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HRTEM study of $Al_xGa_{1-x}N/AlN$ DBR mirrors

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Abstract

In the present work semiconductor quarter wavelength distributed Bragg reflector (DBR) mirrors have been studied by high resolution transmission electron microscopy (HRTEM). The mirrors have been fabricated monolithically by plasma assisted molecular beam epitaxy (MBE) on sapphire (0001) substrates. The samples are conformed of a large number of $Al_xGa_{1-x}N/AlN$ layers with 5.5 and 20.5 periods, both with different aluminium concentration. The samples have been designed utilising spectroscopic ellipsometry (SE) dispersion spectra of previously fabricated single layers. The aim of this work was to determine the distortion of lattice parameters of $Al_xGa_{1-x}N/AlN$ epilayers, since this is important for the later production of vertical cavity surface emitting lasers (VCSELs). Distortions of half periods layers were determined from HRTEM techniques and are compared with the distortion determination using an equilibrium theory and high resolution X-ray diffraction (XRD) measurements.

Keywords: AlN; GaN; High resolution transmission electron microscopy; Distributed Bragg reflector

1. Introduction

The development of laser technology based in III-nitrides compounds is actually centred in the introduction of vertical cavity surface lasers (VCSELs). In order to improve the external efficiencies of these lasers, it is necessary the use of high reflectance mirrors, usually in the form of distributed Bragg reflectors (DBRs). AlN/GaN pairs are used as quarter-wave reflectors stack operating in the blue-green region. Reflectances of 90–99% in AlN/GaN mirrors using from 15 to 25.5 periods have been reported [1,2]. $Al_xGa_{1-x}N/GaN$ pairs can be grown with reflectivity up to 93% in the range of 390–70 nm [3–6]. Both systems (Al, Ga)N/GaN mirrors prohibit the possibility of utilise GaN as an active medium for UV-VCSEL, due to light absorption of the mirror in the emitting region of the active GaN. In order to minimise the absorption when GaN is used as an active medium in DBR structures, it is necessary the use of $Al_xGa_{1-x}N/AlN$ pairs controlling the Al content [7–9].

Another important requirement for the fabrication of DBR nitrides is the large band width of the reflectance peaks. However, due to the mismatch between $Al_xGa_{1-x}N$ and AlN layers, the issue of strain relaxation is of particular importance to optimise the properties of these Bragg mirrors that are to be used in VCSEL structures [4].

In the current work, the strained lattice parameters of $Al_xGa_{1-x}N$ and AlN layers used as quarter-wave DBRs mirrors have been determined using high resolution transmission electron microscopy (HRTEM). The $Al_xGa_{1-x}N/AlN$ layers were monolithically grown by plasma assisted molecular beam epitaxy (PAMBE). Furthermore, we have compared the measured strained lattice parameters with results obtained by high resolution X-ray diffraction (XRD) using an extended bond method [10] and an equilibrium theory [11], allowing the analysis of the evolution of critical thickness across DBR periods.

2. Experimental

In the present work, two $Al_xGa_{1-x}N/AlN$ DBR structures have been studied (samples A and B). The samples

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Table 1
Summary of DBR samples under study (see Fedler et al. [8])

Sample	Periods	x (%)	Thickness of periods design (nm)			Thickness of periods by XRD (nm)			Reflectivity (max %)	Peak (design) (centre nm)
			L	LAlGaN	LAlN	L	LAlGaN	LAlN		
A	5.5	37	84.9	40.3	44.7	85.9	41.5	44.4	53.6	377 (380)
B	20.5	5.6	77.4	35.1	42.3	72.7	33.3	39.4	95.4	353 (362)

were grown in a Riber32 ultrahigh vacuum (UHV) chamber by PAMBE (Addon source) with conventional Knudsen cells for Ga and Al sources. Previously both samples have been designed utilising spectroscopic ellipsometry (SE) dispersion spectra. With the aid of ex-situ SE, n and k functions of the reference sample's $Al_xGa_{1-x}N$ layer were extracted. Detailed design and growth conditions are given in Fedler et al. [8,10].

