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RBS/Channeling study of Er doped GaN films grown by MBE on Si(1 1 1) substrates

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Abstract

The influence of the Ga cell temperature on the quality of GaN films grown by MBE on p-Si(1 1 1) substrates was studied for cell temperatures (T_{Ga}) in the range from 865°C to 922°C using the RBS/Channeling technique. The films were in situ doped during growth with Er at a constant cell temperature. The films show a strong dependence of the crystalline quality on the Ga cell temperature with the best films grown at $T_{Ga} = 915°C$. For temperatures T_{Ga} below 880°C the films showed no channeling effect. The thickness increases linearly with the temperature suggesting that changes in the Ga flux influence the growth process. The decrease of the Ga flux allows the incorporation of higher Er concentrations in the films. The data showed that a maximum value of about 0.35 at% was reached under the chosen growth conditions. The Er ions occupy mainly the Ga sublattice in the films with single crystalline quality. A comparison of the angular scans through the $\langle 0001 \rangle$ and the $\langle 10\bar{1}1 \rangle$ axes with Monte Carlo simulations leads to the conclusion that a majority (~90%) of the Er ions occupies Ga sites. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The move from development of the wide bandgap semiconducting materials into the production of commercially available optical devices in the blue wavelength range has a significant technological interest. The new group III-nitride compounds belong to this class of materials and reveal a great potential for applications namely as LEDs and lasers working in the blue region [1,2]. During the last decade, mainly GaN and to a lesser extent AlN and InN have been subject to an intensive research effort in order to improve their structural quality using different combinations of techniques and substrates. Despite of the work done, the structural and chemical differences between the materials commonly used as substrates (e.g. α-Al_2O_3, Si and

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GaAs) and the nitrides make the growth of defect free films a challenge [3–7]. Nevertheless, even with a large dislocation density (about 10^{10} cm^{-2}) it is possible to produce highly efficient blue LEDs using GaN films [8].

The rare earth doping of the nitrides combines both the optical advantages of the wide band-gap semiconductors (in this case GaN) and the sharp emission properties from atomic transitions in the rare earth 4f levels. Typically, when Er is doped into other III–V and IV–IV semiconductors, only the lowest excited state is reported in the infrared as an optically active transition. In contrast, Er-doped GaN films have been found to emit light in the visible (green) wavelengths from higher energy atomic transitions. This occurs under both optical and electrical pumping [9,10].

Since the growth of films on silicon substrates is very attractive due to the possibility of complete integration into well-established Si technology, we report in this work the influence of the Ga cell temperature (T_{Ga}) on the crystalline quality of GaN films grown by MBE on Si(1 1 1). The films were doped with Er during the growth and the influence of T_{Ga} on the Er concentration incorporated and on the growth velocity of the films was measured. The lattice site location of Er in the wurtzite structure of GaN was studied for the films with the best crystalline quality.

2. Experimental details

Er-doped GaN films were grown in a Riber molecular beam epitaxy MBE-32 system on 2 inch p-Si(1 1 1) substrates. The growth system has been described elsewhere [11]. Solid sources were employed to supply the Ga (7N purity) and Er (3N) fluxes, while an SVTA rf-plasma source was used to generate atomic nitrogen from ultra-high-purity (5N) N_2 gas passed through an UltraPure gas purifier. The films were grown without initial nitridation. Plasma characteristics were kept constant throughout the growth process at 400 W rf power with an N_2 flow rate of 1.5 sccm, corresponding to a chamber pressure of mid-10^{-5} Torr. A GaN buffer layer was deposited for 10 minutes at a temperature of 500°C. Er-doped GaN growth experiments were typically performed for 3 hours, with a substrate temperature of 750°C and a constant Er cell temperature at 1100°C. The Ga cell temperature (T_{Ga}) during growth was varied from 865°C to 922°C corresponding to a beam equivalent pressure of roughly mid-10^{-7} to mid-10^{-6} Torr.

RBS/Channeling studies were performed with a 1 mm diameter collimated beam of $^4He^+$ or $^1H^+$ ions. The backscattered particles were detected at 140° and close to 180°, with respect to the beam direction using silicon surface barrier detectors located in the standard IBM geometry and with resolutions of 13 and 16 keV, respectively. The angular scans were done using a two-axis goniometer and, in order to avoid radiation effects due to the analysing beam, a fresh spot after each measurement was chosen. To reduce the pile-up effect, which would degrade the sensitivity for the Er signal, the beam current was kept below 2 nA. The angular scans were done across the $\langle 0001 \rangle$ and the $\langle 10\bar{1}1 \rangle$ axial directions. Computer simulations were performed using a Monte Carlo code [12] where the wurtzite structure was incorporated in order to simulate the GaN angular scans.

