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High-quality distributed Bragg reflectors based on $Al_xGa_{1-x}N$/GaN multilayers grown by molecular-beam epitaxy

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Distributed Bragg reflectors based on $Al_xGa_{1-x}N$/GaN multilayer stacks have been grown by plasma-assisted molecular-beam epitaxy on GaN templates. The nominal Al composition ranged from 30% to 45%, and the layer thicknesses of the ten-period stack were designed for a target wavelength of 510 nm. Transmission electron microscopy data reveal periodic structures where (Al,Ga)N on the GaN interface is sharper than GaN on the (Al,Ga)N one. X-ray diffraction spectra fitted to a dynamic diffraction simulation model yield an estimate of the layer thicknesses, Al%, and lattice strain. Reflectivity values above 50% at 510 nm have been reproducibly achieved, in very good agreement with the results of the matrix-method simulation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1401090]

High-reflectivity distributed Bragg reflectors (DBRs) are key elements to develop vertical-cavity surface-emitting lasers[1,2] and resonant-cavity light-emitting diodes (RCLEDs).[3,4] DBRs significantly enhance the efficiency of photodetectors,[5] and in general they lead to more efficient, selective, and faster devices.[6]

Given the rather small $Al_xGa_{1-x}N$/GaN refractive-index contrast, the achievement of high-reflectivity/selectivity reflectors based on this material system needs multilayer stacks with many periods and/or a high-Al mole fraction. The lattice mismatch between $Al_xGa_{1-x}N$ and GaN usually leads to cracks in the reflector structure for thick multilayer stacks with a high-Al mole fraction. (Al,Ga)N/GaN DBRs have recently been demonstrated by metal–organic vapor-phase epitaxy (MOVPE) (Ref. 7) and molecular-beam epitaxy (MBE),[8–10] but in all cases, a large number of periods and a large Al mole fraction were needed to reach reflectivities up to 90%.

In this work, ten-period quarter-wave (Al,Ga)N/GaN DBRs, with Al mole fractions from 30% to 45%, and reflectivities up to 50% at 510 nm have been fabricated to be further incorporated in backside (sapphire) emitting RCLEDs for communications through plastic optical fibers.[11] Such a thin reflector will avoid cracks and an excessive voltage drop caused by a large series resistance. In spite of the small refractive-index contrast ($\Delta n = 0.17$ for 45% Al) and the low number of periods, peak reflectivities above 50% have been achieved. High-resolution transmission electron microscopy (HRTEM) and x-ray diffractometry (XRD) provided the structural characteristics of the DBRs. Normal-incidence reflectance spectra, normalized by a standard mirror, were obtained at room temperature with a Perkin-Elmer Lambda 9 spectrophotometer.

The (Al,Ga)N/GaN DBRs were grown on 3–4-μm-thick GaN templates (GaN/sapphire layers grown by MOVPE) by plasma-assisted MBE (Oxford CARS25 rf source). A 100-nm-thick GaN buffer layer was first grown at 680 °C for all reflectors. The nominal thicknesses were 52.8 nm for the GaN layers, and from 55.5 to 56.9 nm for the (Al,Ga)N layers with 30%–45% Al, respectively. The substrate temperature was sharply increased during the growth of the (Al,Ga)N layers from 680 up to 730 °C, without growth interruption. A streaky 1×1 reflection high-energy electron diffraction (RHEED) pattern (hexagonal symmetry) was observed throughout the growth, turning into a 2×2 surface reconstruction, characteristic of a smooth and flat two-dimensional growth front, upon cooling down. A detailed description of the growth system and conditions is given elsewhere.[12]

The cross-section transmission electron microscopy (TEM) image of a ten-period DBR in Fig. 1(a) reveals very good periodicity and uniformity that are unaffected by threading dislocations running along the structure. The corresponding high-resolution image in Fig. 1(b) shows abrupt and smooth heterointerfaces, being the (Al,Ga)N on GaN interface sharper than the GaN on (Al,Ga)N one. This fact was also observed by RHEED when the streaky 1×1 pattern became diffused at the end of the (Al,Ga)N layer growth. The measured layer thicknesses (49.5 nm for GaN; 52 nm for $Al_{0.3}Ga_{0.7}N$) are very close to the nominal values within a ±3 nm dispersion. The extra periodicity observed in the (Al,Ga)N layers, already reported in (Al,Ga)N/GaN multilayers grown by MOVPE,[13] is attributed to the modulation of the Al/Ga ratio due to the sample rotation rate and the Al and Ga cells position (angle) relative to the substrate. Reflectivity

