# The addition of Sb as a surfactant to GaN growth by metal organic vapor phase epitaxy

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The role and effect of the isoelectronic center Sb on the structure and properties of GaN epilayers have been investigated. The gas phase Sb concentration was varied by changing the triethyl antimony/trimethyl gallium mole ratio over a wide range of concentrations while keeping other growth parameters constant. The Sb addition slightly improved the optical and structural properties of GaN epilayer at a low level of Sb incorporation, especially for the films grown under a high group V/III ratio conditions. The addition of Sb resulted in changes in GaN surface morphology, which was further explored by the lateral epitaxy overgrowth (LEO) technique through the changes in the growth rates and the facet formation. The presence of Sb in the gas phase greatly enhanced the lateral overgrowth rate and altered the formation of the dominant facets. Vertical facets to the LEO growth appeared with the addition of Sb under conditions that normally produced sloped sidewalls. While Sb altered the growth facet present during LEO, only a small amount of Sb was incorporated into the GaN, suggesting that Sb acts as a surfactant during the GaN metal organic vapor phase epitaxy growth. Sb addition produces surface conditions characteristic of a Ga-rich surface stoichiometry indicating both a possible change in the reactivity of $NH_3$ and/or enhanced surface diffusion of Ga adatom species in the presence of Sb.  © *2002 American Institute of Physics.*
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## I. INTRODUCTION

GaN and related materials are being developed for applications in short wavelength optoelectronics and high temperature and high power electronics. Due to the lack of suitable substrate, continuous efforts have been made to reduce the high defect density within the GaN films, arising from the difference in lattice parameters and thermal expansion coefficients between the GaN and underlying substrate. The utilization of low temperature grown AlN[1] or GaN[2] buffer layers addressed these issues and dramatically improved the electrical, luminescence, and structural properties of the GaN thin films. These buffer layers provide a high density of nucleation sites and promote the coalescence of the initial GaN islands. The resulting heteroepitaxial growth of GaN then proceeds through a step flow growth mechanism. Most of the lattice mismatch is accommodated by crystalline defects generated near the interface, often appearing as low-angle grain boundaries, between the slightly misoriented GAN grains. These defects in the form of threading dislocations can have a density as high as $10^8 - 10^{10}$ cm$^{-2}$ Recently, several regrowth processes, such as the lateral epitaxial overgrowth (LEO) technique[3–6] and the pendeo-epitaxy technique,[7] have been reported to achieve a significant reduction in the dislocation density ($10^4 - 10^6$ cm$^{-2}$). The dislocation reduction realized through these techniques relies on the blocking of the dislocations in the initial film by the masking layer and the lateral growth of low defect density material over the masked regions. While sharp reductions in defect density have been achieved in these techniques, they typically involve several complicated processes, such as photolithography and dielectric deposition, which could impact yield and cost of the GaN structure.

Other techniques have been used to modify the growth and defect generation in a variety of material systems. In particular, the use of a surfactant during growth has been explored to modify strained-layer heteroepitaxial growth. For example, several studies using surfactants during the growth of SiGe have shown striking results. Antimony (Sb),[8] bismuth (Bi),[9,10] and arsenic (As),[11] segregate to the growth front and alter the surface energy and surface kinetic processes of the growing strained SiGe layer. The use of these surfactants leads to an increase in the epitaxial thickness of the SiGe layer and facilitated layer-by-layer growth. These elemental surfactants are typically characterized with a low vapor pressure, at the growth temperature of interest, and a low solubility within the solid. The resulting segregation to and accumulation on the growth front of these elements give rise to the changes in the surface thermodynamic and/or kinetic properties of the growing surface. As a result, a small amount of surfactant introduced to the growth front can greatly change the growth behavior without a high level of incorporation into the film.

