High quality UV AlGaN/AlGaN distributed Bragg reflectors and microcavities

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ABSTRACT

We demonstrate high-reflectivity crack-free $Al_{0.18}Ga_{0.82}N/Al_{0.8}Ga_{0.2}N$ distributed Bragg reflectors (DBR) and monolithic microcavities grown by molecular beam epitaxy on thick *c*-axis GaN templates. The elastic strain energy in the epilayer is minimized by compensating the compressive and tensile stress in every period of the DBR structure. A 25 period DBR mirror provides a 26nm-wide stop band centered at 347 nm with the maximum reflectivity higher than 99%. The high-reflectivity DBRs can be used to form high *Q*-factor monolithic AlGaN/AlGaN microcavities.

INTRODUCTION

High-reflectivity distributed Bragg reflectors (DBR) in the ultraviolet region are essential for the development of GaNbased 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 challenging 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. Only a few groups have reported high-reflectivity $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ DBRs [1-4].

We demonstrate high-reflectivity crack-free $Al_{0.18}Ga_{0.82}N/Al_{0.8}Ga_{0.2}N$ 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 close to 100 % and a 26nm-wide stop-band centered at 347 nm.

Due to the lattice constant mismatch between GaN and AlN, an $Al_xGa_{1-x}N$ 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 [5]. A typical $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ DBR structure is however 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.

To compensate the stress in the individual layers of the DBR structure and to minimize the elastic strain energy the lateral lattice constant of the structure must match the average lattice constant of the individual layers in the relaxed state. Such structure can be grown on a substrate with a lattice constant equal to the average lattice constant. A relaxed $Al_XGa_{1,X}N$ interlayer, where X is the average Al fraction, can serve as a seeding layer.

Each layer of the DBR structure also must be coherent with the previous layer. Therefore, the Al content x and y of the DBR layers are chosen so the thickness of each layer, determined by the center wavelength of the DBR $d_{1,2} = \lambda_0/4n_{1,2}$, doesn't exceed the corresponding critical thickness. Such DBR structure remains coherently strained with the strain alternating from the compressive in the low Al content layers to the tensile in the high Al content layers. The

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corresponding stress is compensated in each pair of the $\lambda/4$ layers such that a DBR structure can be grown without the formation of cracks.



Fig. 1. Stress compensation in AlGaN/AlGaN DBR and X-ray diffraction spectra of DBR samples with periods 67, 74, 84 nm (top to bottom).

EXPERIMENT

100 μ m thick GaN templates are prepared by hydride vapor phase epitaxy (HVPE) on 2 inch sapphire substrates. The DBR structures are grown on the GaN templates by plasma assisted MBE at 750° C and the background pressure of 2.10⁻⁶ Torr under slightly metal rich conditions at a growth rate of 300 nm/h set by RF power of 400W and nitrogen flow rate of 0.75 sccm. Two Al cells were used for the growth of the alternating AlGaN layers. The cell designated for the high Al content layers is also used for the growth of the interlayer.

The critical misfit defines the thermodynamic boundary between epilayers with a given thickness stable against and susceptible to the dislocation formation. For a mirror with the stop band centered at around 350 nm the thickness of individual DBR layers is $d = \lambda_0/4n \sim 30$ -40 nm. The critical misfit for thickness d = 30 nm is ~0.003 and it corresponds to the variation of ~30% in the Al content of the DBR layers [6]. However, films with thickness exceeding the critical by a factor of two typically remain coherent with the substrate [7].

The Al content *x* is chosen high enough to avoid the interband absorption within the stop band. Taking into consideration these constraints, the following DBR structure was grown: the Al_xGa_{1-x}N interlayer with Al content X = 0.5+/-0.05 is grown on an initial MBE GaN buffer layer; it is followed by an Al_xGa_{1-x}N/Al_yGa_{1-y}N pair of quarter wave layers with x = 0.18+/-0.02 and y = 0.8+/-0.1 repeated (m-1) times; the structure is capped by a $\lambda/4$ layer of Al_xGa_{1-x}N. The misfit between the GaN substrate and the interlayer with Al content X = 0.5 is ~0.013. The corresponding critical thickness: $d_c < 10$ nm $<<\lambda_0/4n$. Therefore the interlayer thickness was adjusted to match one quarter of the central wavelength and to serve as a part of the DBR structure with $m \lambda/4$ pairs.

