. The results show that the photon energy can shift from 3.05 to 3.20 eV within the range of 0–20 Å diffusion length, resulting in a reduction of spontaneous light emission of 17%.

Acknowledgements

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References