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Analysis of biaxial strain in InN(0001) epilayers grown by molecular beam epitaxy

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The in-plane lattice parameters of InN, GaN and Al_2O_3 in a InN/GaN/Al_2O_3(0001) heterostructure have been measured as a function of temperature in the range of 25–350 °C, using high resolution X-ray diffraction. The results reveal that both the GaN and InN crystals follow the in-plane thermal expansion of the Al_2O_3 substrate's lattice and there is no rearrangement of misfit dislocations at the InN/GaN and GaN/Al_2O_3 interfaces. It was also found that either compressive or tensile character of residual biaxial strain is possible for the InN films, depending on the two-dimensional (2D) or three-dimensional (3D) growth mode of InN on the GaN(0001) buffer layer. The tensile strain is inherent to the nucleation and coalescence of 3D islands.

1 Introduction

It has been found that the residual strain in InN films grown on 2–4 µm-thick GaN(0001) buffer layers, grown on Al_2O_3(0001) substrates, correlates with the nucleation and morphology of the InN films [1]. Tensile strain was present in the compact InN films grown on GaN/Al_2O_3(0001) by a two-step growth method. These films were nucleated and grown following a three-dimensional (3D) growth mechanism. As a possible origin of the tensile strain was thought [1] to be a higher in-plane linear thermal expansion coefficient of InN compared to GaN. This assumption, however, would require that the InN and GaN crystals do not follow the thermal expansion/contraction of the Al_2O_3 lattice. This would be possible by a different degree of rearrangement of the two misfit dislocation networks at the InN/GaN and GaN/Al_2O_3(0001) interfaces during cool down, at the end of the growth.

It has thus become important to know whether the InN and GaN crystals follow the thermal expansion/contraction of Al_2O_3 substrate and this was addressed in the present work. This allowed understanding the origin of tensile and compressive stress in the InN epilayers.

2 Experimental details

Several InN epilayers, with nominal thickness between 1 and 10 µm, were grown by nitrogen radio-frequency plasma-assisted molecular beam epitaxy (RF-MBE) [2]. GaN(0001) buffer layers, 2–4 µm thick, grown by metallorganic vapor phase epitaxy (MOVPE) on 300 µm thick *c*-plane Al_2O_3 were used for substrates. One additional InN epilayer was grown on a GaN/6H-SiC(0001) substrate.

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The samples can be classified in three groups. Group A consists of samples where the nucleation and the growth of InN were performed at relatively high temperature (400–430 °C) using equal fluxes of In and active N. On the other hand, group B consists of samples where the nucleation of InN was performed at low temperature (300 °C) using N-rich conditions and, subsequently, the growth was performed either at the same temperature using N-rich conditions or at higher temperature (410 °C) using equal fluxes of In and active N. Finally, group C consists of samples where the nucleation was performed at high temperature (400–500 °C) and subsequently the growth was performed at 500 °C. N-rich conditions were employed for both the nucleation and main-layer growth for the samples of group C. For the additional InN sample which was grown on the GaN/6H-SiC(0001) substrate, the same growth conditions as those of group A samples were used.

The morphology of the InN epilayers was studied by atomic force microscopy (AFM). The values of *a*- and *c*-lattice parameters were determined by high-resolution X-ray diffraction (HRXRD). The diffraction angles of the (0004) and $(10\bar{1}5)$ wurtzite reflections were measured, employing the extended Bond method [3], in order to correct for eccentricity and zero errors [4].

3 Results and discussion

The different growth conditions used for each group of samples resulted in different growth modes of the InN epilayers [2]. The growth mode of the group A samples was two-dimensional (2D), resulting in compact InN epilayers. As it was expected, the same results were obtained for the InN epilayer grown on the GaN/SiC substrate. Compact InN epilayers were also obtained for the samples of group B, but following a three-dimensional (3D) growth mode, through nucleation and coalescence of InN islands. It is important to mention the microcracks observed on the surface of InN for all group B samples [1, 2]. The samples of group C also followed a 3D growth mode, but the InN islands were partially coalesced, forming in that way porous or columnar InN structures. The growth mode and the morphology of InN has been analytically described in previous work [2].

