Importance of strain for green emitters based on (In, Ga)N films of non-polar orientation

Sandip Ghosh* and Holger T. Grahn

1 Department of Condensed Matter Physics and Material Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400005, India
2 Paul Drude Institute for Solid State Eelectronics, Hausvogteiplatz 5–7, 10117 Berlin, Germany

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*Corresponding author: e-mail sangho10@tifr.res.in, Phone: +91 22 22782840; Fax: +91 22 22804610

Wurtzite In$_x$Ga$_{1-x}$N films, with alloy compositions suitable for obtaining green-light emitting diodes (LED) and lasers in the wavelength range between 520 and 550 nm, experience compressive anisotropic in-plane strain when grown on non-polar (1100) M-plane or (1120) A-plane GaN substrates. The results of calculations of the electronic band structure presented here demonstrate that this strain mixes the valence bands and modifies the emission polarization properties in such a way that lasing characteristics will benefit from it. The advantage improves with partial anisotropic strain relaxation. However, both lasing characteristics and light extraction out of a LED will deteriorate when such a film becomes fully relaxed.

1 Introduction

Semiconductor-based white-light generation by combining red, green, and blue light-emitting diodes (LED) and lasers is at present unable to reach its full potential due to the absence of efficient green emitters [1, 2]. While blue emitters based on wurtzite In$_x$Ga$_{1-x}$N/GaN quantum wells are efficient, adding more In to lower the energy gap of the active layer for obtaining green-light emission in the range of 520 to 550 nm leads to a significant drop in the light output for the same input electrical power [3]. This is commonly referred to as the green-gap problem. The recently reported continuous-wave green laser at 524 nm based on C-plane In$_x$Ga$_{1-x}$N/GaN quantum wells had a wall plug efficiency of 2.3% [4]. The use of films with non-polar (1100) M-plane or (1120) A-plane orientation is an alternative being pursued in order to increase the efficiency of group-III-nitride-based emitters in general. The absence of large piezo- and pyro-electric fields in non-polar heterostructures increases their radiative efficiency [5] and also helps to avoid a current-dependent shift of the lasing wavelength. In order to prevent the reduction of radiative recombination due to defects such as misfit and threading dislocations arising from the very large lattice mismatch between the film and the substrate, devices are now being grown on bulk-like GaN substrates. LEDs [6] operating at 527 nm and lasers [7] at 500 nm have been demonstrated using non-polar GaN substrates. Green-light emitting In$_x$Ga$_{1-x}$N still has a fairly large average lattice mismatch (∼3%) with GaN, and recent studies suggest that the resultant strain can lead to defects, which are detrimental for light emission [8]. Therefore, it has been suggested that one needs a growth and device structure strategy which leads to an unstrained In$_x$Ga$_{1-x}$N/GaN active layer of non-polar orientation, where structural defects are minimized. Previous studies have addressed how the light emission characteristics of non-polar blue-emitting In$_x$Ga$_{1-x}$N alloys vary with In concentration [9, 10].

Here we present results of a theoretical investigation, which emphasizes the effects of anisotropic in-plane strain and its partial relaxation on the electronic band structure of non-polar M-plane and A-plane In$_x$Ga$_{1-x}$N films suitable for green-light emission. We show that some amount of strain is in fact essential for obtaining efficient non-polar In$_x$Ga$_{1-x}$N film based green emitters.

2 Electronic band structure calculations

The emission characteristics of a semiconductor light emitter is determined by the nature of its conduction band (CB) and valence bands (VB) in the vicinity of the fundamental energy
gap. In group-III nitrides, the CB is composed of atomic s orbitals with wavefunctions of \( |S \rangle \) symmetry, while their three, closely spaced VBs are formed out of \( p \) orbitals with wavefunctions represented by a linear combination of \( |X\rangle \), \( |Y\rangle \), and \( |Z\rangle \) symmetries. A transition involving a CB state and an \( |X\rangle \)-like, \( |Y\rangle \)-like, or \( |Z\rangle \)-like VB state requires light polarized in the \( x \), \( y \), and \( z \)-direction, respectively. Anisotropic in-plane strain in a non-polar film mixes the different VBs and dramatically changes the polarization properties of the three interband transitions [11]. The point being emphasized in this paper is that such changes in the polarization selection rules will have a strong influence on laser and LED performance. We have used the Bir-Pikus Hamiltonian to calculate the influence of strain on the electronic band structure and the oscillator strengths of the transitions, which determine the polarization selection rules. The procedure is described in Refs. [11, 12]. Here we consider only the lowest-energy transition which dominates the emission process, and determine its relative oscillator strength components \( f_x \), \( f_y \), and \( f_z \) for light polarization in the \( x \), \( y \), and \( z \)-direction, respectively. The material parameter values for GaN and InN are listed in Table 1, the values for In\(_{1-x}\)Ga\(_x\)N were obtained through interpolation. The energy gap bowing parameter of In\(_x\)Ga\(_{1-x}\)N was taken to be 1.4 eV.

