Strain and potential fluctuations effects on $(In, Ga)N/(Al, Ga)N/GaN$ Electroluminescence red shift

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Abstract: Theoretical calculations of potential fluctuations and strain effects are investigated in this paper. Good agreement between the suggested effects and the luminescence bands red shift, observed experimentally for $In_xGa_{1-x}N/Al_yGa_{1-y}N/GaN$ double heterostructure grown on SiC substrate, which shows that the model is simple and more consistent with the experimental results.

PACS: 78.20.Bh-78.60.Fi
Keywords: Potential fluctuations, Strain, Electroluminescence, $(In, Ga)N$ heterostructure.
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I-Introduction

The discovery of the narrow band gap of InN at $0.7eV$ [1,2] opened up many new applications for the nitrides. For example, it has been recognized that the band gap range of $In_xGa_{1-x}N$ alloy system $(0.7 - 3.4eV)$ is an almost perfect match for the solar spectrum, which makes it a potential material for tandem solar cells [3]. Previous studies have demonstrated that $In_xGa_{1-x}N$ alloys exhibit superior radiation resistance electrical and optical properties over than other materials commonly used in tandem solar cells [3,4]. Indeed, the $InGaN$ alloys have attracted much interest as they can be used to cover the emission spectral range from the ultraviolet to the near infrared by varying the InN fraction. But the large difference in interatomic spacing between GaN, AlN and InN gives rise to compositional inhomogeneities (fluctuations) and strains that strongly affect the optical properties of the $InGaN$ heterostructures. The purpose of this work is to investigate the strain and the potential fluctuations effects on the $In_xGa_{1-x}N/Al_yGa_{1-y}N/GaN$ systems electroluminescence.

II-Experimental data

The CREE type 430-DH85 LED commercial for which the schematic diagram is showing in Fig. 1, was used in this work. According to the information supplied by the manufacturer, the active layer $(In, Ga)N$ is situated at $25\mu m$ below the surface top and its thickness is about $10\mu m$. The layers are n and p type doped respectively by implanting silicon Si_{Ga} (n) and Mg_{Ga} (p) but the doping level remains unknown.

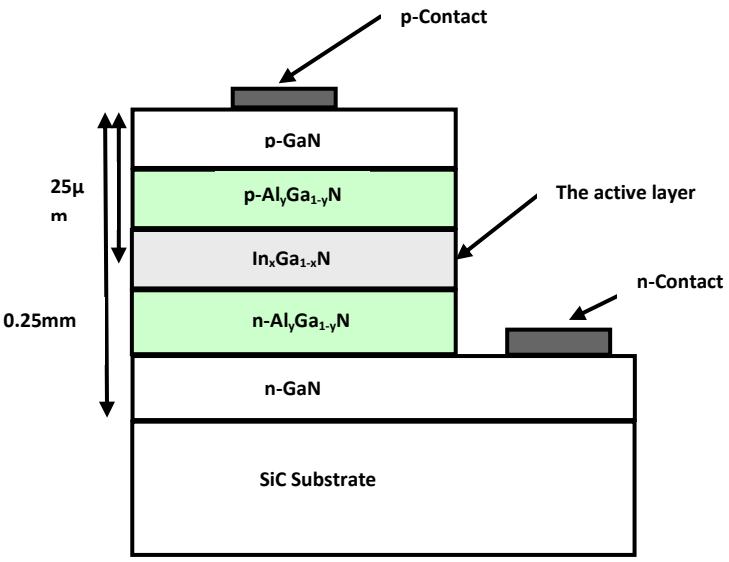


Fig. 1: Schematic structure and composition of $(In, Ga)N$ double hétérostructure according to the information supplied by the manufacturer [5].

III-Theory

In our previous work [5], we have reported that, EL spectra of $(In, Ga)N/(Al, Ga)N/GaN$ structure grown on SiC substrate obtained for forward polarization $(220\mu A, 3.18V)$, show three main structures. Room temperature EL contains the blue luminescence(BL), yellow luminescence (YL) and infra red luminescence(IRL). This later is less studied and less common compared with BL and YL which are located respectively at $2.78eV$ and $2.05eV$. Generally, a broad BL band centered at

$2.88-2.90eV$ is often observed in PL, EL and CL of undoped and Si-doped n-type GaN grown by different techniques [6 − 9]. A BL band, similar in energy position and shape to that observed in undoped and Si-doped GaN, has also been observed in high resistivity C-doped GaN [10]. In one investigation [11], a slight deviation has been observed in that doping with C introduced a BL band peaking at approximately $3.03eV$. In the same context, the YL band has been the topic of literally hundreds of publications [For examples: 12-19] and it is always broad, nearly the Gaussian with $FWHM$ of about $350-450meV$, and structureless even at the lowest temperatures. However, the exact position and shape of this band are sometimes samples dependent. In most of unintentionally and intentionally doped n-type GaN samples obtained by various techniques available, the room temperature PL spectrum contains the YL band peaking at $2.20-2.25eV$. (Reference [5] for more details about BL and YL bands).
Indeed, our experimental results presented in Ref. [5] are inconsistent, generally, with those cited above which concern $h-GaN$ grown on different substrate and obtained by different epitaxial techniques. Speculations about the red shift observed experimentally are discussed in this work. Taking account of the structure nature, the potential fluctuations and strain effects are suggested to explain the experimental red shift.