HRTEM studies of samples have been carried out using the JEOL 2000-EX microscope at 200 kV with an spherical aberration of 0.7 mm and working in the Scherzer focus. The HRTEM images obtained are digitalised and processed for the extraction of lattice parameters of layers and subsequently the strain values in each half period are determined. However, we have compared the strain results obtained by HRTEM with an extensive XRD analysis, which gives precise information about lattice parameters and layer thickness of grown DBR samples. In Table 1 the structure layers and SE design [8] of DBR samples are summarised.

3. Results and discussion

Thermal and lattice mismatch between heteroepitaxial layers generate distortion of parameters and misfit dislocations in the epilayers. To determine the distortion in the epilayers, approaches based in equilibrium theories used in metastable heteroepitaxial semiconductor structures can be used [12,13]. Fischer et al. [12] have proposed an equilibrium theory, which included the elastic interaction between straight misfit dislocations, and obtained the critical thickness (h_c). We have used the Fischer model to determine the h_c in each half period of DBR mirrors. According to the Fischer model, the critical thickness is given by

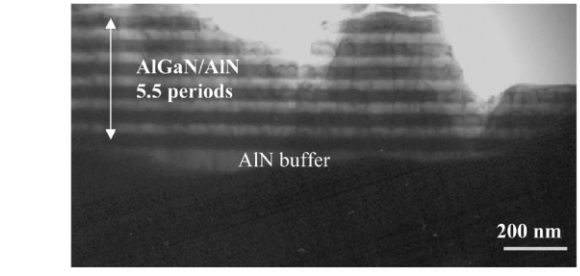
$$\frac{a_0-a_s}{a_s}=\frac{b\cdot\cos\lambda}{2h_c}\left\{1+\left[\frac{1-\frac{\nu}{4}}{4\pi(1+\nu)\cdot\cos^2\lambda}\right]\ln\left(\frac{h_c}{b}\right)\right\} \quad (1)$$

a_0 and a_s denotes the lattice constant of the epilayer and that of the layer underneath, respectively. λ is the angle between the Burgers vector (**b**) and the direction in the interface, normal to the dislocation line. ν is the Poisson constant of epilayer.

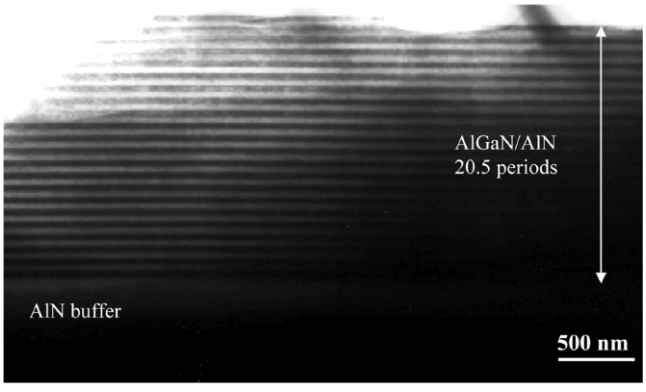
The h_c value of AlN buffer is calculated assuming an underneath layer consisting of relaxed sapphire. The a parameter at the surface of the AlN buffer layer is

Table 2
Calculated critical thickness and DBR layers thickness

Sample	Calculated critical thickness (nm)			Thickness measured from XTEM images (nm)		
	AlN buffer	$Al_xGa_{1-x}N$	AlN	AlN buffer	$Al_xGa_{1-x}N$	AlN
A	1003	16.25	17.71	222±6	33±4	39±4
B		9.08	9.91	241±5	31±3	40±4



(a)



(b)

Fig. 1. Bright field XTEM images near the $\langle 11\bar{2}0\rangle$ zone axis, (a) sample A (5.5 periods) and (b) sample B (20.5 periods).