3. Results and discussion

3.1. Crystalline quality

The RBS spectra obtained in channeling and random directions for the best film studied are shown in Fig. 1. The smooth and regular dechanneling rate over the entire depth probed by the analysing beam (~2 μm) indicates the good epitaxial quality of the film along the growth direction. This result demonstrates good quality of single crystal GaN films on silicon substrates despite the large lattice mismatch. The schematic projections of Fig. 2 show the epitaxial relationship between the wurtzite structure of the GaN film and the diamond structure of silicon. According to these projections, epitaxy can occur in the following directions: Si[1 1 1] ∥ GaN[0 0 0 1] and Si(1 1 0) ∥ GaN($10\bar{1}0$). In this case the in-plane misfit defined as $\eta = (a_{\mathrm{film}} - a_{\mathrm{Si}})/a_{\mathrm{Si}}$ has a value of −17.7% much higher than the value commonly accepted for the growth of good

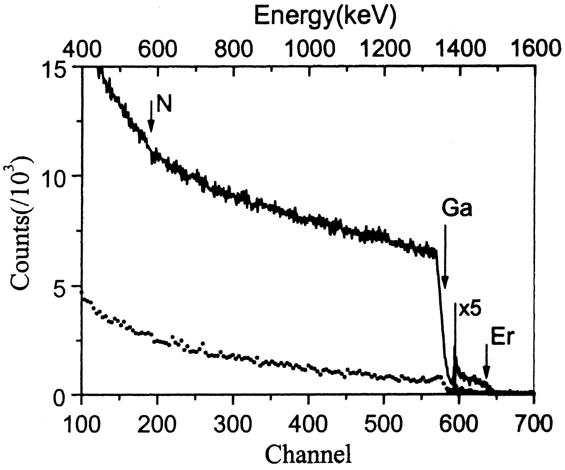

Fig. 1. Random and ⟨0 0 0 1⟩ aligned RBS spectra obtained for the GaN film grown at a cell temperature of 915°C. The good quality of the film is indicated by the low backscattering yield along the ⟨0 0 0 1⟩ growth direction.

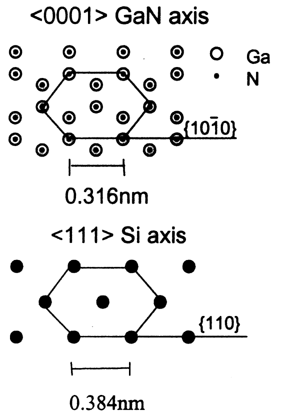

Fig. 2. Schematic illustration of the epitaxial relationship between (1 1 1) silicon and (0 0 0 1) galium nitride.

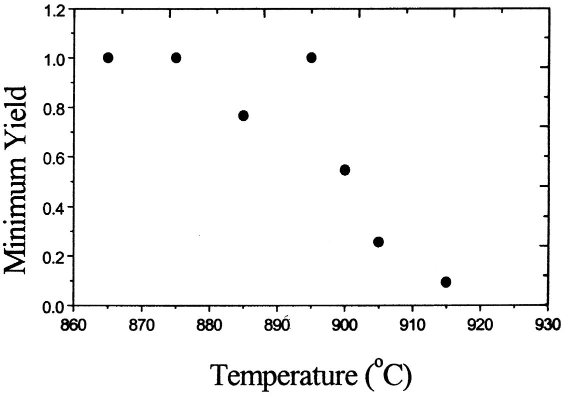

Fig. 3. Minimum yield measured along the ⟨0 0 0 1⟩ of the GaN films versus the Ga cell temperature. Above 900°C the films start to have channeling quality.

epitaxial films ($\leqslant 2\%$). The absence of lattice matching between the two structures suggests the presence of some incoherence in the interface or a high concentration of misfit dislocations necessary to accommodate the interfacial strain. The single crystalline quality of the films becomes worse with a decrease of the Ga cell temperature (T_{Ga}) (Fig. 3). Below 880°C the RBS spectra measured in the expected directions of the *c*-axis showed no sign of a channeling effect. On the other hand, X-ray diffraction (XRD) measurements show strong peaks for the GaN(0 0 0 2) reflection on all films, indicating a respectable crystalline quality. Further the XRD spectra reveal a narrowing of this peak in the films grown at higher temperatures (Fig. 4) indicating an improvement of the film quality in agreement with the RBS/Channeling results. The discrepancy at lower Ga cell temperatures is probably due to a polycrystalline to single crystal transition. An attempt to improve the quality of the best film ($T_{\mathrm{Ga}} = 915$°C) by annealing it for 120 s at 900°C showed no effect.