1.Potential fluctuations effect

The random distribution of the In atoms in GaN host induces sharp and deep potential fluctuations, as it does in $In_xGa_{1-x}N$. Indeed, it is important to consider the potential fluctuations effect while interpreting the experimental results concerning GaN. Significant potential fluctuations originating from Poisson distribution of charge points defects play a very important role in the properties of compensated semiconductors [20,21], are expected because the concentration of free carriers is usually too small to screen them. This effect has been studied theoretically [20] and experimentally [22-24] and the energy of the emission has been simulated by the following expression:
In the case of conduction band (CB) to valence band (VB) transitions [20]:

$$\hbar\omega = E_g - 2\gamma \quad (eV) \tag{1}$$

In the case of donor-acceptor (DAP) transitions [23]:

$$\hbar\omega = E_g - (E_d + E_a) - 2\gamma \quad (eV) \tag{2}$$

where E_g is the band gap energy, γ is the potential fluctuations amplitude, E_a and E_d are respectively the acceptor and the donor energies.

Note that, these equations are obtained by assuming that after excitation the carriers relax quickly to the potential minima (electrons) and potential maxima (holes) of CB and VB respectively. Then they recombine with the probability determined by the degree of wave function overlap of the recombining carriers. In the case of DAP recombination, the carriers are first captured by donors and acceptors resulting in additional terms in Eq. 2. Following this arguments, equations (1) and (2) can be used only when the wave function of at least one of carriers is large enough, namely, compared to the spatial size of potential fluctuations. In the limit of high degree of compensation, the amplitude (γ) and spatial size (r_f) of typical potential fluctuations can be expressed as given by [21]:

$$\gamma = \frac{e^2}{4\pi\varepsilon}\frac{N^{2/3}}{n^{1/3}}$$

$$r_f = \frac{N^{1/3}}{n^{2/3}}$$

Where $N = N_d + N_a$ is the combined concentration of acceptors and donors, n is the free carrier's concentration, e is the electron charge and ε is the semiconductor permittivity.

Fig. 2 shows the typical amplitude of potential fluctuations with combined concentration of carriers $N = 10^{18}$, 10^{19} and $10^{20}cm^{-3}$, as function of free carriers at room temperature. As can be seen from this figure, the typical potential fluctuation amplitude can be very large for a weak concentration of free carriers. For a constant free concentration carriers, the amplitude of potential fluctuation increases as function of the combined concentration of carriers. Evidently, the increase of the amplitude is limited by the band gap energy because the screening increases with the Fermi level approaching the VB and the CB at the extreme points.

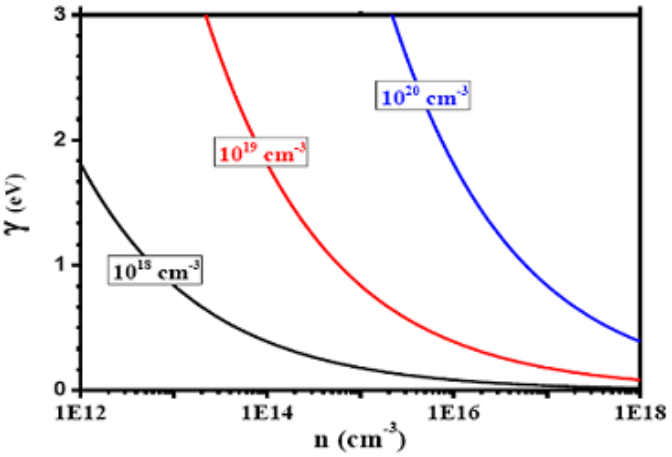


Figure 2: Typical amplitude of potential fluctuations for three combined concentration N and for free concentration less than $10^{18}cm^{-3}$.

2. Strain effect

To express the uniform deformation of a crystal under the strain effect, let consider an orthogonal reference related to the non deformed solid defined by three vectors $\vec{u}_1$, $\vec{u}_2$ and $\vec{u}_3$. In the elastic range approximation, the direction and the length of these vectors ($\vec{u}_i$) change after the deformation is applied.