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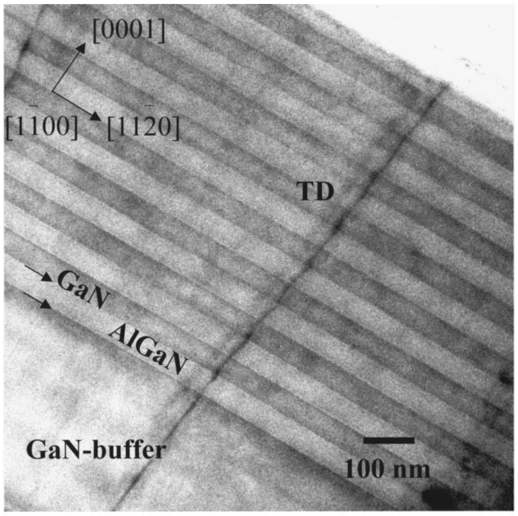
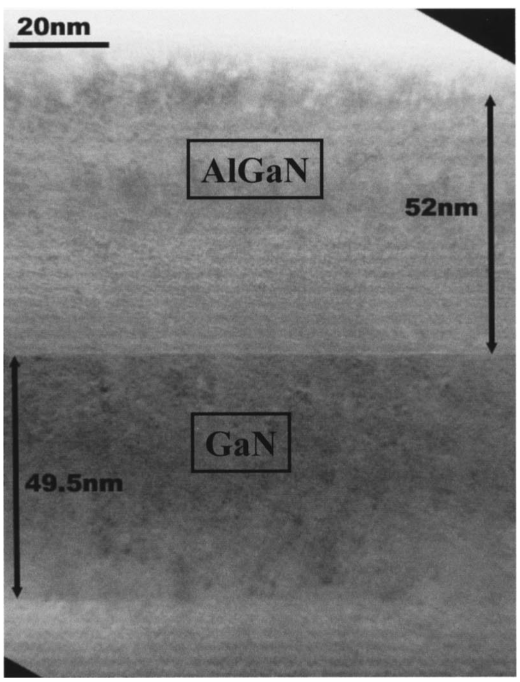


(a)



(b)

FIG. 1. (a) Cross-section TEM image of a ten-period $Al_{0.3}Ga_{0.7}N$/GaN DBR. (b) High-resolution TEM image of a ten-period $Al_{0.3}Ga_{0.7}N$/GaN DBR.

and XRD simulations show that this additional periodicity does not affect the DBR performance. Cracks are observed by optical microscopy on the surface of the DBRs for Al contents above 30%.

High-resolution XRD (HRXRD) spectra and a dynamic simulation program[14] provide an estimate of the layer thicknesses, the Al mole fraction, and the strain state. A very good agreement between measured and simulated XRD spectra is shown in Fig. 2. Sharp and intense satellite peaks confirm the excellent structural quality of the DBRs. A partial relaxation of the (Al,Ga)N layers is found to increase with the Al content. The estimated Al mole fraction is quite close to the nominal values and the layer thicknesses [53 nm for GaN and 56 nm for (Al,Ga)N] are also very close to the nominal and HRTEM-derived values.

Figure 3(a) shows reflectivity spectra measured in two

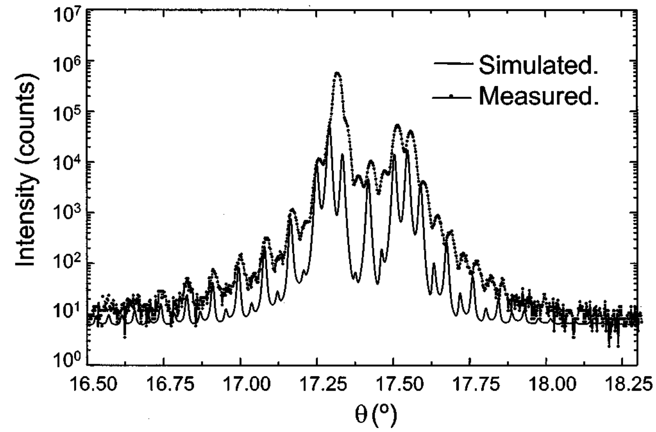


FIG. 2. Comparison between measured and simulated HRXRD spectra for a ten-period $Al_{0.3}Ga_{0.7}N$/GaN Bragg mirror.

