Influence of the structural inhomogeneity on the luminescent properties of nitride multiple quantum wells grown by MOCVD

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Abstract. We investigated GaN/InGaN multiple quantum wells grown by MOCVD for LED application in the blue and green regions. The sample considered was characterized by a significant number of defects on the interfaces between the layers. We examined the heterostructure by means of cathodoluminescence. Due to the composition and the layer's thickness fluctuations on a small and a large scale, we observed peak splitting and broadening. In order to justify our assumption, we compared the experimental results with our theoretical calculations. The theoretical model used is based on the T-matrix formalism.

1. Introduction

The III-nitride layered heterostructures have acquired widespread applications as building blocks in manufacturing of devices for optical communication, high-electron-mobility transistors, ultra-violet lasers and resonant-tunneling-based structures for THz applications [1-3]. Along with the attractive characteristics [4], they also possess very specific ones, such as well pronounced piezoelectric and spontaneous polarizations along the low-symmetry axis. These features should always be taken into account when considering thin III-nitride layers, especially in superlattices and multiple quantum wells. The optical properties of such structures are greatly affected by the presence of macroscopic polarization in the layers. Another important factor that influences the optical properties is the interface roughness, which is manifested as wells with fluctuations [5-7].

In this study, we examined by means of cathodoluminescence an InGaN/GaN multiple quantum well (MQW) grown by MOCVD on a GaN substrate. All measurements were conducted at room temperature. Further, we compared the experimental results with our theoretical calculations based on the model briefly described in [8]. Our main goal was to demonstrate that, despite the idealizations and the simplifications we have made, our calculations are in a satisfactory agreement with the experimental results. We conducted our calculations in the framework of the effective-mass approximation and the T-matrix formalism. To ensure the accuracy desired, the Airy function formalism was used to solve the one-dimensional Schrödinger's equation for the MQW potential.

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2. Theoretical framework and calculation details

The multi-layered structure examined was composed of three layers of $In_xGa_{1-x}N$ (forming the potential wells) alternating with three layers of GaN (forming the potential barriers), grown on a GaN substrate. In order to calculate the levels of the electrons and the holes and, therefore, the optical transition energy, we examined the one-dimensional potential of the MQW. Due to the spontaneous and piezoelectric polarization in the layers, the profiles of the wells and the barriers assume a trapezoidal shape. The magnitudes of the corresponding electric fields were calculated to be [9]:

$$E_{\mathrm{w,b}} = \frac{\left(P_{\mathrm{b,w}} - P_{\mathrm{w,b}}\right) L_{\mathrm{b,w}}}{\left(\varepsilon_{\mathrm{b,w}} P_{\mathrm{w,b}} - \varepsilon_{\mathrm{w,b}} P_{\mathrm{b,w}}\right) \varepsilon_0} \tag{2.1}$$

in the wells and barriers regions, respectively. Here $P_{\mathrm{w,b}}$ represents the total polarization in a layer, $L_{\mathrm{w,b}}$, its thickness, $\varepsilon_{\mathrm{w,b}}$, the relative permittivity of the materials, and ε_0, the permittivity of vacuum. Having determined the potential across the MQW, we found the electron and hole states in the wells (using the effective-mass approximation) and, thereupon, the interband transition energies. In order to perform the calculations, one needs a set of material parameters, which are systematized in table 1. All the parameters of GaN and InN were extracted from [10] The parameters of $In_xGa_{1-x}N$ were calculated following [9] by setting $x = 0.2$:

$$\begin{aligned} E_{\mathrm{g}} &= 3.39 - 2.65x \\ \chi &= 4.26 + 1.67x - 0.67x^2 \\ m_{\mathrm{e}}^* &= 0.2 - 0.08x \\ \varepsilon &= 9.8 + 5.2x \end{aligned}, \tag{2.2}$$

where E_{g} is the energy gap in bulk $In_{0.2}Ga_{0.8}N$ in eV, χ is the electron affinity of the material in eV, m_{e}^* is the electron effective mass in units of m_0 (i.e. free electron mass), and ε is the dielectric constant in units of ε_0.

