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Electronic states properties in GaN/$Al_xGa_{1-x}N$ heterostructures with graded interfaces

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AlGaN/GaN multiple quantum wells (MQWs) are common building blocks for the active regions of UV light emitting diodes. In this work we have studied the influence of well width fluctuations on the bound state energy levels in GaN/AlGaN QW. We studied the influence of the interface roughness and the electric charge due to the internal polarization fields.

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1. Introduction

AlGaN/GaN multiple quantum well (MQW) structures are common building blocks for the active regions of UV light emitting diodes (UV LEDs). The understanding of the radiative recombination mechanisms in these systems is therefore of great interest. AlGaN/GaN quantum wells (QWs), multiple QW stacks (MQWs) or superlattices (SLs) are presently investigated for a number of device applications, such as emitters and detectors, barriers for HEMT structures and electrical contact regions in various devices. [1]

The optical properties of AlGaN/GaN are influenced by strong internal electric fields across the layers, due to spontaneous and piezoelectric polarization effects. [2]

The presence of strong polarization charges at the surfaces and the interfaces is a typical property of the wurtzite III-nitride materials, where the layers are grown along the polar (0001) axis. The spontaneous (sp) and the piezoelectric (pz) polarization play an important role, and for the AlGaN/GaN system these contributions can be of comparable magnitude. These polarisation charges create internal fields in the QWs that influence the optical properties, affecting oscillator strengths of excitons and the position of the corresponding photoluminescence (PL) peaks. Another important effect that influences optical properties is the well/barrier interface roughness, which is manifested as well with fluctuations.

In this study, we theoretically investigate a AlGaN/GaN QWs grown in the (0001) direction, taking into account the interface roughness influence on the electronic states and their dependence on the well width fluctuations and the internal electric field. The calculations are made within the framework of the envelope function approximation.

2. Calculation details

We have calculated the photoluminescence (PL) peak splitting, which is due to the influence of the well width fluctuations on the energy states. Splitting of the peak of about 23meV [3] was experimentally observed by means of PL spectroscopy on a 5 period AlGaN/GaN MQW structure. It was interpreted as the presence of two QW widths dominating the PL spectrum, consistent with the idea that the interface roughness is of the order of one or two monolayers. This splitting is due to the difference in the recombination energies for the different well widths. We have aimed at evaluating this effect by modelling a similar MQW structure, i.e. a MQW consisting of five periods with well width 4.5 nm, separated by $Al_{0.07}Ga_{0.93}N$ barriers of 7nm [3].

In the calculations we use the following parameters: effective electron masses $0.2\,m_0$ for GaN and $0.4\,m_0$ for AlN, heavy hole masses $1.42\,m_0$ for GaN and $3.53\,m_0$ for AlN, light hole masses $0.3\,m_0$ for GaN and $3.53\,m_0$ for AlN, E_g (GaN)=3.47 eV and E_g (AlN)=6.2 eV, E_v=0.066 eV, ΔE_c=0.116 eV and E_g (x) equal to:

$$E_g = xE_g(AlN) + (1-x)E_g(GaN) - x(1-x)b - E_g(GaN) \qquad (1)$$

where x is the chemical composition and b is the bowing parameter, here $b = 0.25$. The values of the effective masses for the ternary compound are taken as a linear interpolation of those for GaN and AlN.

3. Results and discussion

3.1 Influence of the well width fluctuations on the bound states

First we consider a single 4.5nm thick GaN QW between two AlGaN 7 nm thick barriers. With the aim of studying the electron levels as a function of the well width, we have calculated the energies of the bound states and their wave functions for a set of well width fluctuations corresponding to a full c -vector (2 ML = 0.52 nm), ± c/2 -

vector (1ML=0.26 nm) and 2*c* -vector (4 ML = 1.04 nm), without including the effect of the electric field. The results are summarized in Table 1. The energies are calculated from the bottom of the well.

Here the peak splitting is simply the sum of the differences in the electron and heavy hole energy levels between the nominal (4.5 nm) (figure 1) and the disturbed QW.

3.2. Influence of the internal field on the bound states

As a next step, we consider the influence of the internal electric field on the energy levels in the well. To calculate the electric field caused by the polarization, we can neglect the surface induced depletion potential, which in undoped samples should not be appreciable. Then for the internal electric field (*F*) in the GaN wells we have [3] $F_w = (P_b - P_w)L_b/(L_w + L_b)\varepsilon_0\varepsilon$ (2)

and for the barrier

$$F_b = (P_w - P_b)L_w/(L_w + L_b)\varepsilon_0\varepsilon \qquad (3)$$

Here, L_w is the well width, L_b - the barrier width, P_w - the polarization field over the well, P_b - the polarization field over the barrier, ε - the dielectric constant for the material, ε_0 - the dielectric constant for the vacuum.

