High-reflectivity ultraviolet AlGaN/AlGaN distributed Bragg reflectors

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High-quality distributed Bragg reflectors (DBRs) in the ultraviolet region are essential for the development of GaN-based optical devices. In particular, the region around 350 nm is important for devices containing pure GaN as an active medium. The growth of DBRs remains a fundamental challenge in the nitride system. The difficulty lies in maintaining the structural integrity of a relatively thick structure that contains materials with a large lattice constant mismatch and different thermal expansion coefficients. The successful growth of lattice-matched AlGaN/AlInN DBRs with metal-organic vapor phase epitaxy has been reported recently, however, it is yet to be demonstrated using molecular-beam epitaxy (MBE). Only a few groups have reported high-reflectivity Al$_{1-x}$Ga$_x$N/Al$_{1-x'}$Ga$_{x'}$N DBRs.

Due to the lattice constant mismatch between GaN and AlN, an Al$_{1-x}$Ga$_x$N epilayer grown on the GaN substrate experiences in-plane tensile strain. The layer is stable against the introduction of misfit dislocations if its thickness is below the critical thickness defined by the Matthews–Blakeslee criterion. At typical Al$_{1-x}$Ga$_x$N/Al$_{1-x'}$Ga$_{x'}$N DBR structure is much thicker than the critical layer thickness, and the strain in the structure tends to relax by generating a network of cracks, which degrade the optical quality. However, if the DBR structure is designed to alternate between the tensile and the compressive strain in the layers with different Al content, the in-plane stress in the individual layers counteracts and the epilayers maintain coherency with the substrate throughout the structure.

In this letter, we demonstrate high-reflectivity crack-free Al$_{0.15}$Ga$_{0.85}$N/Al$_{0.18}$Ga$_{0.82}$N DBRs in which the low Al content layers are under the in-plane compressive stress and the high Al content layers are under the tensile stress. The structures are grown by MBE on GaN templates. We have produced DBR stacks consisting of up to 25 periods that exhibit no cracks. A 25-period DBR provides the maximum reflectivity higher than 99%. © 2006 American Institute of Physics. [DOI: 10.1063/1.2195547]
diffractometry in 67, 74, and 83 nm as determined by high-resolution x-ray

The room-temperature characteristics of the 74 nm period sample and to 100% (within the experimental error of ±1.5%) for the 25 period sample.

The reflectivity spectra are used to extract the refractive indices and absorption coefficients of the AlGaN layers. To model the wavelength dependence of the refractive indices, we assume a general model of the real part of the dielectric function in the vicinity of the band gap.

\[
\varepsilon(\lambda) = C + A \lambda^{2} \left[ 2 - \left( 1 + \frac{\lambda_s}{\lambda} \right)^{1/2} - \left( 1 - \frac{\lambda_s}{\lambda} \right)^{1/2} \right],
\]

where \( \lambda_s = h\nu / E_g \) is the band-gap absorption edge, and \( A \) and \( C \) are constants that depend on the Al content. The absorption coefficient is assumed to decay exponentially below the band gap according to the Urbach model: \( \alpha(E) = \alpha_0 \exp(E - E_g / \nu_U) \).

By varying the parameters of Eq. (1), reflectivity spectra are calculated using the transfer matrix approach and matched to the experimental data (Fig. 1).

The parameters of Eq. (1) used in the calculations are summarized in Table I. Strongly damped oscillations of the reflectivity on the short-wavelength side of the stop band indicate that the absorption edge of the low Al content layer is located immediately next to the stop band. It allows the determination of the absorption edge \( \lambda_s \) for Al\(_{x}\)Ga\(_{1-x}\)N layers

<table>
<thead>
<tr>
<th>Sample/layer</th>
<th>( E_g (\text{eV}) )</th>
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<tr>
<td>S1/Al(<em>{x})Ga(</em>{1-x})N</td>
<td>3.77</td>
<td>5.35</td>
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width at half maximum of 25 nm and 26 nm, respectively. The maximum reflectivity is verified by the direct measurement of the reflection coefficient using the frequency-doubled emission from a mode-locked Ti-Sapphire laser tuned to 700 nm. The low-temperature spectra are shown in Fig. 2. The maximum reflectivity increases to 95% for the 20 period sample and to 100% (within the experimental error of ±1.5%) for the 25 period sample.

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with high accuracy. The absorption coefficient for Al\textsubscript{0.18}Ga\textsubscript{0.82}N layers above the band gap is assumed to be equal to 

\[ \alpha_0 = 0.63 \times 10^4 \text{ cm}^{-1} \text{ (Ref. [12])} \]

and the Urbach parameter \( E_{U} = 0.045 \text{ eV} \) is adjusted to fit the experimental data.

The calculated reflectivity spectra show a good fit to the experimental data. The corresponding refractive indices modeled by Eq. (1) are shown in Fig. 1. Compared to the values reported in the literature the optical constants determined from the fit appear slightly smaller. The index decrease in the low Al content layers is partly attributed to the strain-induced changes in the band-gap structure. The compressive strain results in a positive shift of the absorption edge \( \Delta E_g \sim 50 \text{ meV} \):

\[
\Delta E_g = \frac{dE}{d\sigma} \Delta \sigma = \frac{E}{1 - \nu} \frac{dE}{d\sigma} \Delta a,
\]

where the strain induced coefficient \( dE/d\sigma = 25 \text{ meV/GPa} \), the bulk modulus \( E = 200 \text{ GPa} \), Poisson’s ratio \( \nu = 0.22 \), and the misfit between the Al\textsubscript{0.18}Ga\textsubscript{0.82}N and the Al\textsubscript{0.5}Ga\textsubscript{0.5}N layer \( f = \frac{dE}{d\sigma} = 0.008 \). The refractive index varies most rapidly in the vicinity of the band gap, and the shift in the band-gap position of the low Al content layers by \( 50 \text{ meV} \) (\( \sim 5 \text{ nm \@ 350 nm} \)) can produce the refractive index decrease of \( \Delta n = 0.03 \). In addition, a variation of several percent in the composition of AlGaN layers would alter the optical constants.

Factors limiting reflectivity include the refractive index contrast between the \( \lambda/4 \) layers and intrinsic absorption in the low Al content layer below the band gap. The maximum reflectivity for a DBR consisting of layers with the refractive indices of sample S2 is shown in the inset of Fig. 2. The maximum reflectivity is calculated as a function of the number of periods \( m \) assuming no absorption below the band gap. The effect of intrinsic absorption can be seen in the shape of the stop band sloped on the short-wavelength side. The maximum reflectivity for a mirror with the intrinsic absorption below the band gap described by the Urbach model decreases by \( \sim 0.5\% \).

In conclusion, we demonstrate high-reflectivity \( 25 \text{ pe-} \lambda \) Al\textsubscript{0.18}Ga\textsubscript{0.82}N/Al\textsubscript{0.5}Ga\textsubscript{0.5}N DBRs centered at \( 347 \text{ nm} \) grown by MBE on thick GaN templates. The structural quality of the DBR layers is maintained by balancing the compressive and tensile strains in each \( \lambda/4 \) pair. This approach results in the lowest elastic strain energy and allows the growth of thick coherently strained DBRs. Reflectivity spectra show a \( 26 \text{ nm wide stop band centered at 347 nm} \) with the maximum reflectivity higher than \( 99\% \). The stop band covers the spectral region corresponding to the exciton energies in bulk GaN and AlGaN/GaN quantum wells, and the DBRs can be used to build microcavities with GaN quantum wells as an active medium.

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