Optical reflectivity spectra of the samples are measured at room temperature and at T = 10 K using a xenon arc lamp. 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.



Fig. 2. Measured and calculated room-temperature reflectivity of a 25-period Al_{0.18}Ga_{0.82}N/Al_{0.8}Ga_{0.2}N DBR (right panel) and measured low-temperature reflectivity of a 20 and 25-period DBRs.

RESULTS

DBR samples are grown with the periods $d_1+d_2 = 53$, 67, 74, and 83 nm as determined by high-resolution x-ray diffractometry in ω -2 θ geometry. The growth conditions were proven to produce sharp interfaces, as confirmed by the x-ray analysis of reference superlattice samples. The homogeneity of the layer thickness throughout the structure is confirmed by cross-sectional scanning electron-microscopy. All samples with the period up to 75 nm exhibit no crack formation. The x-ray diffraction scans show compressive strain in the low Al content layers and tensile strain in the high Al content layers (Fig. 1). The 83nm-period sample developed a network of cracks with an average spacing of $5 - 7 \mu m$ clearly visible in the optical microscope. The x-ray diffraction scan of this sample shows the lattice relaxation in the epilayers.

The room temperature reflectivity characteristics of the 74nm-period mirrors are shown in Fig. 2. The structure produce a well-defined stop band with the maximum reflectivity of 93 +/- 1.5 % for a 20-pair mirror and 99 +/- 1.5 % for a 25-pair mirror. The FWHM of the stopband is 25 and 26 nm respectively. At T = 10 K, 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.

Reflectivity spectra are calculated using the transfer matrix approach and matched to the experimental data. The calculated reflectivity spectra show a good fit to the experimental data. Compared to the values reported in the literature the optical constants determined from the fit appear slightly smaller [8-10]. The index decrease in the low Al content layers is partly attributed to the strain-induced changes in the bandgap structure. The compressive strain results in a positive shift of the absorption edge $\Delta E_g \sim 50$ meV [10]. The refractive index varies most rapidly in the vicinity of the bandgap, and the shift in the bandgap position of the low Al content layers by 50 meV (~5 nm @ 350 nm) can produce the refractive index decrease of $\Delta n = 0.03$. In addition, variation of several percent in the composition of AlGaN layers would alter the optical constants.

DISCUSSION

Stress-compensated AlGaN/AlGaN DBR show substantially better reflectivity characteristics and allow achieving reflectivity higher than 99%. Factors limiting reflectivity in this system include the refractive index contrast between the

 $\lambda/4$ layers and intrinsic absorption in the low Al content layer below the bandgap. The maximum reflectivity for a DBR consisting of layers with the refractive indices extracted from the experimental data is shown in the Fig. 3. The maximum reflectivity is calculated as a function of the number of periods *m* assuming no absorption below the bandgap.



Fig. 3. Peak reflectivity of an $Al_{0.2}Ga_{0.8}N/Al_{0.8}Ga_{0.2}N$ DBR as a function of the number of periods *m* calculated using the optical constants extracted from the experimental data.

Absorption in the proximity of the bandgap results in a small reduction of the reflection coefficient. 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 bandgap described by the Urbach model decreases by $\sim 0.5 \%$ [10].

The refractive index contrast in our structure is close to the highest allowed value. A lower Al fraction in the lowindex layer results in the shift of the absorption edge into the stopband region. A higher Al fraction in the high-index layer results in a larger lattice mismatch and, consequently, the lattice relaxation and crack formation. An alternative approach for high-reflectivity DBR structures is to replace the low-index layers with AlInN layers. An AlInN/AlGaN DBR can be designed to be lattice matched. The index contrast of the lattice-matched AlInN/AlGaN DBR is however lower than in our structures and a comparable reflectivity can only be achieved in structures with more periods.

CONCLUSIONS

In conclusion, we demonstrate high reflectivity 25 period $Al_{0.18}Ga_{0.82}N/Al_{0.8}Ga_{0.2}N$ DBRs centered at 347 nm grown by MBE on thick GaN templates. The structural quality of the DBR layers is maintained by compensating 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 26nm-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 the bulk GaN and AlGaN/GaN quantum wells and these DBRs can be used to build microcavities with GaN quantum wells as an active medium.

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