The new vectors $\vec{u}_{1n}$, $\vec{u}_{2n}$ and $\vec{u}_{3n}$ (n: new)are obtained in the initial reference as function of dimensionless coefficients [25]:

$$\Delta\vec{u}_i = \vec{u}_{in} - \vec{u}_i = e_{i1}\vec{u}_1 + e_{i2}\vec{u}_2 + e_{i3}\vec{u}_{i3}$$

The Hook's low [26] indicates that the strain and deformation of the crystal lattice are deduced from the modulus of the elasticity.

The epitaxial growth of a layer on the other one in a sample such as that studied in this paper generates a biaxial strain which is due to substrate strongly detuned. In this case:

$$\varepsilon_{xx} = \varepsilon_{yy} = -\frac{c_{33}}{2c_{13}}\varepsilon_{zz}$$

It is well known that, the biaxial strain generates modifications on the semiconductors band structure. For the Wurtzite structure (hexagonal), the spin-orbit coupling divides the VB up in two levels:

- The first corresponds to heavy and light holes bands degenerated at Γ point.
- The second shifted by Δ_{SO} corresponds to ''split-off'' band.

Moreover, the non cubicity of this structure gives rise to an electric field (crystal field) which raises the degeneration of the VB between the heavy and light holes at Γ [27-30]. The combined effect of crystal field and spin-orbit coupling is shown schematically on Fig. 3.

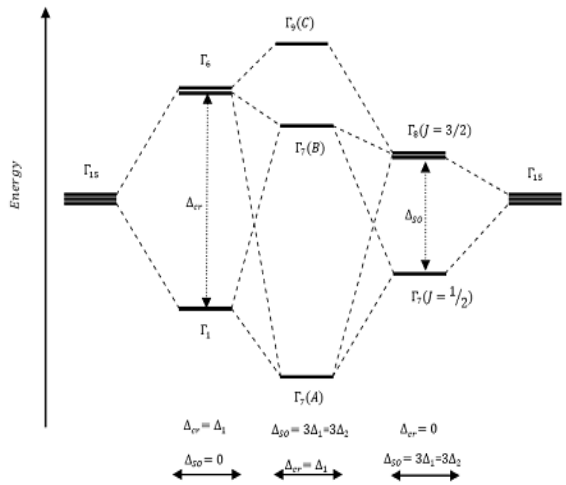


Figure 3: Combined effect of crystal field and spin-orbit coupling on the VB degeneration at Γ point for GaN hexagonal.

The strain dependence of the A, B and C maxima energies of the VB (at Γ) is given as following [31]:

$$E_C(\varepsilon) = (D_1+D_3)\varepsilon_{zz} + (D_2+D_4)(\varepsilon_{xx}+\varepsilon_{yy})$$

$$E_B(\varepsilon) = -\frac{\Delta_1+3\Delta_2}{2} + D_1\varepsilon_{zz}+D_2(\varepsilon_{xx}+\varepsilon_{yy}) + \frac{D_3\varepsilon_{zz}+D_4(\varepsilon_{xx}+\varepsilon_{yy})}{2} + \frac{1}{2}\sqrt{[\Delta_1-\Delta_2+D_3\varepsilon_{zz}+D_4(\varepsilon_{xx}+\varepsilon_{yy})]^2+8{\Delta_3}^2}$$

$$E_A(\varepsilon) = -\frac{\Delta_1+3\Delta_2}{2} + D_1\varepsilon_{zz}+D_2(\varepsilon_{xx}+\varepsilon_{yy}) + \frac{D_3\varepsilon_{zz}+D_4(\varepsilon_{xx}+\varepsilon_{yy})}{2} - \frac{1}{2}\sqrt{[\Delta_1-\Delta_2+D_3\varepsilon_{zz}+D_4(\varepsilon_{xx}+\varepsilon_{yy})]^2+8{\Delta_3}^2}$$

We notice that the energies' origin is taken at the unconstrained VB maximum.

ε_{ij} : The strain tensor component.

D_i : Potential deformation

$\Delta_1 = \Delta_{cr}$ and $\Delta_2 = \Delta_3 = \frac{\Delta_{SO}}{2}$

The CB minimum energy is expressed as function of the strain as follow:

$$E_{CB_{min}}(\varepsilon) = E_g(\varepsilon=0) + \Phi_D\varepsilon_{zz}$$

Where $E_g(\varepsilon=0)$ is the band gap energy of unconstrained material and Φ_D is the dilatation component of the CB potential deformation.
Then, the energies of transitions between the BC minimum and the BV is given by:
$\hbar\omega_i = E_{CB_{min}}(\varepsilon) - E_i(\varepsilon)$