This present study focuses on the use of Sb as a surfactant during the growth of GaN using metal organic vapor phase epitaxy (MOVPE). Sb has been reported to serve as a surfactant during molecular beam epitaxial growth of an InGaAs(N):Sb/GaAs quantum wells system and led to improvement in the long-wavelength semiconductor laser performance.[12,13] In these cases, the addition of Sb resulted in an increase in the critical thickness at which the growth mode changes from two-dimensional (2D) to three-

dimensional (3D) growth. Isovalent doping with antimony has also been used during the bulk growth of GaAs in order to reduce the dislocation density through impurity hardening. In the latter case, the Sb was incorporated at low concentrations under moderately As-rich conditions.[14] An optimal Sb concentration was found to result in a reduction in the dislocation density and a reduction in the concentration of intrinsic deep centers such as EL2 and EL5 within the GaAs crystal. In this article, the role and effect of Sb during GaN MOVPE growth has been studied through the addition of triethylantimony into the GaN growth ambient over a wide range of gas phase antimony concentrations during the conventional two-step growth of GaN. Antimony addition resulted in a change in the surface morphology and roughness during GaN growth. The observed modifications in GaN microstructure were additionally explored by the LEO technique by noting the changes in facet formation and the lateral-to-vertical growth rates due to the presence of Sb in the gas phase. We found that a small Sb addition led to a remarkable increase in the lateral overgrowth rate and resulted in vertical facets under conditions that normally produce triangular sidewalls. Such changes in growth behavior are related to the alterations in the growth surface chemistry due to the presence of Sb on the GaN growth front.

## II. EXPERIMENTAL PROCEDURE

GaN:Sb thin films were grown within a horizontal MOVPE reactor operated at a pressure of 76 Torr with rf heating. Trimethylgallium (TMGa), triethylantimony (TESb), and $NH_3$ were used as precursors in Pd-diffused hydrogen carrier gas. C-plane sapphire was used as substrate and heated in a flowing $H_2$ ambient to 1100 °C for 10 min prior to the growth. A "two-step" growth process was employed, involving a low temperature GaN buffer layer followed by the high temperature growth. Sb was not introduced during the buffer layer growth in order to ensure that the GaN had a consistent initial growth surface. The buffer layer was deposited at a growth temperature of 525 °C with a group V/III ratio of ~6000. The "as-grown" buffer layer was then heated at a rate of 25 °C per minute to 1050 °C and annealed at 1050 °C for 10 min. The annealed buffer layer thickness was optimized to about 20 nm. The high temperature growth step was kept at 1050 °C with a group V/III ratio of about 3000. TMGa mole fraction within the reactor was ~$10^{-4}$. The Sb impurity was only introduced into the reactor during the high temperature growth step. The gas phase Sb concentrations were varied from TESb/TMGa molar ratios of 0, 0.0075, 0.015, 0.03, 0.06, 0.12, and 0.24. All these films were ~1.2 $\mu$m in thickness.

The GaN:Sb LEO growth was carried out on a 1.2 $\mu$m MOVPE GaN epilayer grown on a c-plane sapphire substrate. $SiN_x$ films were used as the masking layer. Patterning of the masking layer was performed using conventional photolithography and wet etching. A parallel stripe pattern was aligned in the $\langle 1\bar{1}00 \rangle$ GaN direction with a window opening width of ~1 $\mu$m and a line spacing of ~10 $\mu$m. The LEO sample was heated to the growth temperature in an $NH_3$ ambient. Once the substrate reached the growth temperature,

TMGa and TESb precursors were introduced into the reactor. The TMGa mole fraction within the reactor was ~$10^{-4}$. The gas phase Sb concentrations were varied from a Sb/Ga mole ratio of 0.015, 0.03, and 0.06. The growth temperature was varied over the range of 1000 to 1100 °C. The gas phase group V/III ratio was varied from 1000 to 7000. Additional LEO samples were grown in which the change in growth habit or facet formation was investigated. In these samples, TESb was either added to or removed from the growth ambient during LEO growth and compared to both undoped as well as GaN:Sb LEO growth.

