Strain and crystallographic tilt in uncoalesced GaN layers grown by maskless pendeoepitaxy

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The strain in thin GaN layers grown by maskless pendeoepitaxy has been investigated using high-resolution x-ray diffraction and finite-element simulations. The crystallographic tilt of the free-hanging wings was determined to result from the strain relaxation of the seed stripes along [0001]. The impact of the dimensions of the pendeostructure and of the formation of crystal defects on the expected wing tilt is discussed. © *2002 American Institute of Physics.*
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Lateral epitaxial overgrowth (LEO) and pendeoepitaxy have been shown to significantly reduce the density of threading dislocations in GaN layers grown on highly lattice mismatched substrates such as sapphire or SiC.[1–3] The laterally growing wing regions of these structures are often crystallographically tilted relative to the seed region. For the case of LEO, this has been attributed to threading dislocations which form a grain boundary along the edge of the mask.[4,5] Several groups have also investigated maskless pendeoepitaxy in which the growth starts from the $\{11\bar{2}0\}$ sidewalls and the (0001) surface of unmasked GaN stripes.[6,7] Strain and tilt in these structures have not yet been investigated in detail. However, maskless materials are assumed to be different compared to either LEO or pendeoepitaxy with masks on the stripes, since any interactions between a mask and the GaN wings as a result of differences in the coefficients of thermal expansion, adhesion or the cross diffusion of atoms are excluded. Recent temperature-dependent high resolution x-ray diffraction (HRXRD) experiments have shown that the wing tilt in maskless pendeoepitaxy samples grown in this research is primarily thermally induced,[8] which is opposite to the findings for LEO.[9] Using HRXRD and finite-element (FE) simulations, we have determined in this study that the wing tilt in uncoalesced GaN layers grown by maskless pendeoepitaxy results mainly from the relaxation of the strain in the GaN seed stripes.

GaN stripes along $[1\bar{1}00]$ having a rectangular cross section were etched from 1 μm thick GaN layers grown by metalorganic vapor phase epitaxy on 0.1 μm thick AlN buffer layers previously deposited on 6H–SiC (0001) substrates. The subsequent overgrowth process was stopped before the wings coalesced into a layer. A representative cross-sectional scanning electron microscopy (SEM) micrograph of the resulting structure is shown in Fig. 1. The initial stripe widths s were in the range from 3.1 to 4.8 μm. Due to variations in the overgrowth conditions, the final wing width w and the final stripe height h varied for the investigated samples within the ranges 0.6–3.6 and 0.9–3.0 μm, respectively. Details of the growth process can be found elsewhere.[10] HRXRD measurements were performed using a Philips X'Pert MRD diffractometer equipped with a fourfold Ge(220) monochromator and a threefold Ge(220) analyzer. Two-dimensional FE simulations were conducted using the software FElt version 3.05.[11]

A typical HRXRD reciprocal space map of the GaN (0002) reflection recorded with the diffraction plane perpendicular to the stripe direction is shown in Fig. 2. The intensity distribution contains three separate peaks. The center peak can be attributed to the stripe region and the two outer ones to the left and right wings, respectively. The separation of the peaks along the q_x-axis corresponds to different orientations of the c-axis of the three regions, i.e., it is the manifestation of the wing tilt. It should be noted that a corresponding tilt was not observed if the diffraction plane was parallel to the stripes. The tilt angles of the wings relative to the stripes are in the range 0.05°–0.17° for the samples under investigation. These values are smaller than numbers typically reported for thin layers grown by LEO or pendeoepitaxy involving the use of a SiO_2 mask which are on the order of 1°.[4,12,13] The peak separation along the q_z-axis in Fig. 2 reveals that the c-axis lattice parameter of the wing regions is larger than that of the stripe region.

The wing tilt appears to be strain induced, as indicated by the results presented in Fig. 3. The c-axis lattice parameter of the stripes decreases with increasing wing tilt. In contrast, the a-axis lattice parameters of the stripes perpendicular to the stripe direction do not exhibit any clear correlation to the wing tilt, the data of which are not shown here. Figure 3 also shows that the c-axis lattice parameter of the wings is always larger than that of the stripes. Moreover, it slightly decreases with increasing wing width. The primary conclu-

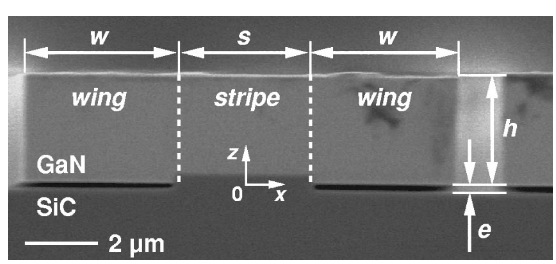

FIG. 1. Cross-sectional SEM micrograph of an uncoalesced GaN layer grown by maskless pendeoepitaxy.