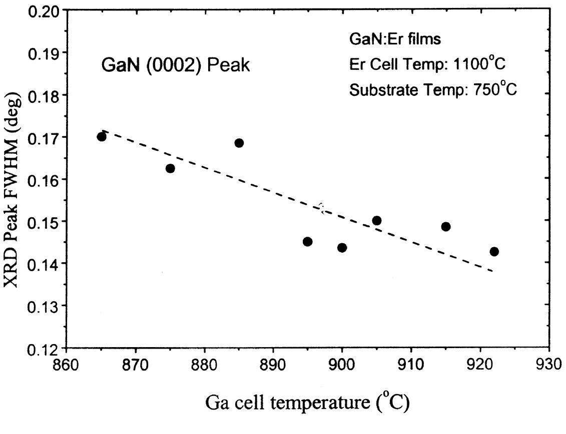

Fig. 4. Influence of the Ga cell temperature on the width of the (0 0 0 2) GaN peak. The decrease of the FWHM indicates the improvement of the film crystallinity.

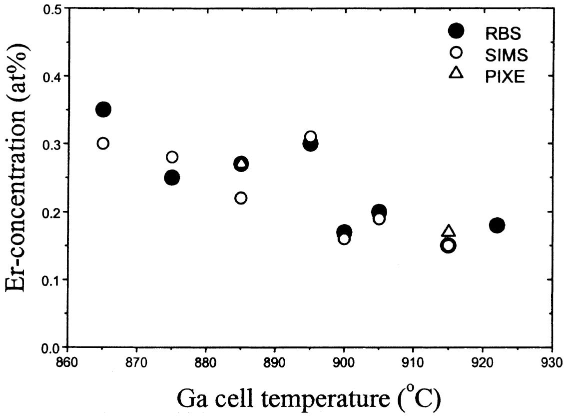

Fig. 5. Er concentration measured in the films. The decrease of the concentration is related with the increase of the growth velocity.

The rectangular shape of the Er profile observed in Fig. 1 shows that Er is homogeneously distributed throughout the film. The concentration of Er in the films has a maximum value of 0.35 at% and decreases with the increase of the temperature of the Ga cell as can be seen in Fig. 5. The values obtained by RBS were confirmed by SIMS and PIXE measurements also shown in Fig. 5. Since the temperature of the Ga cell controls the Ga flux, a reduction of the film thickness for lower cell temperatures is observed. It is possible that this reduction of GaN:Er film growth rate allows the incorporation of an increasing amount of Er. Another explanation for higher Er concentrations at lower T_{Ga} values could be site competition epitaxy between Er and Ga atomic species. Higher Ga fluxes lead to greater amounts of Ga adatoms on the surface reducing the number of sites available for Er at a constant Er flux. Despite the change in the growth velocity, the stoichiometry of the GaN films remains 1:1 within 5%.

3.2. Erbium lattice location

From the reduction of the Er scattering yield observed in the $\langle 0001\rangle$ aligned spectrum (Fig. 1) it can be concluded that Er occupies substitutional sites of the GaN lattice. Detailed angular scans through the $\langle 0001\rangle$ and the $\langle 10\bar{1}1\rangle$ axes were carried out in the films with channeling quality to determine the Er lattice site unambiguously. For these scans windows were set such as to include Ga and Er located in a depth between 5 and 80 nm. The corresponding Er and Ga scans (Fig. 6(a) and (b)) show a complete overlap indicating that Ga and Er are subjected to exactly the same flux distribution of the channeled ion beam in both axes. Thus, it can be concluded that the majority of the Er ions are located in regular lattice positions. In contrast to the $\langle 0001\rangle$ axis where there are mixed rows of Ga and N, the scan across the $\langle 10\bar{1}1\rangle$ axis (Fig. 6(b)) distinguishes between Er on Ga or N positions. In the $\langle 10\bar{1}1\rangle$ axis we have pure Ga and N rows as depicted in the projections of Fig. 6(d). The different atomic numbers of Ga and N result in different steering potentials for the respective rows leading in turn to angular scans with very different widths as can be seen in the simulated curves (Fig. 6(c)). Simulations of the $\langle 0001\rangle$ axial scan with an average potential for the mixed Ga + N rows yield just one width. The best agreement with the experimental data was obtained by assuming that 88% of the Ga atoms occupy regular lattice sites and 12% are in random positions. For the Er atoms, the fit yielded values of 84% occupying Ga lattice sites and 16% random sites. These findings agree with previous studies on Er implanted single crystalline GaN films grown on sapphire [13].

