Effects of compressive strain on optical properties of $In_xGa_{1-x}N/GaN$ quantum wells

N. Khan and J. Li[a)]
Department of Physics, Kansas State University, Manhattan, Kansas 66506-2601

(Received 3 July 2006; accepted 29 August 2006; published online 13 October 2006)

$In_{0.2}Ga_{0.8}N/GaN$ multiple quantum well (MQW) blue light emitting diode (LED) structure was grown on a specially designed sapphire substrate (with increasing thickness from the edge to the center within a single wafer). X-ray diffraction revealed that the GaN lattice constant c decreases continuously from the edge to the center, indicating a continuous variation in the compressive strain. The spectral peak positions of the electroluminescence (EL) spectra exhibited a blueshift when probed at the edge as compared to the center, which is a direct consequence of the continuous variation in the compressive strain across the wafer. Based on the experimental results, a ratio of elastic stiffness constants (C_{33}/C_{13}) for GaN was deduced to be $\sim 5.0 \pm 1.0$, which was in agreement with the calculated value of ~ 4.0. A linear relation of the EL emission peak position of LEDs with the biaxial strain was observed, and a linear coefficient of 19 meV/GPa characterizing the relationship between the band gap energy and biaxial stress of $In_{0.2}Ga_{0.8}N/GaN$ MQWs was also obtained. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2362587]

Current intensive research on III nitrides has led to rapid progress in optoelectronic devices such as blue/green light emitting diodes (LEDs) and laser diodes (LDs) and high power electronic devices. To further improve the performance of nitride-based optoelectronic and microelectronic devices, a better knowledge of its growth kinetics, surface dynamics, and strain or stress states due to difference in lattice mismatch and thermal expansion coefficients between the epitaxial layers and the substrate is needed.[1–3] Mechanical stresses are known to considerably influence semiconductor band gaps and effective masses of electrons and holes.[4] Several groups have studied the effects of stress or strain on the optical properties of $In_xGa_{1-x}N/GaN$ multiple quantum wells (MQWs) subjected to variable amount of lattice mismatch induced strain by changing In content or QW width.[5–7] However, there is no report on the strain induced variation in the band gap of $In_xGa_{1-x}N/GaN$ MQWs, which is important for the design of improved nitride LED structures.

In this letter we report on the effects of compressive strain on the optical properties of blue LEDs grown by metal organic chemical vapor deposition (MOCVD). We used a wafer polishing method to design a single substrate having the thickness increasing continuously from the edge ($\sim 350\ \mu m$) to the center ($\sim 450\ \mu m$) to study the effects of varying geometrical shape induced strain on the optical properties of blue LEDs. X-ray diffraction (XRD) was employed to characterize the crystalline structure and strain in GaN epilayers. The ratio of elastic stiffness constants (C_{33}/C_{13}) for GaN was deduced to be $\sim 5.0 \pm 1.0$, which was in agreement with the calculated value of ~ 0.4.[8] Electroluminescence (EL) spectra were measured to study the optical properties of $In_{0.2}Ga_{0.8}N/GaN$ MQW. A linear coefficient which describes the variation of $In_xGa_{1-x}N$ band gap per unit stress was obtained.

$In_{0.2}Ga_{0.8}N/GaN$ MQW LED structure was grown by MOCVD on a 2 in. specially designed sapphire substrate. Simultaneously growth in the same reactor on flat sapphires was also carried out for comparison studies. A low temperature GaN buffer layer with thickness ~ 30 nm was deposited at $\sim 530\ °C$ prior to the growth of $\sim 3\ \mu m$ GaN with Si doping of $3 \times 10^{18}\ cm^{-3}$ at $\sim 1100\ °C$. Then an $In_{0.2}Ga_{0.8}N/GaN$ (3 nm/8 nm) MQW with 8 periods and lastly $\sim 0.25\ \mu m$ Mg-doped GaN were deposited at $\sim 1040\ °C$ on the GaN/sapphire template.

The most direct approach for studying strain or crystalline structure in epitaxial GaN is through XRD measurements.[9] The inset of Fig. 1 shows schematically the top view of the specially designed substrate. The GaN lattice constant c was deduced from the GaN (0002) peak position. It increases continuously from the center of the wafer towards the edge, and has the same trend in all directions, A, B, C, and D, as shown in Fig. 1. GaN in plane lattice constant a was calculated from the (104) peak position, and an

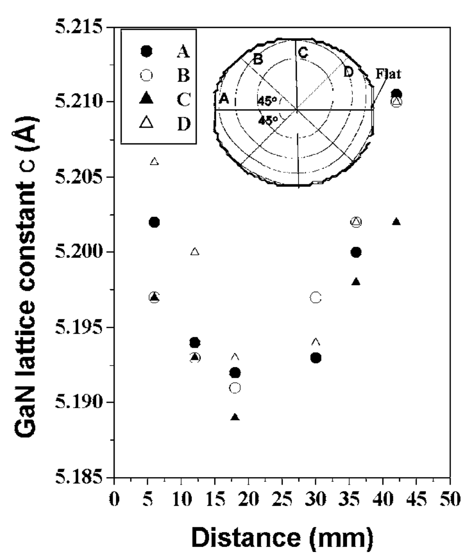

FIG. 1. GaN lattice constant c vs the wafer position, along directions A, B, C, and D, deduced from the GaN (0002) XRD peak in the blue LED wafer grown on a specially designed sapphire substrate. The wafer edges are taken as the references.

