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LETTER

Growth temperature dependence of strain in a GaN epilayer, grown on a *c*-plane sapphire substrate

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Despite the large mismatch in the lattice constants and thermal-expansion coefficients between the epilayer and the sapphire substrate, GaN epilayer is commonly grown on a *c*-plane sapphire substrate due to the lack of other suitable substrates [1–3]. The GaN epilayer on a *c*-plane sapphire substrate is widely grown with the use of the two-step metalorganic chemical vapor deposition (MOCVD), employing an AlN [4] or a low-temperature GaN buffer layer [5].

It was reported that a biaxial strain and a hydrostatic strain could coexist in the GaN epilayer [6, 7]. In GaN, the biaxial stress is due to thermal mismatch stress and growth [6–10]. The growth stress can be caused by lattice mismatch, island coalescence, grain growth, or surface stress [8–10]. Some in-situ measurements on the growth stress have been reported during MOCVD of GaN [8–10]. The internal hydrostatic strain was shown to have been introduced by the presence of point defects, which can be compressive or expansive depending on their size [6, 7].

A study was reported on a high-resolution X-ray diffraction (HRXRD) strain–stress analysis of a GaN/sapphire heterostructure grown through molecular beam epitaxy (MBE), particularly in the deformation state, depending on the relative content of N in the $Ga_{1-x}N_x$ buffer layer by Harutyunyan et al. [11]. In the authors previous study [12], the strain analysis of a GaN epilayer with different growth times on a *c*-plane sapphire substrate via a two-step growth, using low-pressure, metalorganic chemical vapor deposition was conducted on the basis of precise measurement of the lattice parameters, using HRXRD.

In this continuing study, the growth temperature dependence of the residual strain in a GaN epilayer at room temperature on a *c*-plane sapphire was studied. The final growth temperature in a fixed two-step MOCVD was varied from 850 to 1,050 °C. The *c*- and *a*-lattice parameters were measured using HRXRD, followed by the out-of-plane and in-plane strains. We have extracted the levels of biaxial and hydrostatic components of strain in the GaN films on sapphire.

An undoped GaN epilayer was grown on a *c*-plane sapphire substrate in a horizontal MOCVD reactor at a low pressure of 300 Torr, as described in the authors' previous articles [12, 13]. We employed a two-step growth method of GaN—consisting of the deposition of the low-temperature GaN buffer layer and high-temperature GaN epitaxial growth. The growth temperature of the high-temperature GaN was varied from 850 to 1,050 °C so that the temperature dependence of the strain of the GaN epilayer induced after the two-step MOCVD growth process could be studied. The V/III ratios were 2,740 and 1,370 for buffer growth and the main high-temperature growth, respectively [12]. The growth rate was fixed at 0.07 μm/min; as such, the thickness of the GaN layer that was grown for 20 min was estimated to be 1.5 μm.

The *c*-lattice and *a*-lattice parameters of the GaN epilayers were measured with a ω-2θ scan of the wurtzite GaN epilayer through triple-axis, HRXRD, to obtain precise measurements (PANalytical X'Pert PRO MRD), as described in the authors' previous article [12].

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The unstrained *c*-lattice and *a*-lattice parameters obtained from a reference were used to measure the out-of-plane and in-plane strain components [12]. Leszczynski et al. [14] reported the lattice parameters of the homoepitaxial GaN layers using HRXRD. The unstrained *c*-lattice and *a*-lattice parameters were 0.51850 nm and 0.31878 nm, respectively [14].

The strains and biaxial stresses in the GaN epilayers prepared at the different growth temperatures were measured and extracted. Table 1 shows the strains and biaxial stress in the GaN epilayers. A convention—that the strains are negative if the epilayer is under compression and positive if it is under tension—was used [15]. The GaN epilayer on the (0001) sapphire substrate exhibits in-plane isotropic elastic properties, and its in-plane deformation state can be described by a single strain component [11].

The measured strain in the *c*-direction, ε_c, corresponds to the out-of-plane strain component, while the measured strain in the *a*-direction, ε_a, corresponds to the in-plane strain component [11, 12]. The obtained values of ε_c and ε_a are superpositions of the biaxial strain components, $\varepsilon_c^{(b)}$ and $\varepsilon_a^{(b)}$, respectively, and of the hydrostatic strain component ε_h [6, 7, 11, 12]. And the hydrostatic strain, ε_h, can be determined from the Poisson ratio, ε_c, and ε_a [11]. The Poisson ratio, on the other hand, can be determined from the elastic constants, C_{13} and C_{33} [11, 16], as described in the authors previous article [12].

The Poisson ratio and elastic constants cited in the previous reports [12, 16] were then used to extract the biaxial and hydrostatic strain components of each sample. Table 1 shows the out-of-plane (in the *c*-direction) and in-plane (in the *a*-direction) biaxial strain components, $\varepsilon_c^{(b)}$ and $\varepsilon_a^{(b)}$, respectively, and the hydrostatic strain, ε_h.

The in-plane biaxial stress in the GaN epilayer, σ_f, can be calculated from the product between and $\varepsilon_a^{(b)}$ and M_f, the biaxial elastic modulus [11], as described in the authors previous paper [12].

Table 1 shows that the samples with different growth temperatures had a negative measured (i.e., total) in-plane strain, ε_a, in the GaN epilayer, except for the 850 °C sample. The order of magnitude of all the measured in-plane strain values was 10^{-3}. The negative strain implied that the epilayer was under compression.