Proceeding from the above parameters and considering (2.1), we calculated the band offsets and the potential profile of the structure. The alternating layers of GaN and $In_{0.2}Ga_{0.8}N$ had thicknesses of $L_{\mathrm{b}} = 10\,\mathrm{nm}$ and $L_{\mathrm{w}} = 4\,\mathrm{nm}$, respectively. The offset in the conduction band was calculated to be $\Delta E_{\mathrm{C}} = 0.3\,\mathrm{eV}$ and the offset in the valence band, $\Delta E_{\mathrm{V}} = 0.26\,\mathrm{eV}$. A plot of the potential profile of the MQW examined, as well as the electron (E1) and heavy hole (HH1) ground states, are shown in figure 1.

The transition $\mathrm{E1} \rightarrow \mathrm{HH1}$ as calculated to have an energy of 2.81 eV, which corresponds to a wavelength of $441\,\mathrm{nm}$. In order to estimate the influence of the structural inhomogeneity of the $In_{0.2}Ga_{0.8}N$ layers (the wells), we performed the same calculations for MQW structures with different

Table 1. Parameters of GaN and $In_{0.2}Ga_{0.8}N$.

Parameter	GaN	$In_{0.2}Ga_{0.8}N$
Bandgap energy E_{g} (eV)	3.39	2.86
Electron affinity χ (eV)	4.26	4.56
Effective mass (m_0)		
electron m_{e}^*	0.2	0.18
heavy hole m_{hh}^*	1.4	1.55
Dielectric constant ε (ε_0)	9.8	10.84
Total polarization P ($\mathrm{C\,m^{-2}}$)	-0.03	-0.062
Lattice constant c (Å)	5.19	5.6

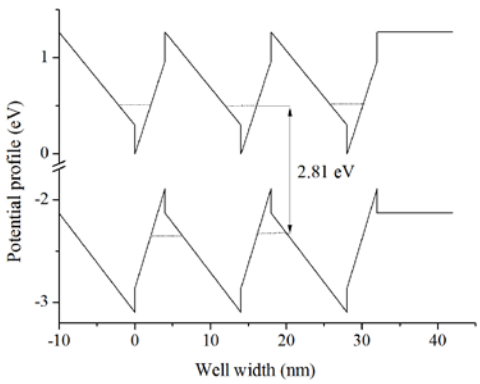

Figure 1. Potential profile across the growth axis of three-period $In_{0.2}Ga_{0.8}N$/GaN MQW. The ground electron and hole levels, along with the transition energy, are also depicted.

well widths. We considered well-width fluctuations of ± 2 monolayers (ML), i.e. $\pm c_{\mathrm{InGaN}}$, and kept all other parameters the same throughout the calculations.

3. Results and discussion

The luminescent spectrum shown in figure 2 was obtained from the sample considered above. Two distinct peaks are clearly observed. The leftmost peak on figure 2(a) is observed at $\lambda = 364\,\mathrm{nm}$. This wavelength corresponds to the bandgap of GaN, hence the peak is due to transitions between the band edges in the GaN substrate. The second peak is wider and split at $\lambda = 425\,\mathrm{nm}$ and $\lambda = 441\,\mathrm{nm}$. It is attributed to the transition $\mathrm{E1} \rightarrow \mathrm{HH1}$ in the MWQ. The calculation results indicate a transition energy of $E_{E1\rightarrow HH1} = 2.81\,\mathrm{eV}$ or $\lambda = 437\,\mathrm{nm}$ for the quantum wells with a nominal width ($L_{\mathrm{w}} = 40\,\mathrm{nm}$). For the quantum wells whose width is increased by 2 ML, the transition energy is calculated to be $E^{+2}_{E1\rightarrow HH1} = 2.72\,\mathrm{eV}$ or $\lambda = 456\,\mathrm{nm}$, while for wells whose width is decreased by 2 ML, the results are $E^{-2}_{E1\rightarrow HH1} = 2.95\,\mathrm{eV}$ or $\lambda = 420\,\mathrm{nm}$. All results are plotted over the measured luminescent spectrum on figure 2(b).