[a)]Electronic mail: jingli@phys.ksu.edu

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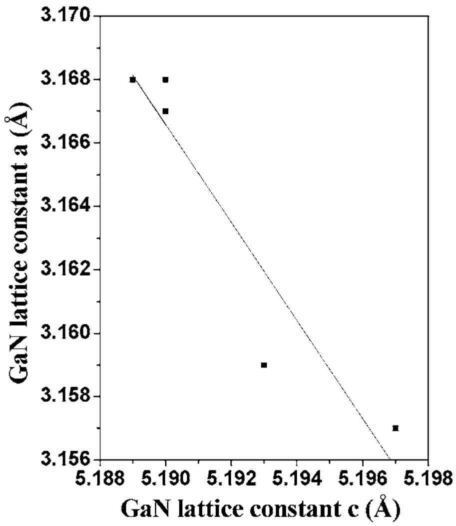

FIG. 2. GaN lattice constants c vs a deduced from the GaN (0002) and (104) XRD reflection peaks in the blue LED wafer grown on a specially designed substrate.

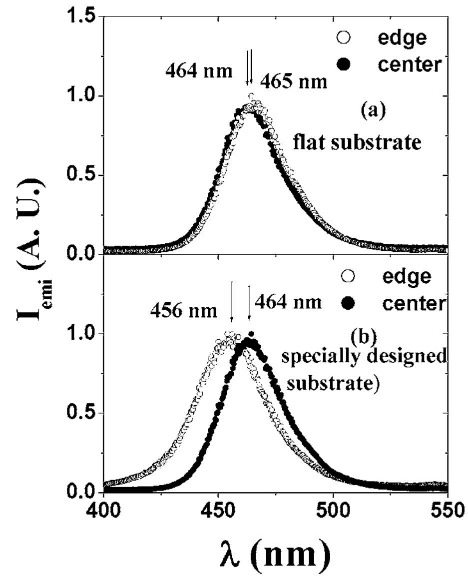

FIG. 3. EL spectra of blue LEDs grown on (a) flat and (b) specially designed substrates.

inverse relation between lattice constants c and a was observed. For comparison, no variations in (0002) and (104) GaN peak positions for LED wafers grown on flat sapphire substrates were observed. The measured variation of GaN lattice constants c and a for LED wafer grown on the specially designed substrate was related to the compressive strain, which was larger at the edges as compared to the center. This difference in strain is most likely induced by the geometrical shape of the substrate, as it possesses a continuous thickness variation. Nevertheless, the growth on such a substrate allows us to probe the effects of strain on the optical properties within a single wafer.

The ratio of elastic stiffness constants for GaN epilayer can be deduced from our experimental data of GaN lattice constants c and a. We consider the case of biaxial strain along the c axis for GaN. The corresponding stress tensor follows Hooke's law as

$$\sigma_{xx} = (C_{11} + C_{12})\varepsilon_{xx} + C_{13}\varepsilon_{zz}, \quad (1)$$

$$\sigma_{zz} = 2C_{13}\varepsilon_{xx} + C_{33}\varepsilon_{zz}, \quad (2)$$

where $\varepsilon_{xx}=(a-a_0)/a_0$ and $\varepsilon_{zz}=(c-c_0)/c_0$, and a (a_0) and c (c_0) are strained (unstrained) lattice constants.

The biaxial strain parallel to the c axis is characterized by vanishing forces in this direction, $\sigma_{zz}=0$, for all layers in a multilayer structure.[4,8] Using this condition and Eq. (2) we have

$$a = (1 + C_{33}/2C_{13})a_0 - (a_0C_{33}/2c_0C_{13})c. \quad (3)$$

As shown in Fig. 2, GaN lattice constant a is plotted against lattice constant c. From linear fitting of our data with Eq. (3), we obtained $(1+C_{33}/2C_{13})a_0=11.19\pm1.61$ and $(a_0C_{33}/2c_0C_{13})=1.55\pm0.31$ which both gives $C_{33}/C_{13} \sim 5.0\pm1.0$, which is in agreement with the calculated value, $C_{33}/C_{13}\sim4.0$.[8]

EL spectra were probed across the entire LED wafer and Fig. 3 shows representative results. For LEDs grown on the flat sapphire substrates, as illustrated in Fig. 3(a), the variation in EL emission peak positions is negligibly small across the entire flat 2 in. wafer. However, as shown in Fig. 3(b), for LEDs grown on the specially designed sapphire substrate, the EL spectral peak positions exhibit a shorter wavelength (~456 nm) at the edges as compared to those at the center, ~464 nm. This is a direct consequence of the fact that the compressive strain is larger at positions close to the edges than those close to the center, consistent with the XRD results shown in Fig. 1. It is known that the band gap energy of a nitride epilayer is affected by the residual stress in the film. A tensile stress will result in a decrease of the energy band gap while a compressive strain causes an increase of the band gap.[2,10,11] So a larger compressive strain results in an EL emission peak position moving towards shorter wavelength.