### 3 Results and discussion

Figure 1(a) shows the variation of the strain components of an In\(_x\)Ga\(_{1-x}\)N film on an \( M \)-plane GaN substrate as a function of In concentration for pseudomorphic epitaxial growth. The range of In concentration considered is one over which the energy gap of the pseudomorphic in-plane strain tensor components \( \varepsilon_{xx} \) and \( \varepsilon_{yy} \), as well as the out-of-plane strain tensor component \( \varepsilon_{zz} \), in In\(_x\)Ga\(_{1-x}\)N films on \( M \)-plane GaN substrate as a function of the In concentration suitable for green emission. (b) Emission wavelength as determined by the lowest-energy interband transition in such strained (solid line) and fully relaxed (dashed line) In\(_x\)Ga\(_{1-x}\)N films at 298 K. The green emission band is schematically indicated. The inset sketches the wurtzite unit cell indicating the relevant crystal planes and the choice of coordinates. (c) The relative oscillator strength components \( f_x \) and \( f_z \) of the lowest-energy interband transition in the strained films for \( x \) and \( z \) polarizations, respectively. For this In concentration range, \( f_y = 0 \).

#### Table 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>GaN(^{(b)})</th>
<th>InN(^{(b)})</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c ) (Å)</td>
<td>5.1851</td>
<td>5.7064 [14]</td>
</tr>
<tr>
<td>( a ) (Å)</td>
<td>3.1893</td>
<td>3.5376 [14]</td>
</tr>
<tr>
<td>( E_g ) (eV)</td>
<td>3.436</td>
<td>0.65 [16]</td>
</tr>
<tr>
<td>( E_{exc} ) (meV)</td>
<td>26</td>
<td>3 [16]</td>
</tr>
<tr>
<td>( \Delta_D ) (meV)</td>
<td>9.2 [15]</td>
<td>19 [17]</td>
</tr>
<tr>
<td>( \Delta_E ) (meV)</td>
<td>18.9 [15]</td>
<td>5 [17]</td>
</tr>
<tr>
<td>( C_{12} ) (GPa)</td>
<td>390</td>
<td>223</td>
</tr>
<tr>
<td>( C_{13} ) (GPa)</td>
<td>145</td>
<td>115</td>
</tr>
<tr>
<td>( C_{14} ) (GPa)</td>
<td>106</td>
<td>92</td>
</tr>
<tr>
<td>( C_{15} ) (GPa)</td>
<td>398</td>
<td>224</td>
</tr>
<tr>
<td>( \alpha ) (eV)</td>
<td>(-44.5 ) [11]</td>
<td>(-7.2 )</td>
</tr>
<tr>
<td>( D_{1} ) (eV)</td>
<td>(-41.4 ) [11]</td>
<td>(-3.7 )</td>
</tr>
<tr>
<td>( D_{2} ) (eV)</td>
<td>(-33.3 ) [11]</td>
<td>4.5</td>
</tr>
<tr>
<td>( D_{3} ) (eV)</td>
<td>(-3.6 ) [15]</td>
<td>(-4.0 )</td>
</tr>
</tbody>
</table>

\(^{(a)}\) Under the quasi-cubic approximation \( D_3 = D_2 = D_1 = -D_1/2 \), \( \Delta_1 = \Delta_2 \), and \( a_{ij} = a \). For InN, \( \alpha \) was obtained using \( a = a_1 + D_1 \), \( a_1 \) being the hydrostatic deformation potential.

\(^{(b)}\) Unless indicated otherwise, the values are derived from Ref. [13].