The structural quality of the InN epilayers was studied by HRXRD rocking curve (RC) measurements of the symmetric (0004) and asymmetric $(10\bar{1}5)$ reflections. In Fig. 1, a typical HRXRD $\omega-2\theta$ scan around the InN (0004) diffraction and the RCs (inset of Fig. 1) for the (0004) and the $(10\bar{1}5)$ diffractions are shown. The full width at half maximum (FWHM) values of the RCs around the InN(0004) diffraction for all samples varied between 330 and 880 arc seconds.

The lattice parameters, as measured by HRXRD, are plotted in Fig. 2. As it is observed, all data points can be well fitted by a straight line. This linear dependence of *c* on *a* is attributed to built-in in-plane biaxial strain in the InN epilayers. Group A samples (denoted by circles) presented the lowest *a* and the highest *c* values, while group B samples (denoted by rhombs) presented the highest *a* and the lowest *c*

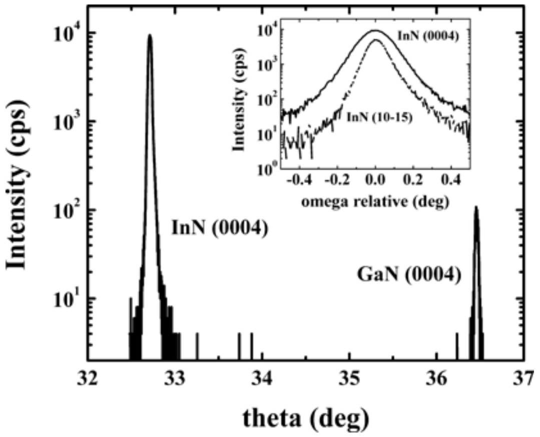

Fig. 1 X-ray diffraction $\omega-2\theta$ scan around the InN(0004) reciprocal space point of a sample belonging to group A. In the inset, the RCs around the InN(0004) diffraction (solid line) and the InN$(10\bar{1}5)$ diffraction (dashed line) are presented.

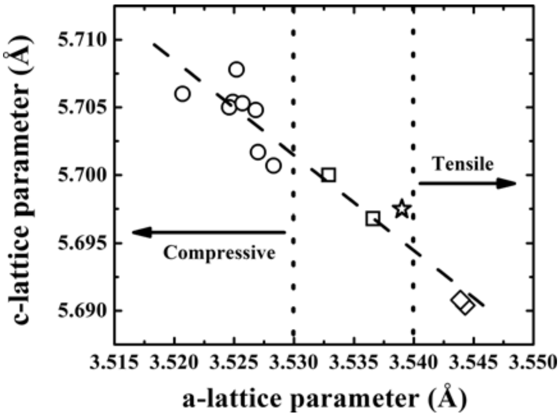

Fig. 2 Plot of the *c* versus *a*-lattice parameters, determined by HRXRD, for all InN epilayers. The samples of group A, group B and group C are denoted by circles, rhombs and squares, respectively. The star corresponds to a sample grown on a GaN/6H-SiC substrate. As it is described in the text, the samples of group A are under compressive stress, while those of group B are under tensile stress. The group C samples and the one grown on SiC are considered to be the least strained.

values. Group C samples (denoted by squares) and the one grown on GaN/SiC substrate (denoted by a star) presented intermediate values. The origin of the in-plane biaxial strain was analyzed on the basis of three stress components.

The first stress component results from the non-relaxed part of misfit strain between InN and GaN. The second stress component originates from the higher in-plane linear thermal expansion coefficients of GaN and Al_2O_3 compared to InN. The third stress component is a tensile one and has been associated with elastic deformation of the crystal to fill the gaps between randomly placed islands during coalescence [5]. An alternative explanation for the development of tensile stress is based on the gradual creation of misfit dislocations at the edges of the islands during their growth [6].

Whatever the real origin of the *tensile* stress component is, the latter appears to dominate in the InN epilayers of group B samples. The overall tensile strain in those epilayers is manifested through the presence of microcracks on their surface, which is typical of layers grown under tensile stress. On the other hand, the *tensile* stress component in the InN epilayers of group A and C samples is expected to be negligible or absent, due to the different growth mode.