The Sb solid concentration within the GaN thin film was measured by secondary ion mass spectroscopy (SIMS). Structural properties of the layers were measured from the GaN (0002) and $(10\bar{1}4)$ rocking curves by double crystal x-ray diffraction. An atomic force microscope (AFM) was used to determine the surface morphology. Photoluminescence (PL) spectra were obtained at 20 K using a He–Cd pump laser at an incident pump power density of ~0.2 W/cm$^2$. Film thickness was optically determined. Scanning electron microscopy (SEM) was used to determine the morphology of LEO stripes.

## III. RESULTS

### A. Nonpatterned GaN growth

The SIMS measurements indicate that only a small amount of Sb was incorporated into GaN thin films even grown at high Sb/Ga gas phase ratios. For a sample grown at a high Sb/Ga mole ratio of 0.12, the Sb solid concentration in GaN epilayer was determined to be ~$2 \times 10^{16}$ cm$^{-3}$. This result suggests that the distribution coefficient of Sb impurity within GaN, defined as the ratio of the Sb/Ga mole ratio in the solid to that in the gas phase, was estimated to be around $10^{-6}$. The low incorporation rate agrees with the known low solid solubility of Sb in a GaN solid.[15]

The Sb addition affected the surface morphology of the GaN epilayers. The typical surface feature size increased with Sb addition, as determined from the AFM micrographs shown in Fig. 1, where images of both undoped and Sb-doped GaN surfaces are obtained in deflection mode by AFM. The Sb-doped samples were grown with Sb/Ga mole ratios of 0.06, 0.12, and 0.24 in the gas phase. At a high Sb gas phase concentration, surface features were observed as triangular shaped hillocks, which are seen in Fig. 1(d). Energy dispersive x-ray spectroscopy (EDS) was used to determine the elemental composition of these hillocks. No chemical differences in the concentration of Ga, N, O, or Sb were detected between these hillocks and the field regions of the GaN film, at the level of the EDS sensitivity, indicating that these features are of the same composition but have developed a morphological instability at the high Sb gas phase concentrations. The Sb signal level for all samples was at the detection limit of the EDS, which is less than ~1–10 ppm in the solid or $10^{16}$–$10^{17}$ cm$^{-3}$.

The optical properties of the GaN:Sb layers were determined by low temperature PL operated at 20 K. The PL spectra are shown in Fig. 2 for an undoped film and an Sb-doped film grown using a Sb/Ga ratio of 0.12 in the gas
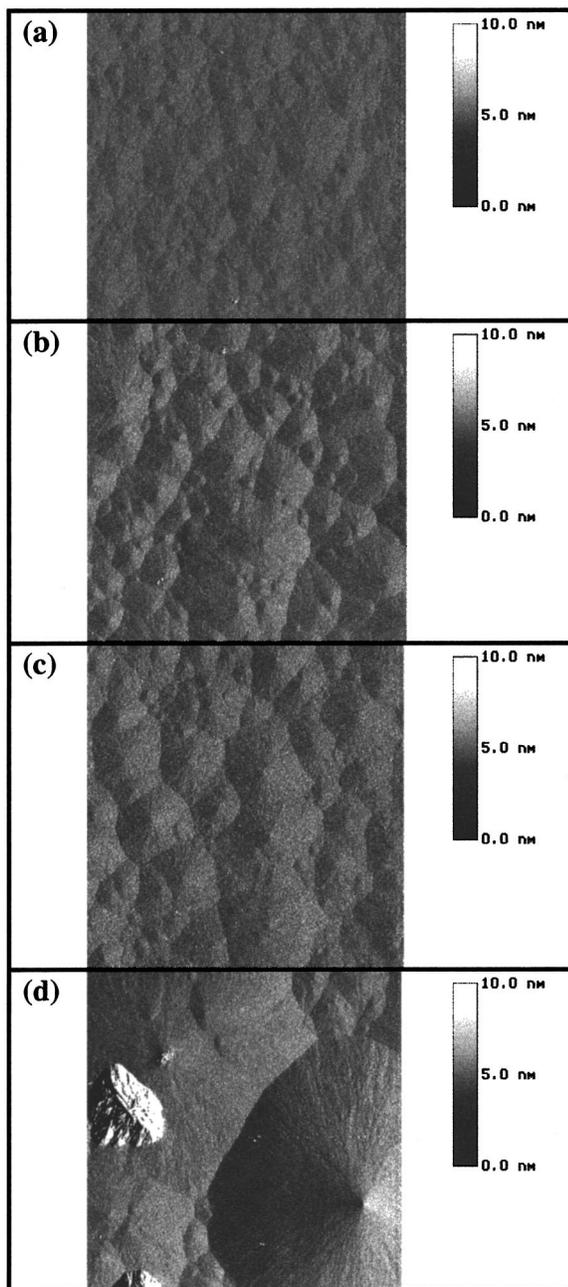
FIG. 1. AFM images of the surface morphology for samples grown without (a) and with Sb co-introduction obtained in deflection mode. The Sb-doped samples were grown under a gas phase Sb/Ga ratio of (b) 0.06, (c) 0.12, and (d) 0.24. The scan sizes are of $100 \times 100$ $\mu m^2$. The Z range is 10 nm. The typical feature size increased with Sb addition to the gas phase.