The angular scan along the $\langle 10\bar{1}1\rangle$ axis exhibited a reduced channeling quality and was fitted with a fraction of 30% of Er and Ga in regular lattice sites. The poor channeling quality of the $\langle 10\bar{1}1\rangle$ axis is mainly due to the surface condition and the columnar structure of the films whose influence on the channeling effect is enhanced by the large tilt angle (~47°) between the beam direction and the surface normal.

4. Conclusions

Er doped GaN films with single crystalline quality were grown on Si(1 1 1) substrates by MBE. The film quality is strongly dependent on the Ga cell temperature. The best films were grown at 915°C. The maximum concentration of Er homogeneously distributed in the films is 0.35 at%. The growth velocity increases with the Ga cell temperature and is

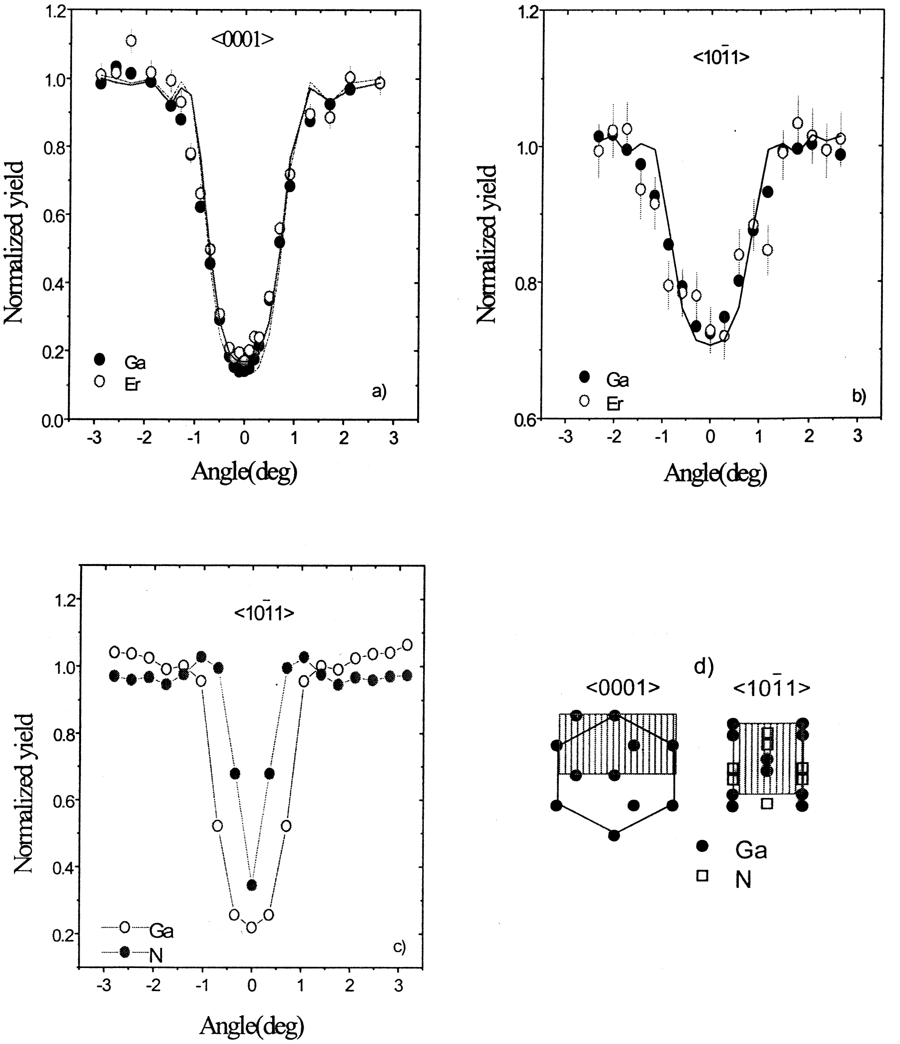

Fig. 6. (a), (b) Angular scans along the ⟨0001⟩ and ⟨1 0 $\bar{1}$ 1⟩ axes for the film grown at 915°C. The dashed and continuous curves are the results of the theoretical simulations. The curves expected for Ga and N along the ⟨1 0 $\bar{1}$ 1⟩ are represented in (c). The dashed regions in (d) are the unit cells used in the simulation program.

accompanied by a reduction of the Er concentration. The Ga:N stoichiometry of the films is 1:1 within 5%. Close to 90% of the Er incorporated in the GaN lattice occupies substitutional Ga sites. The quality of the films could not be improved by further annealing treatments at 900°C.

Acknowledgements

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