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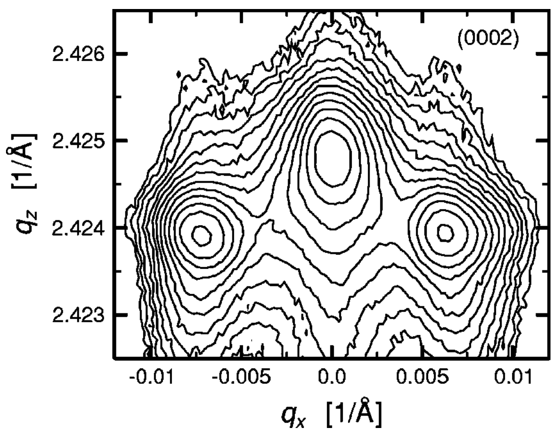

FIG. 2. HRXRD reciprocal space map of the GaN (0002) reflection.

sion from these data is that the tilt of the wings is caused by the relaxation of the compressive strain along the z-axis in the stripes, and it is not affected by the strain along the x-axis.

Two-dimensional FE simulations of the strain distribution in pendeostructures have been performed to clarify the origin of the wing tilt. The model corresponded to the geometry shown previously in Fig. 1. The thin AlN nucleation layer between the GaN and the SiC is omitted for simplicity. The thickness and the width of the SiC substrate were set to 5 and 12 μm, respectively, which was tested to be sufficiently large for an accuracy of $\pm 2\%$ of the stresses in the GaN. The sidewalls and the bottom surface of the SiC were fixed against displacements along the the x- and z-axes, respectively. The strain was assumed to be induced during cooling of the structure from the growth temperature to room temperature by the mismatch in thermal expansion coefficients between GaN and SiC. Using the parameters listed in Table I and assuming a cool-down of $\Delta T = 1000$ K, the mismatch along the a-axis between GaN and SiC was calculated to be $f_x = (\alpha_{\mathrm{GaN}} - \alpha_{\mathrm{SiC}})\Delta T = 1.1\times 10^{-3}$.

Figure 4 shows calculated strain profiles and displacements for a selected set of sample dimensions. The stripe has

TABLE I. Parameter values used for the FE simulations: E is Young's modulus along the a-axis, ν is the Poisson ratio along the c-axis, and α are the linear thermal expansion coefficients along the a-axis.

	E (GPa)	ν	α (K^{-1})	Refs.
GaN:	306	0.203	5.6×10^{-6}	14, 15
6H–SiC:	473	0.086	4.5×10^{-6}	16, 17

partially relaxed, as the strain ϵ_{xx} in this region is considerably smaller than the mismatch f_x. Moreover, the strains in the stripe are inhomogeneous along the c-axis normal: The highest in-plane tensile strain ϵ_{xx} remains at the GaN/SiC interface ($z = 0.1$ μm) due to the closeness of the strain-inducing substrate. This tensile strain decreases toward the GaN surface ($z = 2.0$ μm) and becomes compressive or in a state of ''overrelaxation'' which is a known phenomena in striped films on foreign substrates.[18] Moreover, the strain ϵ_{xx} in the stripe decreases toward the stripe/wing interface. Most parts of the wings are unstrained along the x-axis because they hang freely above the SiC surface. The suggested differences in the strain between the stripe and the wing agree with the HRXRD results shown in Fig. 2. The lower part of Fig. 4 shows the calculated displacements along the z-axis of the structure. The GaN wings tilt away from the SiC surface as the stronger relaxation, i.e., the lateral contraction of the stripe surface relative to the stripe interface region results in a trapezodial cross section in the stripe. The wings simply continue the crystallographic orientation of the tilted sidewalls of the stripe and tilt upward. Unfortunately, the direction of the wing tilt cannot be extracted from HRXRD measurements as those shown in Fig. 2.

The FE simulations were performed for different sets of dimensions of the pendeostructure that are shown for the general case in Fig. 1. The wing width w and the etch depth e into the SiC substrate were found to have only a minor influence on the wing tilt. However, the tilt depended

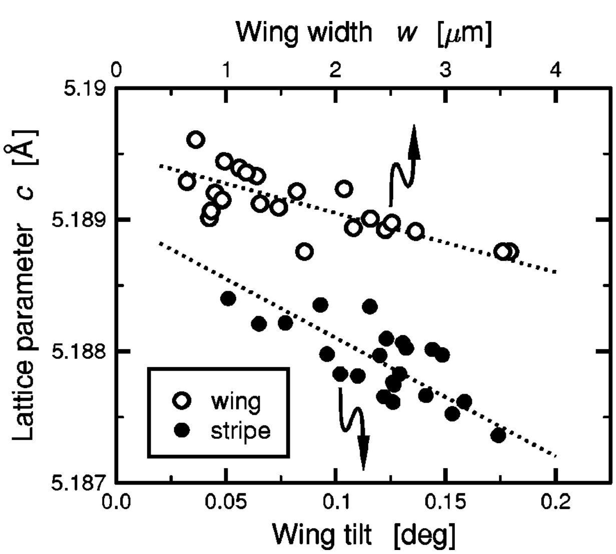

FIG. 3. Lattice parameters c for the stripes (filled circles) and wings (open circles) of different samples vs the wing tilt and wing width, respectively. The dotted lines are guides to the eye.