phase. The band edge emission of undoped GaN was at 3.473 eV with a full width at half maximum (FWHM) of 14 meV, which contains both free and bound exciton transitions. The Sb-doped GaN films showed additional emission peaks at 3.360 and 3.306 eV. The intensity of these peaks increased with Sb gas phase concentration, suggesting that these peaks are related with the presence of Sb in the bulk of the GaN film. These Sb-related peaks could be attributed to the radiative recombination of an exciton bound to the Sb isoelectronic-hole trap in analogy to the previously reported results on Bi doping in GaN.[16,17]
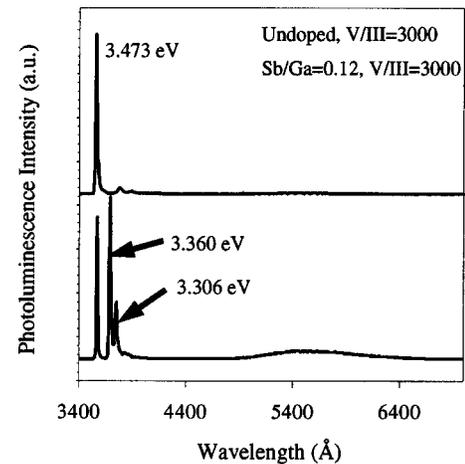


FIG. 2. Low temperature (20 K) PL spectra of an undoped GaN epilayer and an Sb-doped GaN epilayer. The Sb/Ga gas phase ratio was 0.12. The appearance of additional near-band-edge peaks are associated with transition related to the Sb incorporated into the films.

The presence of Sb in the growth ambient resulted in changes in the PL spectra for the GaN films grown under high group V/III ratio conditions ($>7000$). The blue luminescence (BL) band centered around 2.9 eV and the deep-level yellow luminescence (YL) band centered at 2.2 eV were observed in the PL spectra of undoped GaN epilayers grown under a group V/III ratio of 7000. The Sb addition at high concentrations ($>0.12$) suppressed the intensity of the BL and YL in the spectra of the GaN:Sb samples as shown in Fig. 3.

