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Thermal annealing effects on the optical gain of InGaN/GaN quantum well structures

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Abstract

In this work, the variation of the optical gain in the InGaN/GaN quantum well after thermal annealing is simulated. The potential profile change of the quantum well resulting from the interdiffusion of Ga and In atoms across the interface of the well and the barrier during the thermal treatments is assumed to follow Fick's law. The results show that the thermal annealing can induce an increase of the optical gain in the InGaN/GaN quantum well. The maximum optical gain can be obtained at a diffusion length of 0.4 nm of In and Ga atoms. However, an excessive annealing may result in decreasing the optical gain. There is a good agreement between the experimental data in literature and the optimized diffusion length studied in this work.

Keywords: GaN; InGaN; Annealing; Quantum well; Interdiffusion; Gain

1. Introduction

GaN is a promising material for light emitting devices in the violet–blue–green region. Quantum well (QW) structures are often used for GaN-based light-emitting diodes and lasers. Up to now, most of the commercial GaN epitaxial layers are grown by metalorganic chemical vapor deposition. The typical growth temperatures of InGaN, GaN and AlGaN layers are 800, 1020 and 1020 °C, respectively [1]. After the growth of the epitaxial layers, a thermal annealing at 700 °C is employed to convert the as-grown p-type GaN layer into a uniform highly p-type GaN layer [1]. To obtain high hole concentrations in the p-layer, ion implantation and diffusion techniques are also considered. A thermal activation at 1000 °C for 5 min after Mg or Zn ion implantation is employed [2–4]. Diffusion with Mg at 1000 °C for 60 min can also be used for the same intention [5]. To realize the ohmic contacts between metals and semiconductors, thermal annealing at 450–950 °C for 60 min is performed [4,6–8]. During the expitaxial growth of InGaN/GaN MQW structure and the fabrication of devices, InGaN layers undergo several high-temperature treatments. The distribution of the indium composition and the strain in the QW may be changed due to the In and Ga interdiffusion across the interface of the QW and the barrier after these thermal treatments. This leads to a change of the optical properties of the QW [9–13]. After the sample was annealed, a blue shift of the PL peak has been observed [11–13] and the photoluminescence (PL) intensity is increased [13]. In this work, we investigate theoretically the variation of the optical properties in InGaN/GaN QW resulting from the interdiffusion of In and Ga atoms across the interface of the QW and the barrier.

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2. Calculation procedures

The thermal treatments can induce an In and Ga interdiffusion across the interface of barrier and well. In general, the diffusion mechanism of the atoms is described by Fick's law. After thermal treatment, the step-like potential profile of the quantum well is transformed into a gradient one. In this calculation, we assume that the electrical potential variation of the quantum well in the direction of the crystal growth (direction z) follows Fick's law. The potential profile can be described as [10]

$$V(z) = \frac{w_{dp}}{2}\left[\mathrm{erf}\left(\frac{L_w + 2z}{2L_d}\right) + \mathrm{erf}\left(\frac{L_w - 2z}{2L_d}\right)\right] \tag{1}$$

where z denotes the coordinate along the crystal growth direction. w_{dp} is the potential difference between the well and barrier for conduction or valence band which is defined by the indium composition of the QW and Vegard's law, i.e. $w_{dp} = (E_g^{barrier} - E_g^{well}) \times$ (band offset parameter). $E_g^{barrier}$ and E_g^{well} are the band-gap of the barrier and well, respectively. L_w is the well width before the diffusion process, L_d is the diffusion length which is $2 \times \sqrt{Dt}$, D is the diffusion coefficient, and t is the time of diffusion.

The variation of the optical properties due to the In and Ga interdiffusion were calculated for $In_{0.1}Ga_{0.9}N$ and $In_{0.2}Ga_{0.8}N$ single quantum well (SQW) structures. The strong built-in piezoelectric field is considered in this calculation. However, the value of the piezoelectric field in the InGaN/GaN QW depends not only on the indium composition but also on the heterojunction structure [14]. For simplifying the calculation, we assume that the piezoelectric field is proportional to the indium composition in the QW and that the piezoelectric field in the InN/GaN heterostructure is 0.55 V/nm in [0 0 0 1]-direction [14]. Therefore, the piezoelectric field in $In_{0.1}Ga_{0.9}N$ and $In_{0.2}Ga_{0.8}N$ QW is 0.055 and 0.11 V/nm, respectively. The gradient potential profile in QW calculated by Eq. (1) is inclined due to the piezoelectric field. The potential profile with consideration of the interdiffusion and piezoelectric effects is used in the time-independent Schrödinger equation to obtain the distribution of electrons or holes in the region of the quantum well by the finite-difference method [15]. The optical gain spectra were obtained by the standard calculation procedure [15]. The effective mass of electron and hole is $0.2m_0$ and $1.56m_0$, respectively [16], m_0 being the electron mass. The value of the band offset parameter used in this study is 38:62 that we reported recently, as deduced from the optical pumping spectra of the high-indium composition InGaN/GaN quantum well [17].

3. Results and discussion

Fig. 1 shows the potential profile of the conduction band for the 3 nm-wide $In_{0.1}Ga_{0.9}N$/GaN QW with the 0 and 0.6 nm diffusion length (L_d), respectively. For the QW without interdiffusion effect ($L_d = 0$ nm), the step-like potential profile is inclined due to the strong piezoelectric field. With the interdiffusion effect, the QW potential profile is transformed into a gradient one at increasing diffusion length.