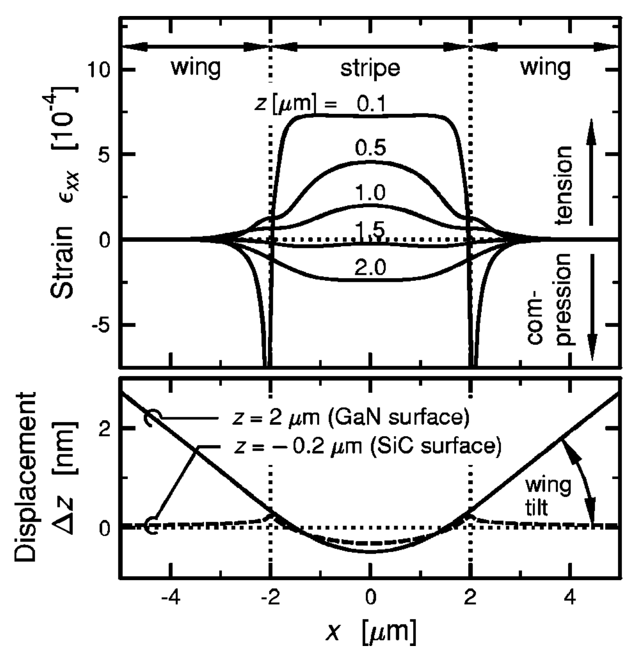

FIG. 4. Linescans of the strain along the x-axis and the displacement along the z-axis as determined by FE simulations for a pendeostructure with $s = 4$ μm, $w = 3$ μm, $h = 2$ μm, and $e = 0.2$ μm.

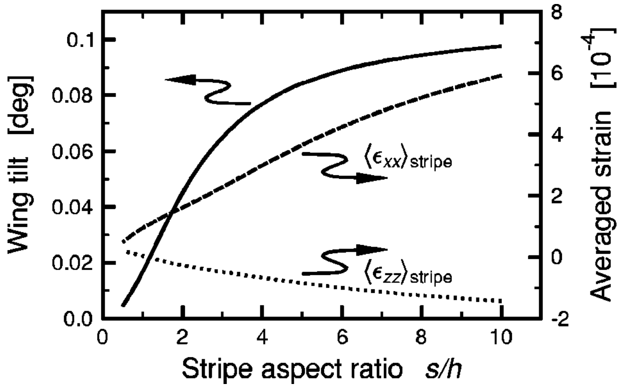

FIG. 5. Wing tilt (solid line) and strains along the x-axis (dashed line) and the z-axis (dotted line) averaged over the stripe region as determined by FE simulations in relation to the stripe aspect ratio for a pendeostructure with $w=3$ μm and $e=0.2$ μm.

strongly on the stripe width s and the stripe height h. Moreover, the stripe aspect ratio s/h, not its absolute size, determines the strain distribution. Figure 5 shows that the wing tilt should decrease if the stripe becomes more narrow and taller. Pendeostructures with the largest wing tilt are also expected to exhibit the largest strains in the stripe region along both the x- and z-axes as Fig. 5 further indicates. The latter fact agrees with the experimental findings presented in Fig. 3. However, the missing correlation of the a-axis lattice parameters of the stripes to the wing tilt mentioned earlier does not.

Plotting the experimental tilt values versus the stripe aspect ratio revealed no clear correlation. This raises the question regarding what else, apart from its dimensions, determines the strains in the stripe and consequently the wing tilt. It should be recalled that all the pendeostructures discussed here were grown under different conditions such as temperature and reactant flow rates. Some of the data indicate that the wing tilt decreases with increasing V/III ratio. Moreover, temperature dependent HRXRD measurements suggest that although the wing tilt decreases significantly with increasing temperature, a rest tilt remains at the growth temperature whose value varies from sample to sample.[8] Therefore, we speculate that the strains in the stripe are both thermally induced and influenced by defects whose density and/or distribution are determined by the growth conditions. For example, threading dislocations might be a source of a tilt-inducing strain, particularly if they propagate from the stripe region into the wing region. The determination and the evaluation of the defect structure is the subject of ongoing investigations.

In conclusion, experimental data have shown that the crystallographic tilt of the GaN wing regions fabricated by maskless pendeoepitaxy is induced by the strain in the stripes along their c-axis. This agrees with theoretical simulations which indicate that the c-plane stress is partially relieved resulting in nearly unstrained wing regions. Differences between theory and experiment were found for the in-plane strains and the impact of the stripe dimensions on the wing tilt. The point and extended defects generated in the GaN during growth are assumed to play as an important role in the formation of strains as does the mismatch in the coefficients of thermal expansion between GaN and SiC.

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