The structural properties of GaN:Sb films, characterized by the FWHM of (0002) and (10$\bar{1}$4) rocking curves, are shown as a function of the Sb/Ga gas phase ratio in Fig. 4. These films had approximately the same thickness of 1.2 $\mu m$. At relatively low Sb gas phase concentrations of 0.03, the crystalline quality was slightly improved as indicated by narrowing of the FWHM of $\sim$70 arcsec in both symmetrical
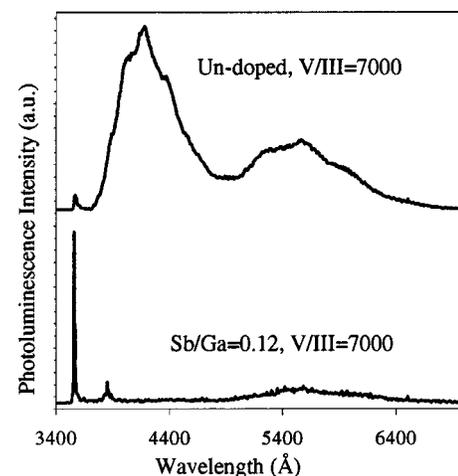


FIG. 3. Low temperature PL spectra of undoped and Sb-doped GaN epilayers grown under a high group V/III ratio of $\sim$7000. The Sb/Ga gas phase ratio was 0.12. Sb addition to the gas phase leads to a reduction in the blue- and yellow-band emissions for samples grown at this high group V/III ratio.
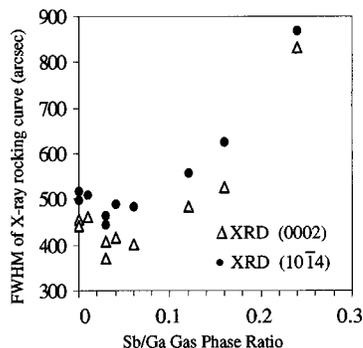
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FIG. 4. The structural properties of GaN:Sb films, characterized by the FWHM of (0002) and (10$\bar{1}$4) rocking curves, as a function of Sb/Ga mole ratio in a gas phase. An improvement in the structural properties of the GaN films is realized at Sb/Ga ratios less than ∼0.06.



FIG. 6. SEM micrographs of GaN LEO growth after (a) 1 h growth without Sb; (b) 30 min of growth with an Sb/Ga concentration of 0.06 followed by an additional 30 min of undoped growth; (c) 30 min of undoped GaN growth followed but an additional 30 min of growth with an Sb/Ga concentration of 0.06; and (d) 1 h growth with Sb/Ga concentration at 0.06. The addition or removal of Sb from the growth environment affects a change in the presented facet at the LEO growth.

and asymmetrical rocking curves when compared to the undoped GaN. At high Sb additions (>0.12), the x-ray linewidth increased over the undoped case.

## B. Patterned GaN growth

The changes in microstructure were also studied by the lateral epitaxial overgrowth technique. These results, previously reported in part, are summarized here.[18] A significant change in growth rates and facet formation was observed when adding Sb into the gas phase. An increase in the lateral overgrowth rate and a decrease in vertical growth rate were observed when increasing Sb/Ga gas phase ratio from 0 to 0.015, 0.03, and 0.06 as shown in Figs. 5(a)–5(d). These cross-sectional SEM images of undoped and GaN:Sb LEO stripes were obtained from samples grown under 1025 °C. For undoped growth, the uncoalesced LEO GaN exhibited a triangular cross section. The cross-sectional profile gradually changed from a triangular to trapezoidal shape, and then finally to rectangular shape with an increase in the Sb/Ga gas phase ratio. The vertical facets were obtained and identified as {11$\bar{2}$0} planes at high Sb/Ga ratio (>0.06) growth conditions. Additionally, the LEO stripe sidewalls are smoother in the GaN:Sb case than the undoped case.

The appearance of specific growth facets during LEO growth can be controlled through the introduction of Sb. In Fig. 6, TESb was introduced into the growth ambient after a period of 30 min of Sb-free growth [Fig. 6(b)] and TESb was removed from the growth ambient after 30 min and with additional undoped GaN LEO growth [Fig. 6(c)]. These samples are compared to an equivalent period of either continuous undoped or GaN:Sb growth [Figs. 6(a) and 6(d), respectively].