For the well with, L_w = 4.5 nm, L_b = 7 nm, ε = 10 for GaN, and ε = 8.5 for AlN, we have $F_w = -4.2\times10^5$ V/cm, and $F_b = 2\times10^5$ V/cm. For this case we have calculated the energy states and their wave functions for the same set of well width fluctuations. The results are presented in Table 2.

Table 1. The energy of the first level for electrons (E1), light (LH1) and heavy holes (HH1) for different well widths in meV.

Well width [nm]	3.5 (-2c)	4 (-c)	4.25 (-c/2)	4.5	4.75 (+c/2)	5 (+c)	5.5 (+2c)
E1	44	40	37	35	32	30	27
LH1	-18	-16	-15	-14	-14	-13	-12
HH1	-9	-8	-7	-7	-6	-6	-5
Recombination energy [eV]	3.523	3.517	3.514	3.511	3.508	3.506	3.501
Peak splitting [meV]	12	6	3	0	3	5	10

Table 2 . The energy of the first level for electrons (E1), light (LH1) and heavy holes (HH1) for different well widths in meV, with an internal electric field.

Well width [nm]	3.5 (-2c)	4 (-c)	4.25 (-c/2)	4.5	4.75 (+c/2)	5 (+c)	5.5 (+2c)
E1	105	103	102	101	100	99	97
LH1	-60	-60	-60	-60	-60	-59	-59
HH1	-46	-46	-46	-46	-46	-45	-45
Recombination energy [eV]	3.463	3.445	3.437	3.429	3.422	3.414	3.4
Peak splitting [meV]	34	16	8	0	7	15	29

Here the field significantly increases the peak splitting. In this case, the peak splitting is calculated from the equation

$$E = |\ hv_n - hv\ | \qquad (4)$$

where the recombination energy hv for the disturbed well (hv_n for the nominal well) is:

$$hv = E_g(GaN) - L_w F_w + E_e + E_h \qquad (5)$$

E_e (E_h) is the energy of the first level for electrons (holes). Figure 2 shows the first energy levels E_1 and HH_1 and the wave function for the 4.5 nm well.

As we can see from the results presented in sections 3.1 and 3.2, the energy of the levels decreases when the well becomes wider. The increase of the width fluctuations results in an increasing difference between the energy levels for the 4.5nm and the disturbed QW, which leads to a larger peak splitting. Adding an electric field increases the electron and hole confinement energies. The peak splitting is also increased in the case of the presence of an electric field. However, the main contribution to the peak splitting comes from the term L_wF_w in the equation (5).

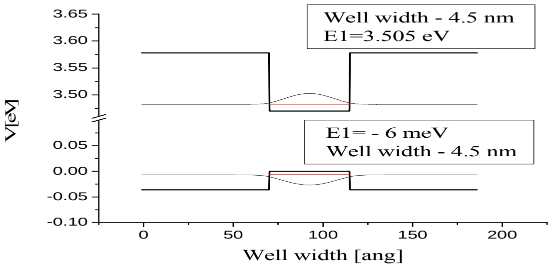

Fig. 1. The energy of the first level and the wave function for electrons and heavy holes without an internal electric field.

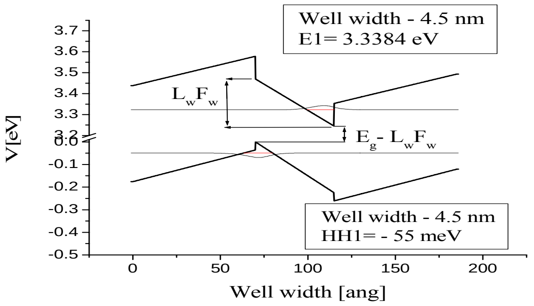

Fig. 2. The energy of the first level and the wave function for electrons and heavy holes for electric fields F_w *-*4.2×10^5 *V/cm, and* $E_b = 2\times10^5$ *V/cm.*

4. Conclusions

We have estimated the effects of interface roughness and the internal field on the recombination energies in AlGaN/GaN QWs. As a result we found that:

- The energy of the levels increases with the presence of an electric field.
- With the narrowing of the well, the energy levels increase.
- An increase in the well width fluctuations increases the peak splitting.
- The electric field increases the differences between the energy levels corresponding to the different well widths, leading to a larger PL peak splitting.

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