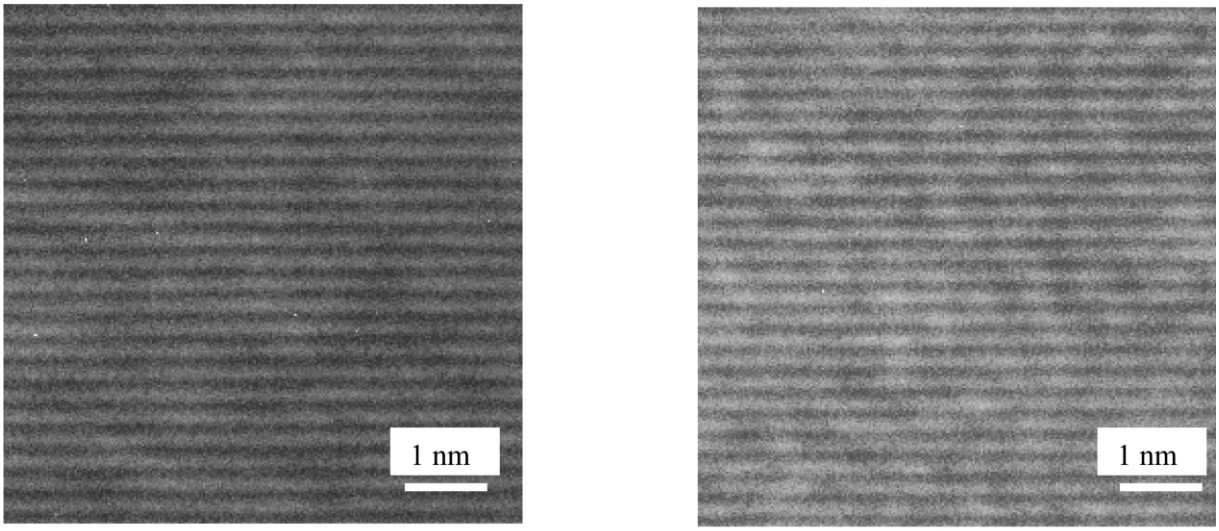


Fig. 2. HREM images showing fringes corresponding to {0002} planes of two half period layers for sample B: (a) $Al_xGa_{1-x}N$ and (b) AlN.

calculated by the equation that relates the dependence of h_c proposed by Chinkyo et al. [11].

$$a = a_0 + \frac{h_c}{h}(a_s - a_0) \quad (2)$$

where a is the strained in-plane lattice parameter of the epilayer, h is the thickness of the epilayer, a_0 and a_s are the unstrained epilayer and the base lattice constants, respectively. Subsequently, the h_c of each half period of $Al_xGa_{1-x}N$ and AlN were determined making an iterative calculation of a_s.

The distortion measured in the present work has been carried out on the c parameter of $Al_xGa_{1-x}N$ and AlN half period layers. The measurements of c parameters is related to the distortion of the a parameter expressed in Eq. (2), as follows [11]:

$$c = c_0 + \frac{c_0 \nu}{a_0}(a_0 - a) \quad (3)$$

where c_0 is the relaxed lattice constant of the epilayer. The results of critical thickness calculation and the thickness of half periods measured from cross-section transmission electron microscopy images (XTEM) are presented in Table 2. Fig. 1 shows XTEM images from both studied DBRs where their stacked layers are visible.

The critical thickness calculated in both samples is below the experimental growth thickness for AlN and $Al_xGa_{1-x}N$ layers. This results indicates that the relaxation processes of $Al_xGa_{1-x}N$ and AlN layers have begun. Starting from calculated critical thicknesses and the calculated a parameter, the distortion in direction $\langle 0001 \rangle$ in the layers is determined; these results are graphically represented in Fig. 3. The dashed lines of Fig. 3 correspond to the calculated c distorted lattice constants of $Al_xGa_{1-x}N$ and AlN half period layers.