## IV. DISCUSSION

This study indicates that Sb can act as a surfactant during GaN MOVPE growth. The low solid solubility of Sb in GaN is a result of the large difference in the thermochemical properties, such as the covalent radii and electronegativity, between the GaN and Sb. As a result of the low solubility, Sb should segregate to the growth surface and result in changes in the surface properties and surface processes during the growth. There is a dynamic equilibrium between the deposition of Sb on the growth front and the evaporation of Sb from the growth front. Elemental antimony has a 1 Torr vapor pressure at 1050 °C. It is, therefore, expected that in the absence of appreciable Sb incorporation in the growing film, the effects noted in both the patterned and non-patterned growth are attributable to the Sb on the GaN growth front. The Sb surface concentration is higher than expected based on the measured Sb incorporation into the bulk GaN film. It is this Sb surface concentration that affects changes in the surface energy and surface kinetic processes. The impact of the Sb on the surface is confirmed by the change in facet formation during LEO as indicated in Fig. 6. The presented facet could be changed during growth through the addition or elimination of Sb from the gas phase.

Several mechanisms have been described, both experimentally and theoretically, for the influence of surfactants on the growth rate, behavior, and resulting morphology.[19–23] Thermodynamic factors and kinetics both play roles in the determining the influence of the surfactant within a particular
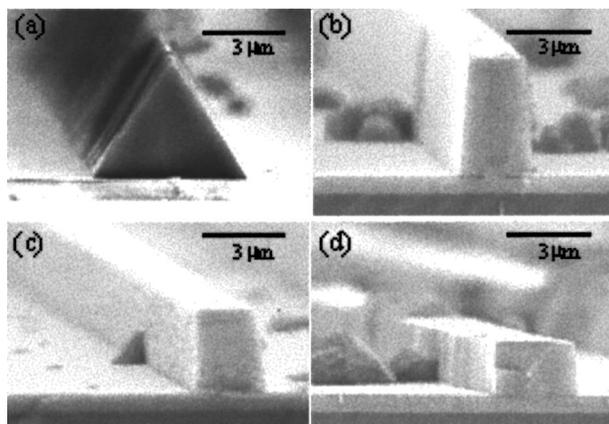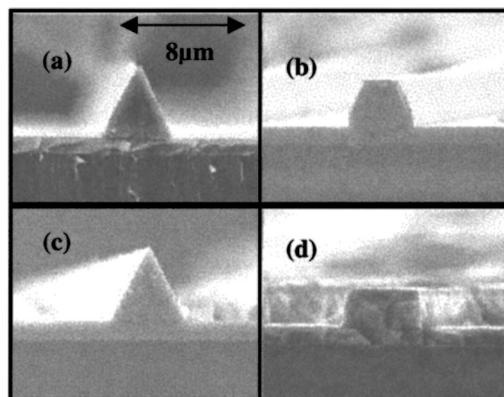


FIG. 5. Cross-sectional SEM images of (a) undoped and (b)–(d) Sb-doped LEO islands grown at 1025 °C. The Sb/Ga mole ratios were (b) 0.015, (c) 0.03, and (d) 0.06 in the gas phase. At a constant growth temperature and group V/III ratio, the Sb induced a change from sloped to vertical facets.

materials system. While there has been a substantial amount of work on the effects of surfactant addition in the growth of more well understood systems, such as SiGe growth on Si,[19] there does not appear to be a consensus on the specific role of all surfactants in affecting the fundamental processes of surface transport and adatom diffusion and subsequent incorporation. The thermodynamic influence of Sb as a surfactant would be expressed as a reduction in the surface energy of the growing surface. The structure and energetics of the undoped GaN surface has recently been studied through the first-principles total energy calculations by Neugebauer *et al.*[24] These calculations, while being carried out for undoped GaN, show that the most thermodynamically stable reconstructions exhibit excess Ga atoms on the top surface. The change in the surface energy and the equilibrium elemental composition of the GaN:Sb surfaces has yet to be determined.