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Figure 1 (online color at: www.pss-b.com) (a) Variation of the pseudomorphic in-plane strain tensor components \( \varepsilon_{xx} \) and \( \varepsilon_{yy} \) as well as the out-of-plane strain tensor component \( \varepsilon_{zz} \), in In\(_x\)Ga\(_{1-x}\)N films on \( M \)-plane GaN substrate as a function of the In concentration suitable for green emission. (b) Emission wavelength as determined by the lowest-energy interband transition in such strained (solid line) and fully relaxed (dashed line) In\(_x\)Ga\(_{1-x}\)N films at 298 K. The green emission band is schematically indicated. The inset sketches the wurtzite unit cell indicating the relevant crystal planes and the choice of coordinates. (c) The relative oscillator strength components \( f_x \) and \( f_z \) of the lowest-energy interband transition in the strained films for \( x \) and \( z \) polarizations, respectively. For this In concentration range, \( f_y = 0 \).

If the polarization lies in the film plane, light can be easily extracted through the top surface (along \( y \)-direction) in an LED. In contrast, for an emission polarization perpendicular to the film plane, light would travel within the film and be reabsorbed, resulting in a poor light extraction out of an LED [18]. If the active region of an edge-emitting laser (EEL) is based on such a film with a large \( f_x \) and the cavity is defined along the \( z \)-direction, then there would be a beneficial lowering of the threshold current for lasing. In vertical-cavity surface-emitting lasers (VCSEL) based on \( C \)-plane films, fixing the emission polarization is a problem. With these strained \( M \)-plane films as active regions, the...
VCSEL, polarization direction will be naturally fixed along the x-direction.

However, for In concentrations in the range $x = 0.25–0.4$, the pseudomorphic in-plane compressive strain in films grown on an $M$-plane GaN substrate is very high. Consequently, strain relaxation will occur in films of practically useful thickness such as a 10-nm-thick quantum well. In addition, the in-plane strain in $M$-plane films is anisotropic. Therefore, for a given In concentration, one needs to obtain results for a range of values of the in-plane strain tensor components $\varepsilon_{xx}$ and $\varepsilon_{zz}$. As a representative case, we have chosen the In concentration to be $x_{\text{In}} = 0.3$. The basic nature of the following results is also valid for other $x_{\text{In}}$ needs to obtain results for a range of values of the in-plane strain tensor components $\varepsilon_{yy}$ and $\varepsilon_{zz}$. For pseudomorphic growth on an $M$-plane GaN substrate, $\varepsilon_{xx} = -3.17\%$, $\varepsilon_{zz} = -2.93\%$, and $\varepsilon_{yy} = 2.15\%$, with light emission at 496 nm. These high strain values are not sustainable, and the film will typically relax to a state with a mismatch of the lattice constants along directions parallel and perpendicular to the c-axis will ensure a final anisotropic strain state with $\varepsilon_{xx} \neq \varepsilon_{zz}$. The dashed line represents a strain relaxation trajectory where the magnitudes of $\varepsilon_{xx}$ and $\varepsilon_{zz}$ decrease proportionally. Although it is not necessary that the final strain state of the partially relaxed film will lie on this line, it will be somewhere close to this line. Such a partially relaxed film will have an emission wavelength corresponding to the lowest-energy transition as a function of strain $\varepsilon_{xx}$ and $\varepsilon_{zz}$ for an $M$-plane In$_{0.3}$Ga$_{0.7}$N film.

Figure 2 displays the variation of the emission wavelength corresponding to the lowest-energy interband transition as a function of strain $\varepsilon_{xx}$ and $\varepsilon_{zz}$ for an $M$-plane In$_{0.3}$Ga$_{0.7}$N film. For pseudomorphic growth on an $M$-plane GaN substrate, $\varepsilon_{xx} = -3.17\%$, $\varepsilon_{zz} = -2.93\%$, and $\varepsilon_{yy} = 2.15\%$, with light emission at 496 nm. These high strain values are not sustainable, and the film will typically relax to a state with $\varepsilon_{xx} \neq \varepsilon_{zz}$. The dashed line represents a strain relaxation trajectory where the magnitudes of $\varepsilon_{xx}$ and $\varepsilon_{zz}$ decrease proportionally. Although it is not necessary that the final strain state of the partially relaxed film will lie on this line, it will be somewhere close to this line. Such a partially relaxed film will have an emission wavelength corresponding to the lowest-energy transition as a function of strain $\varepsilon_{xx}$ and $\varepsilon_{zz}$ for an $M$-plane In$_{0.3}$Ga$_{0.7}$N film. Figures 2(a) and 2(b) show $f_x$ and $f_z$, respectively, over a smaller range of strain values in (c) and (d) is much smaller than in (a) and (b).