The EL emission energy peak position as a function of GaN lattice constant c can be extracted from the experimental data such as those shown in Figs. 1 and 3. A linear dependence of the emission energy on the lattice constant c is apparent. After a linear fit of the data as is shown in Fig. 4, the band gap energy of $In_{0.2}Ga_{0.8}N/GaN$ QWs can be ex-

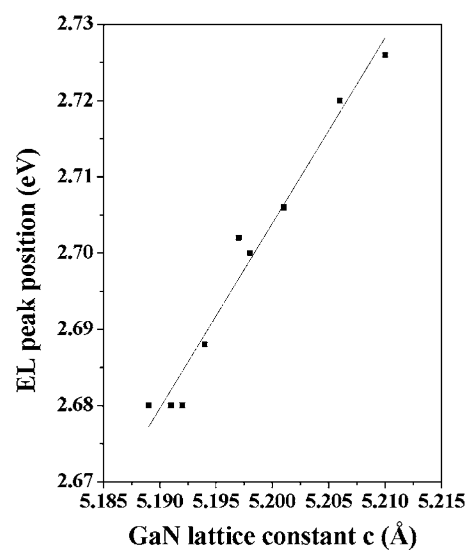

FIG. 4. EL spectral peak position of blue LEDs wafer vs GaN lattice constant c.

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pressed in terms of the change in GaN lattice constant according to

$$E_g = 2.67 + 2.43\Delta c, \quad (4)$$

where $\Delta c = c - c_0$, which represents the change in GaN lattice constant. Here $E_{g0} = 2.67$ eV defines the emission energy of $In_{0.2}Ga_{0.8}N$/GaN MQWs without stress. The biaxial stress dependence of the band gap energy can be expressed as

$$E_g = E_{g0} + B\sigma_{xx} \text{ (eV)}, \quad (5)$$

where E_{g0} and σ_{xx} are unstrained band gap energy and biaxial stress, respectively. B is the linear coefficient characterizing the relationship between the band gap and biaxial stress.[2]

Again considering the case of biaxial strain along the c axis of $In_{0.2}Ga_{0.8}N$ which is characterized by vanishing forces in this direction, $\sigma_{zz} = 0$. The relationship between two components ε_{xx} and ε_{zz} of the strain tensor follows with a coefficient of $-C_{33}/2C_{13}$ and Eq. (1) will take the form

$$\sigma_{xx} = -[C_{13} - (C_{11} + C_{12})C_{33}/2C_{13}]\Delta c/c_0. \quad (6)$$

Here the negative sign represents the compressive stress,[12] C_{13}, C_{11}, C_{12}, and C_{33} are the elastic stiffness constants, and Δc is the lattice constant change of $In_{0.2}Ga_{0.8}N$. We found the elastic stiffness constants of $In_{0.2}Ga_{0.8}N$ by assuming the linear relation between the elastic stiffness constants of GaN and InN. For $In_{0.2}Ga_{0.8}N$ alloy, $C_{11} = 350$ GPa, $C_{12} = 137$ GPa, $C_{13} = 109$ GPa, and $C_{33} = 355$ GPa. Equation (6) can be written as $\sigma_{xx} = 129\Delta c$ and Eq. (5) as follows:

$$E_g = 2.67 + 129B\Delta c, \quad (7)$$

since Δc of $In_{0.2}Ga_{0.8}N$ is unknown, so if we assume that Δc of $In_{0.2}Ga_{0.8}N$ is comparable to that of Δc of GaN, we can compare Eq. (7) and Eq. (4) to get the linear coefficient B of $In_{0.2}Ga_{0.8}N$, which we found was ~19 meV/GPa.

In summary, we have studied the strain effects on the emission properties of InGaN/GaN MQWs through the use of a single blue LED wafer that possesses a continuous variation in compressive strain. Based on the experimental results, a ratio of elastic stiffness constants (C_{33}/C_{13}) for GaN was deduced to be $\sim 5.0 \pm 1.0$, which was in agreement with the calculated value of ~4.0. A linear relation of the EL emission peak position of LEDs with the biaxial strain was observed, and a linear coefficient of 19 meV/GPa characterizing the relationship between the band gap energy and biaxial stress of $In_{0.2}Ga_{0.8}N$/GaN MQWs was also obtained.

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