Our recent first-principles calculations[25] investigating the effect of Sb on the mobility of N adatoms and the surface chemistry of GaN surfaces suggest that Sb adatoms are far more mobile than N adatoms on a Ga-terminated GaN(0001) surface. The periodic self-consistent gradient-corrected density functional theory calculations yield an estimate for the Sb diffusion barrier of $\sim 0.6$ eV ($2 \times 2$ unit cell), whereas the corresponding estimate for the N diffusion barrier is $\sim 1.0$ eV. Because of the low mobility of N adatoms the recombination of two N adatoms to form $N_2$ is kinetically limited.[24,26] On the other hand, Sb adatoms are more mobile, and as a result they can react with N adatoms much easier, forming SbN through an exothermic reaction. Although the SbN species are strongly bound to the Ga-terminated GaN(0001) surface, they still diffuse much faster on the surface than N adatoms do (diffusion barriers $\sim 0.7$ and 1.0 eV, respectively). One possible mechanism we are currently investigating theoretically would involve a reaction between an SbN species and a N adatom to yield $N_2$, which would desorb immediately at the usual growth temperatures, and a free Sb adatom. That Sb adatom could then react with another N adatom, form an SbN, and repeat the same cycle. According to this mechanism, Sb essentially acts as a "fast" carrier for N adatoms, supporting a catalytic cycle leading to $N_2$ desorption from the surface. Importantly, only a small amount of Sb would be needed for the above cycle to operate, which is in accord with the fact that the vapor pressure of Sb is several orders of magnitude higher than that of Ga, and hence one would not expect a significant surface coverage for Sb under usual growth conditions. It is worth noting here that we find Sb incorporation into the bulk of the GaN to be energetically unfavorable, and, therefore, we propose that Sb acts as a surfactant. Therefore, Sb can be viewed as an efficient medium for reducing the surface coverage of N for a given group V/III reactant feed ratio. Alternatively, Sb can impede $NH_3$ decomposition on the GaN surface, leading, again, to surface conditions characteristic of a Ga-rich surface stoichiometry. We plan to investigate possible effects of Sb on $NH_3$ decomposition on GaN surfaces using first-principles calculations. The surface stoichiometry determines many of the growth behaviors and processes through changes in surface kinetic processes such as adsorption/desorption, diffusion,

and adatom incorporation. The presence of a surfactant layer has been proposed to both enhance and impede the surface diffusion processes altering the GaN surface morphology through these changes in surface chemical composition.[19] Changes to the Ga-adatom mobility and incorporation rate will directly affect the growth rate, surface morphology, and defect generation and propagation in the GaN layer. The change in surface feature size in the nonpatterned GaN:Sb growth, indicates that one influence of the Sb as a surfactant is the change in the surface diffusion rate of Ga adatoms on the surface. As the diffusion rate increases, the feature size characteristic of the surface morphology increase. Growth conditions favoring the Ga-rich surface composition are associated with such an increase in the surface diffusion rate. Similar behavior has been seen in molecular beam epitaxy grown GaN in the presence of Sb, albeit at a much lower temperature of 900 °C.[27]