where $i \equiv A, B, C$

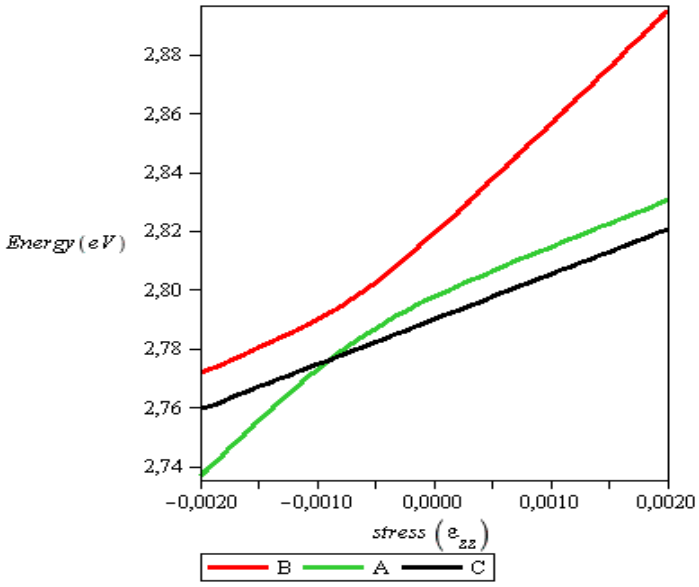
The $h-GaN$ elastic constants and the potential deformation have been studied within the framework of the above concept both theoretically and experimentally [32-34]. However, the results dispersion leaves us a large domain for choosing these constants. Gil et al [31] were the first which present a quantitative correlation between experimentally energies and the strain state. In the same context, To correlate the experimental results and theoretical calculations, especially taking into account the measurements made on samples under strain and measured parameters by X-ray

diffraction, several studies have been reported subsequently [35-38]. In this work, we have used the literature data, particularly, the values proposed by the [35,37] authors which concern the strain $h-GaN$ measurements obtained on SiC substrate. For C_{13} and C_{33} coefficients, we have used those cited in reference [39]. The parameters in ternary $In_xGa_{1-x}N$ used in this calculation are assumed to be linear combinations of those of binary GaN and InN. The result obtained for the strain dependence of A, B and C transitions corresponding to $x = 14\%$ is presented in Fig. 4.

Figure 4: The energies of A, B and C transitions as function of strain for the indium composition equal to 14%.

3. Discussion

It appears from the results presented above that the displacement to lower energies observed experimentally can be explained by the suggested effects. A very significant potential fluctuations effect is showing in Fig. 2, especially, for weak free concentrations. The more the combined



concentrations of acceptors and donor increased, the more the potential fluctuation is very important. In this case, a sizable portion of free carriers would be captured by donors and acceptors before they thermalize respectively to the potential minima or maxima. The broadening and shift to lower energies at low current density injected would be governed by the ratio between the wave-function size and the slope ($^{2\gamma}/_{r_f}$) of the potential fluctuations at this point. The larger this ratio, the larger the broadening and the shift would be. In the one hand, the results obtained for the average slope of the potential, $^{2\gamma}/_{r_f}$ as function of the free concentration carrier (not shown here), depicts that it is very small so that the wave-function size of order of $1nm$ or less can hardly cause any broadening and shift of the EL bands more than $20meV$ due to the potential fluctuations. In the other hand, the slope increases as function of the carrier concentration, i.e., with increasing the current density injected in the structure. In this trend, with increasing of the injected current density, we would expect the shift of the EL bands not to higher but to lower energies, unless the potential fluctuations and the wave-function sizes are comparable.

As can be seen in Fig. 4, the strain effect is very important and can affect the position, the shape and the broadening of the EL bands. For the structure as that reported in [5] in which the layers are grown on the others, one can speculate that the results are affected by the strain effect.

However, in all report concerning, especially, the BL bands in $GaN:Mg$ grown on silicon carbide or saphir cited above, increasing the excitation intensity (PL spectra) resulted in shifts only to higher energies (blue energies). Probably, in the case of the wide-band gap semiconductors, the short-range potential fluctuations resulting in transitions between local minima and maxima can be used as a qualitative argument compared to the excitation intensity effect .i.e., the shift to higher energies is due to the screening of the potential fluctuations in the structure less constrained. For our results related to $In_xGa_{1-x}N$ structure ($x = 0.14$), we can say that the combined effects of strain and potential fluctuations play a very important role in broadening and shift to lower energies unless for a current density used in this work less than $500\mu A$.

4. Conclusion

In this paper, speculation about the red shift of the EL bands obtained from $(In,Ga)N/(Al,Ga)N/GaN$ systems is presented. The strain and potential fluctuations effects are investigated. We have shown that the EL bands red shift can be explained by these effects.

Acknowledge

The authors would like to thank Professor C. Carlone and M. Aubin from ''Département de physique de la faculté des sciences de l'université de Sherbrooke (Canada)'' for their technical and experimental advices.

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