Temperature dependent HRXRD measurements were employed to evaluate the effect of the *thermal* stress component on the in-plane biaxial strain of InN epilayers. Namely, the variation of the in-plane *a*-lattice parameter of InN, GaN and Al_2O_3, as a function of temperature in the range of 25–350 °C, was studied systematically for a sample belonging in group A. That sample consisted (from top to bottom) of 10 μm InN/4 μm GaN/300 μm $Al_2O_3(0001)$ and the results are shown in Fig. 3. It is obvious that, within the experimental error of the measurements, the same temperature dependence is observed for the in-plane lattice parameters of the InN and GaN epilayers as well as the Al_2O_3 substrate. Approximating the temperature dependence of the in-plane lattice parameters with linear functions, practically identical

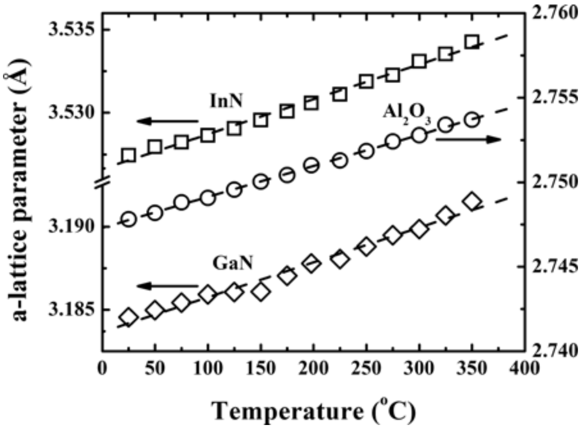

Fig. 3 Temperature dependence of the in-plane lattice parameters of all three layers of a sample belonging to group A, as measured by HRXRD. The structure of the specific sample is 10 μm InN/4 μm GaN/300 μm Al_2O_3. It is observed that both the InN and GaN epilayers follow the in-plane thermal expansion of the Al_2O_3 lattice.

apparent in-plane linear thermal expansion coefficients, $\Delta a/(a\,\Delta T)$, of Al_2O_3, GaN and InN could be determined: $6.6 \times 10^{-6}\,K^{-1}$ for Al_2O_3, $6.7 \times 10^{-6}\,K^{-1}$ for GaN and $6.0 \times 10^{-6}\,K^{-1}$ for InN. The in-plane linear thermal expansion coefficients reported in the Ref. [7] for these three crystals are $7.5 \times 10^{-6}\,K^{-1}$, $5.6 \times 10^{-6}\,K^{-1}$ and $3.6 \times 10^{-6}\,K^{-1}$ for Al_2O_3, GaN and InN, respectively.

Thus, it is obvious that both the InN and GaN(0001) epilayers follow the in-plane thermal expansion of the Al_2O_3 lattice. As a result, a compressive *thermal* strain component develops in the InN epilayer. This indicates that the dislocations are not sufficiently mobile in both the InN and GaN epilayers at temperatures up to 350 °C, so that they could result in rearrangements of the MD networks to accommodate any temperature induced strain variations.

After all, the InN epilayers of group A samples must be compressively strained. This is consistent with the lowest *a* and the highest *c* values of those samples compared to the samples of group B and C. In the InN epilayers of group C samples, the *thermal* stress component is expected to be limited due to their limited contact to the substrate, while in the InN epilayers of group B samples, it is expected to be compensated by the *tensile* strain component. In addition, due to the fact that the in-plane linear thermal expansion coefficient of 6H-SiC [$(3.2 - 4.2) \times 10^{-6}\,K^{-1}$] [8] is very close to that of InN, the *thermal* stress component in the InN epilayer grown on GaN/SiC substrate is expected to be limited, justifying in that way why this sample presented higher *a* and lower *c* values than those of group A samples.

The reported findings allowed the accurate determination of the strain-free *c*- and *α*-lattice constants, as described elsewhere [2].

4 Conclusions

A compressive thermal stress component is imposed to the InN epilayers due to the higher in-plane linear thermal expansion coefficient of Al_2O_3 compared to InN. A tensile stress component, related to the coalescence mechanism between adjacent InN islands, is dominant in the epilayers grown in 3D mode.

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