Figures 3(a) and 3(b) display $f_x$, $f_z$, and $f_y$ for emission from a compressively strained $M$-plane In$_{0.3}$Ga$_{0.7}$N film as a function of in-plane strain tensor components $\varepsilon_{xx}$ and $\varepsilon_{yy}$. The white dot indicates the pseudomorphic strain state when grown on an $M$-plane GaN substrate $\varepsilon_{xx} = -3.17\%$ and $\varepsilon_{yy} = -2.93\%$. The dashed line indicates the trajectory of strain relaxation for a proportional decrease in $\varepsilon_{xx}$ and $\varepsilon_{yy}$. The color scheme has only an approximate correlation with the emission wavelength. Note that the displayed range of strain values in (c) and (d) is much smaller than in (a) and (b).
$\varepsilon_{xx} = \varepsilon_{zz} = 0$, one obtains $f_x = f_y = 0.5$ as expected for perfect wurtzite symmetry. Thus green-light emission from an $M$-plane In$_{x}$Ga$_{1-x}$N film with very small strain values will exhibit neither an emission with a large polarization along the $x$- nor along the $z$-direction, which is detrimental for EEL or VCSEL applications. Moreover, since in this case a significant out-of-plane $f_z$ component occurs, it is also detrimental for light extraction out of an LED.

It is important to note that incorporating high concentrations of In in non-polar In$_{x}$Ga$_{1-x}$N films has been a technological challenge [20]. However, recent reports show that up to 32% In incorporation is achievable, resulting in emission at 535 nm [21]. In addition, strain relaxation in the active layer through the generation of defects such as threading and misfit dislocations is detrimental for light emission. An increase of the emitted light intensity at 535 nm was achieved in $M$-plane In$_{0.32}$Ga$_{0.68}$N films by growing them on a much thicker In$_{x}$Ga$_{1-x}$N base layer with a lower In concentration [21]. This procedure reduces the effective lattice mismatch between the active layer and the base on which it is grown. This can lead to defect-free films with small in-plane anisotropic pseudomorphic strain, which is sufficient for the oscillator strength-related advantages presented in this paper.

Finally, we note that, apart from the reports of green lasing [4] using $C$-plane In$_{x}$Ga$_{1-x}$N films on GaN substrates, growth on an appropriate thick alloy base for achieving defect-free active layers has also been suggested for $C$-plane films [22]. Therefore, we briefly consider the case of $C$-plane In$_{x}$Ga$_{1-x}$N films, where the in-plane strain is compressive, but $\varepsilon_{xx}$ and $\varepsilon_{yy}$ are now equal in sign and magnitude. This isotropic in-plane strain preserves the high symmetry in the $x$–$y$ plane, and for the lowest-energy transition in $C$-plane films one obtains $f_x = f_y = 0.5$ and $f_z = 0$ in the In concentration range suitable for green-light emission. While this is acceptable for conventional LED applications, we see that strongly polarized emission in strained $M$-plane films, where $f_x$ or $f_y$ can easily become 1, represents a 100% improvement over $C$-plane films for EEL applications. In addition, devices based on $C$-plane films continue to exhibit undesirable current-dependent shifts of the emission wavelength. Thus, from the point of view of the oscillator strength, $M$-plane or $A$-plane films under anisotropic compressive in-plane strain have a fundamental potential for a better performance than $C$-plane films of similar crystalline quality.

4 Summary and conclusion In conclusion, we find that valence band mixing in anisotropically strained non-polar $M$-plane and $A$-plane In$_{x}$Ga$_{1-x}$N films on GaN substrates with alloy compositions suitable for green-light emission can result in complete polarized emission along a direction in the film plane. This strain-induced effect is an additional advantage for EEL and VCSEL applications, apart from the advantage arising from the absence of large piezo- and pyro-electric fields in non-polar films. However, this advantage for EEL and VCSEL is lost in unstrained or almost relaxed films, where the lowest-energy transition acquires a significant out-of-plane polarization component, which is also detrimental for LED applications. Note that small amounts of strain are not necessarily detrimental for the film quality in terms of defect generation. In fact, there are suggestions that some defects reported earlier in group-III-nitride films were in fact artifacts of electron microscopy measurements [23].

References