The hydrostatic strain, ε_h, showed positive values at 850 °C and 900 °C, and negative values from 950 to 1,050 °C. At 1,050 °C, the hydrostatic strain was -1.38×10^{-4}, whose magnitude was one order smaller than the biaxial strain in the *a*-direction, $\varepsilon_a^{(b)}$, and the total in-plane strain, ε_a. Thus, the hydrostatic component became minor in the total in-plane strain at 1,050 °C.

From 1,000 to 1,050 °C, the total in-plane strain, the hydrostatic strain, and the extracted biaxial in-plane strains, all became of the same compressive type.

Figure 1 shows the measured in-plane strain, ε_a, the biaxial in-plane strain component, $\varepsilon_a^{(b)}$, the hydrostatic strain component, ε_h, and the calculated thermal strain, $\varepsilon_{\text{thermal}}$, as functions of the growth temperature.

Since the thermal-expansion coefficient of GaN ($5.6 \times 10^{-6}\ \text{K}^{-1}$) is much smaller than that of sapphire ($7.5 \times 10^{-6}\ \text{K}^{-1}$) [1], compressive stress can be induced in the GaN epilayer. The thermal strain, $\varepsilon_{\text{thermal}}$, can be calculated from the thermal-expansion coefficients, derived from the post-growth cooling from the high growth temperature to room temperature.

Figure 1 shows a tendency for the magnitude of the difference between the in-plane biaxial component, $\varepsilon_a^{(b)}$, and the thermal strain, $\varepsilon_{\text{thermal}}$, to decrease as the growth temperature increases.

At 1,050 °C, the total in-plane strain, ε_a, seemed to be governed by the biaxial strain, $\varepsilon_a^{(b)}$, because the hydrostatic strain, ε_h, was one order of magnitude smaller than the in-plane biaxial strain, $\varepsilon_a^{(b)}$. Also, with increasing growth temperature, the biaxial strain, $\varepsilon_a^{(b)}$, and the thermal strain, $\varepsilon_{\text{thermal}}$, became much closer in magnitude, as can be seen in Fig. 1.

The highest growth temperature in the metalorganic chemical vapor deposition of GaN on *c*-plane sapphire was most effective in reducing the hydrostatic strain. At such a maximum temperature, the total in-plane strain was dominated by the biaxial strain component. Also, the biaxial

Table 1 Strains and biaxial stress in the GaN epilayers, with different growth temperatures, on a (0001) sapphire substrate grown by a two-step growth method using low-pressure MOCVD

Growth temperature (°C)	Measured strain in *c*-direction ε_c	Measured strain in *a*-direction ε_a	Hydrostatic strain ε_h	Biaxial strain in *c*-direction $\varepsilon_c^{(b)}$	Biaxial strain in *a*-direction $\varepsilon_a^{(b)}$	Biaxial stress σ_f(GPa)
850	-6.56×10^{-4}	2.16×10^{-3}	3.24×10^{-4}	-9.80×10^{-4}	1.84×10^{-3}	–0.88
900	3.39×10^{-3}	-2.42×10^{-3}	1.38×10^{-3}	2.02×10^{-3}	-3.79×10^{-3}	–1.81
950	-1.99×10^{-3}	-1.54×10^{-3}	-1.83×10^{-3}	-1.56×10^{-4}	2.93×10^{-4}	1.40
1,000	-1.66×10^{-3}	-2.45×10^{-3}	-1.93×10^{-3}	2.74×10^{-4}	-5.14×10^{-4}	–0.25
1,020	-1.31×10^{-3}	-3.86×10^{-3}	-2.20×10^{-3}	8.85×10^{-4}	-1.66×10^{-3}	–0.80
1,050	1.04×10^{-3}	-2.35×10^{-3}	-1.38×10^{-4}	1.18×10^{-3}	-2.21×10^{-3}	–1.10

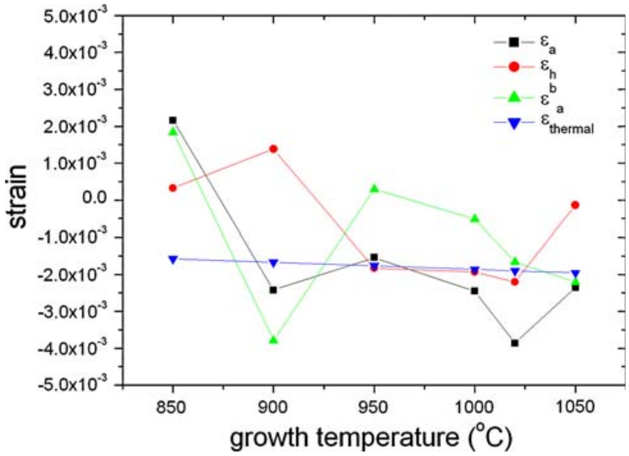

Fig. 1 The measured in-plane strain, ε_a, the biaxial in-plane strain component, $\varepsilon_a^{(b)}$, the hydrostatic strain component, ε_h, and the calculated thermal strain, $\varepsilon_{thermal}$, as functions of the growth temperature

strain component seemed to be governed mainly by the post-growth thermal cooling. The observation that the calculated value of thermal strain and the measured biaxial strain approach each other with increase in growth temperature shows that relaxation of any sort and growth stress contributions diminish with increasing growth temperatures.

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