The distortion of the c parameter has directly been measured in experimental images obtained by HRTEM from the central zones of the half period layers. The HRTEM images are obtained in three beam conditions, using the transmitted, 0002 and $000\bar{2}$ reflections. In this way, fringes corresponding to the {0002} planes are observed. From these images, the measurement of distortion in c parameters of AlN and $Al_xGa_{1-x}N$ layers can be determined. The procedure is based in the tracing of perpendicular profiles to (0002) planes, measuring the distances among maximum peaks and determining the c parameter distortions.

Fig. 2 shows two HRTEM images that correspond to the central zone of $Al_xGa_{1-x}N$ and AlN half periods of sample B. This type of HRTEM image was utilised to carry out the strain measurements for samples A and B.

The parameters of unstrained $Al_xGa_{1-x}N$ layers have been calculated using Vegard's law. The average distortions of half periods layers obtained from HRTEM images are indicated in Fig. 3 with black colour squares.

However, high resolution (002) XRD $\theta/2\theta$-scan of the DBRs have been used as a comparative technique to measure the distortions of c parameter in half periods layers and thickness of DBR layers. The details of these XRD measurements is reported in Fedler et al. [8]. The values of distortions measured by XRD are indicated with red colour circles in Fig. 3. These XRD results are compared in this figure with the measured data by HRTEM and with the calculated using an equilibrium

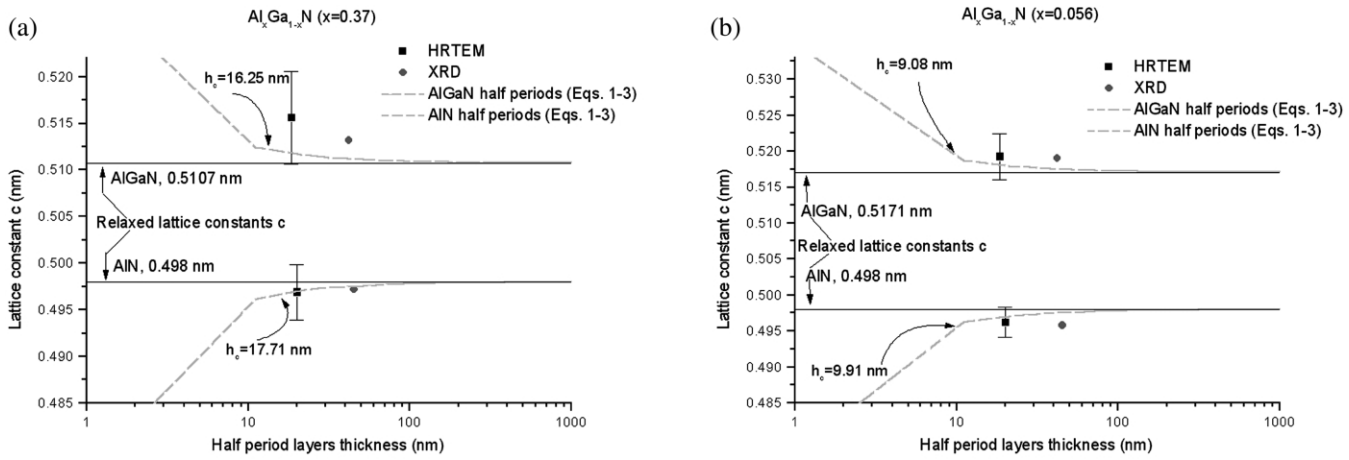


Fig. 3. Distortion of c lattice parameter of $Al_xGa_{1-x}N$ and AlN half periods in samples: (a) A and (b) B.

theory calculations [12]. Good agreement is found among calculated strained lattice parameters and measured by HRTEM and XRD techniques.

4. Conclusions

In the present work, the strain in DBR mirrors conformed by $Al_xGa_{1-x}N/AlN$ pairs (5.5 and 20.5 periods) have been studied from equilibrium theory and measured by HRTEM and high resolution XRD. The equilibrium theory calculations and XRD measurements permit to precisely determine the distortion of c lattice parameters in the $Al_xGa_{1-x}N$ and AlN layers. Good agreement is reached when strain in the half period layers of the DBRs calculated from equilibrium theory is compared with strain measured by HRTEM and XRD techniques.

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