DBRs differing on the Al content and layer thicknesses to fit the target wavelength of 510 nm. The higher peak reflectivity and bandwidth of the second DBR rely on the higher refractive-index contrast,[15] whereas the superimposed oscillations are due to Fabry–Pérot interferences in the GaN buffer and the sapphire substrate. Standard transmission matrix-method simulations[16] were performed to fit the experimental reflectivity spectra, neglecting the absorption in the (Al,Ga)N layers and assuming an infinite thick sapphire substrate. Refractive-index data were obtained from a fit of the transmission spectra to the Sellmeier equation,[17] and the

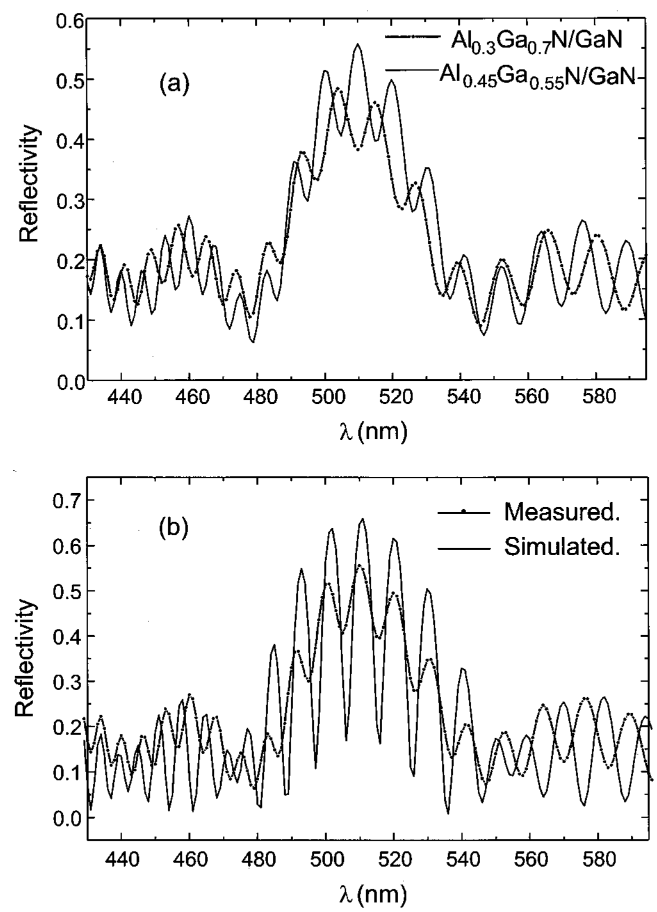


FIG. 3. (a) Reflectivity spectra of two DBRs with different Al compositions, both centered at 510 nm. (b) Comparison between measured and simulated reflectivity spectra of an $Al_{0.45}Ga_{0.55}N$/GaN DBR.

layer thicknesses were derived from the quarter-wave criteria ($n_i d_i = \lambda/4$). Figure 3(b) shows very good agreement between simulated and experimental spectra for an $Al_{0.45}Ga_{0.55}N/GaN$ DBR. Small deviations in the position and intensity of the bandpass satellite peaks may be due to interface roughness and to inaccuracies in the refractive-index values used.

In summary, although a low number of periods and a rather low-Al mole fraction were used, DBRs with reflectivities above 50% at 510 nm have been reproducibly grown by MBE. When MBE proceeds almost homoepitaxially (on GaN templates), it provides an optimal interface abruptness control and a reduction of the surface roughness of the whole structure compared to the template one. DBRs grown by MBE are key elements to fabricate RCLEDs, whose active region may be grown by MBE or MOVPE. An excellent periodicity, uniformity, and interface abruptness have been achieved. An accurate growth rate control leads to very close nominal and experimental layer thicknesses, allowing a very high reproducibility.

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