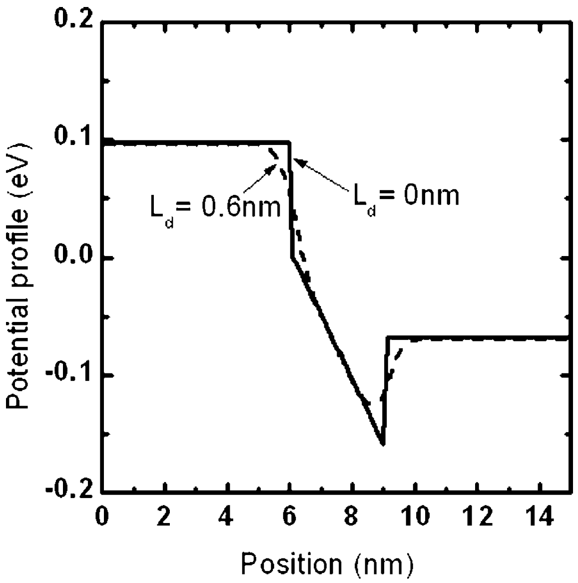

Fig. 1. Conduction band diagram for 3 nm-wide $In_{0.1}Ga_{0.9}N$ QW under 5.5×10^{-2} V/nm piezoelectric field with $L_d = 0$ and 0.6 nm.

Fig. 2 shows the optical gain as a function of the In diffusion length for the 3 nm-wide QW with 10% and 20% indium composition. The current density in the calculation is 1600 and 800 A/cm^2 for the $In_{0.1}Ga_{0.9}N$

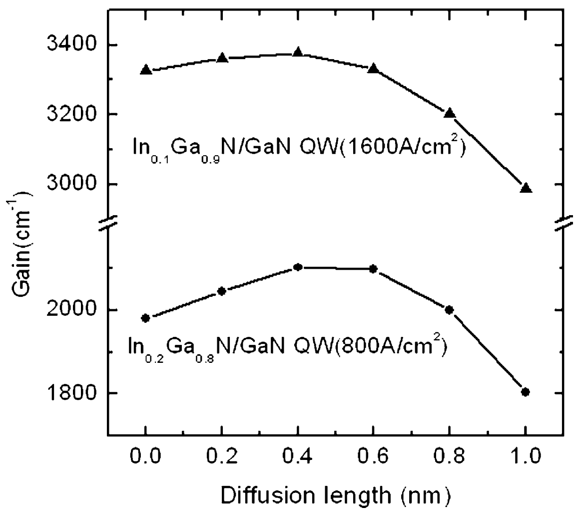

Fig. 2. Variation of the optical gain for (a) $In_{0.1}Ga_{0.9}N$ and (b) $In_{0.2}Ga_{0.9}N$ QW with different diffusion length under the current density of 1600 and 800 A/cm^2, respectively.

and $In_{0.2}Ga_{0.8}N$ QW, respectively. The result shows that for both QWs with 10% and 20% indium composition, the optical gain increases as the diffusion length increases from 0 to 0.4 nm. The maximum optical gain is obtained for a diffusion length of 0.4 nm. As the diffusion length is greater than 0.4 nm, the optical gain decreases severely as the diffusion length increases. The increase of the optical gain originates principally from the fact that as the diffusion length increases to 0.4 nm, the "effective" well width decreases leading to the increase of the overlap of the electron and hole distributions (transition probability). At a diffusion length larger than 0.4 nm, the decrease of the optical gain originates from the flattening of the quantum well. This indicates that the quantized energy of the conduction band becomes close to the energy difference between the barrier and the well leading to decrease of the confinement of the electrons in QW. This results in a decrease of the electron–hole transition probability. These results provide a theoretical analysis to the increase of the PL intensity of the InGaN/GaN quantum structures due to the thermal annealing [13].

In Ref. [12], the thermal annealing was performed to the InGaN/GaN quantum well structures from 900 to 1050 °C for 10 min. The diffusion coefficients have been reported to be 2×10^{-6} and 1×10^{-4} nm^2/s for the annealing at 900 and 1050 °C, respectively [12]. By following the Arrhenius expression, the diffusion coefficient can be described as $D = 1.93 \times 10^9 \exp(-40473/T)$ nm^2/s. T is the annealing temperature in Kelvin. In Ref. [14], the PL intensity increases as the annealing temperature increases from 900 to 1000 °C. However, the annealed sample at 1050 °C shows a severe decrease of PL intensity. The maximum PL intensity occurred after the annealing treatment between 1000 and 1050 °C for 10 min. The corresponding diffusion lengths can be obtained by the Arrhenius expression to be 0.27 and 0.48 nm, respectively. There is an agreement between these experimental data and the calculated diffusion length in this work for the maximum optical gain at 0.4 nm. These results reveal quantitatively that there may be a maximum optical gain of the QW with the diffusion length around 0.4 nm. Thermal treatments at high temperature for about 10 min are often performed during the fabrication of the laser. Therefore, the result of this study shows that the thermal treatments during the fabrication of the laser can significantly influence the performance of the devices. An additional thermal treatment after the growth of the epitaxial layers could help determine whether the optical gain can be improved.

4. Summary

In this work, we investigate the optical gain variation of InGaN/GaN QW for different diffusion conditions. The maximum optical gain can be obtained as the diffusion length of the indium is 0.4 nm. The result shows a good agreement with the experimental results in literature. The results can help to increase the optical gain of InGaN/GaN QW laser and LED.

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