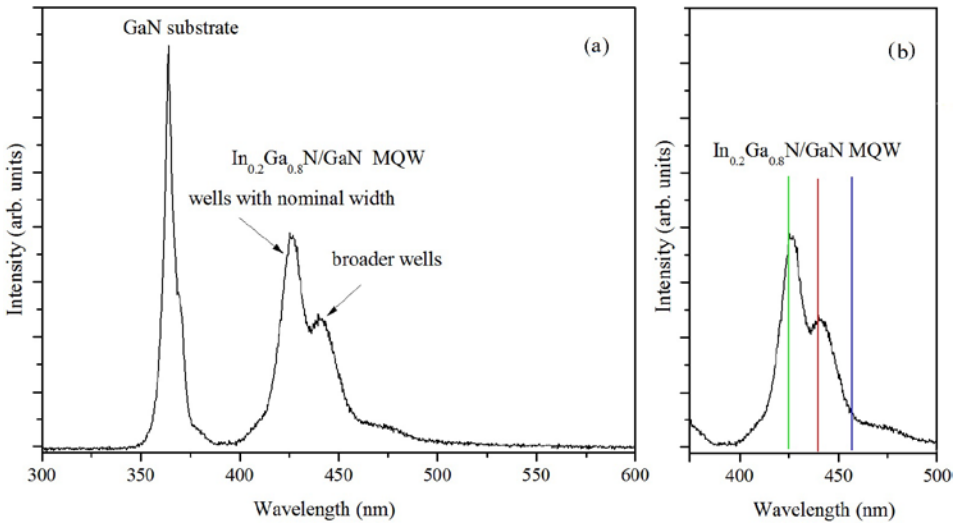

Figure 2. (a) Room temperature cathodoluminescent spectrum of $In_{0.2}Ga_{0.8}N$/GaN MQW. The first peak is attributed to the transitions between the band edges in the GaN substrate. The second peak is due to the optical transitions in the MQW. The split in the second peak is attributed to fluctuations in the InGaN layer; (b) $\mathrm{E1} \rightarrow \mathrm{HH1}$ transition wavelength, calculated for: nominal width of the wells (red line); wider wells (blue line); narrower wells (green line). The corresponding wavelengths are depicted over the spectrum of the MQW.

The splitting observed in the luminescent spectrum is most likely due to fluctuations in the InGaN well width, which inevitably occur during the growth process. This assumption is supported by the fact that the difference of $110\,\mathrm{meV}$ between the peaks (in the measured spectrum) is very close to the difference of $90\,\mathrm{meV}$ between $E_{E1\rightarrow HH1}$ and $E^{+2}_{E1\rightarrow HH1}$, or to the difference of $130\,\mathrm{meV}$ between $E_{E1\rightarrow HH1}$ and $E^{-2}_{E1\rightarrow HH1}$. In our theoretical results, we observed a certain tendency toward the lower transition energies, which is most likely due to a composition ratio that differs from the nominal during the growth process, or to the chosen set of band parameters. For example, a higher value of the InGaN bandgap energy would have resulted in higher transition energies. Apart from this, our calculations are in a good agreement with the experimental results.

4. Conclusions

We examined both theoretically and experimentally the transition energies in InGaN/GaN MQW grown by MOCVD. We calculated the optical transition energy taking account of the well-width fluctuations. The splitting of the peak that corresponds to the $E1 \rightarrow HH1$ transition was explained by the well-width fluctuations. The luminescence spectrum observed supported our theoretical results, although the latter showed a certain shift toward the lower energies. This might be corrected in further calculations by choosing another set of parameters or by changing the composition ratio.

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References

[1] Beeler M, Trichas E and Monroy E 2013 *Semicond. Sci. Technol.* **24** 074022-48
[2] Cho A, Sivco D, Ng H, Gmachl C, Tredicucci A, Hutchinson A, Chu S and Capassco F 2001 *J. Crystal Growth* **227-228** 1-7
[3] Camacho A S, Gutiérrez R M and Ardilla G 2005 *Microelectr. J.* **36** 922-7
[4] Monemar B 1999 *J. Mater. Sci.: Mater. Electr.* **10** 227-54
[5] DeCuir A, Fred E, Passamore B, Muddasani A, Manasrech M, Xie J, Morkoç H, Ware M and Salamo G 2006 *Appl. Phys. Lett.* **89** 151112-14
[6] Dimitrov S, Valcheva E and Donchev D 2007 *Nanosci. & Nanotechnol.* **7** 115-8
[7] Paskov P, Bergman J, Darakchieva V, Paskova T, Monemar B, Iwaya M, Kamiyana S, Amano H and Akasaki I 2005 *Phys. Stat. Sol.* C **2** 2345-8
[8] Asenova I and Valcheva E 2012 *J. Phys.: Conf. Series* **398** 012014
[9] Piprek J 2007 *Nitride Semiconductor Devices* (Weincheim: Willey-VCH) p 354
[10] Vurgaftman I and Meyer J 2003 *J. Appl. Phys.* **94** 3675-96