The modification in the kinetic processes also leads to alterations in growth characteristics during the surfactant-mediated epitaxial growth. The role of the surfactant is generally considered to affect either the diffusion rate of the adatoms, to influence the attachment and detachment energy at the step, and to change the exchange and de-exchange energy barriers on terrace. Kandel and Kaxiras suggested that the exchange energy between the surfactant and growing atom would be much higher than the diffusion energy barrier, since the former case involves interlayer atomic motion and the breaking of chemical bonds.[21,23] Therefore, they proposed that enhanced diffusion on the surfactant-passivated surface is likely a universal characteristic. The enhanced diffusion rate would promote the step flow growth as observed in many cases of surfactant-mediated growth. For some surfactants that were observed to lead to an increase in the density of island formation, it has been suggested that the steps could be passivated by surfactants without the necessity of a reduced diffusion. In these cases, the de-exchange of the single atoms lying beneath the surfactant layer is considered to be coincident with the exchange process, allowing a steady state to be reached between the two processes of exchange and de-exchange. The adatom concentration atop the surfactant layer could remain appreciable, which may fast diffuse on the surfactant-passivated surface to the step, allowing for a step-flow growth and leading to a smooth surface despite the presence of many islands.

In the case of GaN, Neugebauer *et al.* determined that the diffusion barriers of Ga and N adatoms on the Ga-terminated {0001} surface are about 0.2–0.7 and 0.9–1.5 eV, respectively.[24] However, under N-rich conditions, the activation energy for diffusion of a Ga adatom on the N-terminated {0001} surface increased from 0.7 to 1.8 eV.[24] A nitrogen-rich surface stoichiometry is concluded to significantly reduce the mobility of Ga adatoms. If the Sb surfactant leads to a lower N-to-Ga ratio on the surface, these conditions would favor enhanced Ga surface diffusion, which may be the driving force for the increased feature size in AFM image with Sb surfactant concentrations.

The influence of the Sb addition appears to lower the nitrogen coverage at the surface, relative to the undoped case, at a given group V/III ratio. This appears to create

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conditions that lead to results that are more typical of growth at lower group V/III ratios at given growth temperatures or at higher temperatures at a given group V/III ratio. The effective group V/III ratio at the growth front can influence several factors associated with the GaN growth and materials properties, such as defect formation and impurity incorporation. An enhanced diffusion rate for Ga adatoms is consistent with the increase in the lateral overgrowth rates seen in the LEO growth in Fig. 5. Generally, conditions of low nitrogen activity have been associated with an enhanced surface diffusion rate for Ga adatoms.[24] For undoped LEO growth, sloped $\{1\bar{1}01\}$ facets were typically observed at lower growth temperatures. The sidewalls of the undoped-LEO stripes, grown at these lower temperatures was uneven and had "zig–zag"-like features. When adding Sb surfactant, an increase in the lateral overgrowth rate and a decrease in vertical growth rate were evidenced. Vertical facets $\{11\bar{2}0\}$ were obtained and sidewalls became smooth in these Sb-doped LEO stripes. Our previous LEO growth study and many other reports have shown that when increasing the growth temperature and/or decreasing the group V/III ratio, the sloped facets constantly changed to vertical facets.

The conclusion is that the presence of Sb at the surface is supported by the suppression of the YL band with Sb introduction. Some YL emission was found to involve a deep trap at 1 eV above the valence band in the recombination path,[28] supporting that the gallium vacancy and related complexes as deep acceptors are probably the origin of the YL as suggested by Neugebauer and Van de Walle.[29] It was also previously reported that the YL can be substantially reduced by growing GaN under a Ga-rich condition or doping GaN with Ge or Mg.[30] In this study, the suppression of YL by Sb doping seems to agree with previous conclusions that the Sb addition may lead to Ga-rich surface conditions. It should be noted that the origin of the YL band has been attributed to a variety of sources. The YL band itself often appears to be a compound peak containing several broad peaks that can merge into the broad defect luminescence often noted.[31,32]

## V. SUMMARY

The introduction of Sb into the GaN growth environment during MOVPE leads to changes in the growth behavior and materials properties. These changes have been associated with both an enhanced adatom surface diffusion and an increased Ga/N surface stoichiometry. An enhanced lateral overgrowth rate and improved surface morphology results from small additions of Sb to the growth environment with little Sb being incorporated into the growing GaN film.

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