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The role of Si in GaN/AlN/Si(111) plasma assisted molecular beam epitaxy: polarity and inversion¹

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Abstract

The microstructure, polarity and Si distribution in AlN/GaN layers grown by plasma assisted molecular beam epitaxy (PAMBE) on Si(111) was assessed by scanning transmission electron microscopy (STEM). Samples grown under both metal- and nitrogen-rich conditions contained defects at the AlN/Si interface which suggest formation of an Al-Si eutectic. Correlated with this, interfacial segregation of Si was found in the samples. It is proposed that Si is dissolved in a eutectic layer floating on the AlN surface under metal-rich conditions. This Si is then incorporated into the film if the growth becomes nitrogen-rich, either intentionally or due to plasma source transients. These Si-rich layers appear to induce inversion of the nitride from nitrogen- to metal-polarity, and uncontrolled variations in the Si concentration cause occasional nonuniformity in the resulting inversion.

1. Introduction

GaN holds great potential for next-generation high frequency, high-power electronics and for room temperature, solid-state, single-photon sources.¹⁻³⁾ A key requirement for viable commercialization of these devices is a low cost, large area, easily integrable substrate. Silicon is the obvious choice to meet this need but is not without challenges. It is well known that large mismatches in lattice parameter and thermal expansion coefficient pose difficulties for GaN epitaxy on Si and modified growth techniques are being developed to overcome them.²⁾ Also established is the use of an AlN nucleation layer to avoid “meltback etching,”^{4,5)} which results from the low temperature of the Si/Ga eutectic (29.77 °C).⁶⁾ However, a potential issue for AlN buffer layers is formation of the Al-Si eutectic, which at 577 °C is substantially below typical temperatures used for AlN growth (~1000 °C for metal organic chemical vapor deposition, 800 °C for molecular beam epitaxy (MBE)).⁷⁾

There have been reports of Al-Si eutectic formation during plasma assisted MBE (PAMBE) AlN growth on both Si(111) and SiC substrates.⁸⁻¹⁰⁾ Based on thermodynamic analysis it has been proposed that liquid Al containing Si, in concentrations from 12 % at the eutectic temperature up to 30 % Si at 840 °C, is present on the AlN surface during growth under Al-rich conditions.¹⁰⁾ This liquid Al layer is likely responsible for the smoother surfaces of AlN

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films grown on SiC by PAMBE under metal-rich conditions;¹¹⁾ for the Al droplets formed on AlN under very metal-rich conditions,^{9–12)} and for the improved structural quality and surface morphology of AlN layers grown by PAMBE with Si doping at concentrations from 10^{20} to $5 \times 10^{21} \text{ cm}^{-3}$.^{13,14)} Al–Si eutectic formation is also consistent with the reported suppression of Si dopant incorporation and concomitant surface accumulation of Si in AlN layers grown under Al–rich conditions.¹⁵⁾ In the same study Si incorporation under N–rich conditions was found to be homogeneous, suggesting no eutectic phase transport of the Si dopant.¹⁵⁾

It has been a common practice in PAMBE growth of AlN buffer layers on Si substrates to predeposit several monolayers (ML) of Al on the Si surface, to avoid amorphous silicon nitride formation and promote N–polarity.^{9,15)} Based on the studies described above, it seems likely that this procedure would lead to eutectic formation, which might be avoided by an initial nitridation of the Si surface. However, formation of the Al–Si eutectic during initial stages of PAMBE growth of AlN on Si has been clearly demonstrated for both N–rich and Al–rich starting conditions, along with models for subsequent surface segregation of Si during AlN growth under both growth conditions.¹⁰⁾ Also, in a recent publication we described holes and hillocks at the Si/AlN interface, which suggest eutectic formation, under both metal and nitrogen–rich growth conditions.¹⁷⁾

Related to these observations, it has been recognized that Si can induce polarity reversal in GaN.^{8,18–20)} In fact, deposition of Si at monolayer levels has been used to induce N–polar NWs on Ga–polar GaN template substrates.²¹⁾ Yet, while there is considerable evidence for a Si containing layer on the AlN surface during growth, the possible influence of Si on the polarity of AlN buffers and subsequent GaN layers has not been previously explored.

We report here the morphology and Si distribution in GaN/AlN layers grown by plasma PAMBE on Si(111). Three different growth conditions were examined, all of which showed evidence of Al–Si eutectic formation and subsequent interfacial incorporation of Si. The results are consistent with a model in which, under metal–rich conditions, Si is present in a eutectic layer floating on the AlN growth surface. When nitrogen–rich conditions arise, either deliberately or due to nitrogen flux transients, the Si is locked into the layer. These Si–rich transition regions initiate inversion from N–polarity to metal–polarity, and these inversions are sometimes laterally inhomogeneous due to uncontrolled variation in the Si concentration.

2. Experimental procedure

AlN nucleation layers and subsequent GaN films were grown on Si(111) substrates by PAMBE. Details of the growth system and conditions for obtaining Al- and N-polar AlN have been described previously.¹²⁾ Three samples were studied and their growth conditions are given in Table 1. As noted in the table, there are large uncertainties in the reported fluxes. For nitrogen the uncertainties are related both to startup transients, which have been shown to be as large as 35 % for atomic nitrogen and to extend for up to 30 min,²²⁾ and to similarly large run to run variations.²²⁾ Flux transients are especially important for PAMBE nitride growth on Si where, unlike homoepitaxial nitride growth, it is not possible to

stabilize the nitrogen plasma by running it for extended periods before starting growth. Once the plasma is started two processes are possible: either the group III–nitride growth must start or the plasma will nitride the Si substrate surface.²³⁾ The nitrogen fluxes reported here were measured at equilibrium, many hours after plasma source startup, and are, therefore, likely different from the actual N–fluxes during the short AlN layer growths which are complete before the N–flux stabilizes. Likewise, the reported Al–fluxes were estimated from calibration runs performed periodically, but at varying times relative to the sample growths. This combined with long term drift of the growth conditions resulted in uncertainties in the reported Al–flux values of up to 20 %, not accounting for flux transients. The Ga–flux was calibrated more frequently, by *in-situ* reflectance spectroscopy,¹²⁾ resulting in a lower uncertainty of 6 % for this flux.

For the first sample the AlN buffer was grown under nominally metal–rich conditions, that is with a relatively low V/III ratio, to promote N–polarity. This sample will be referred to as the Low V/III Sample. For the second sample a thin layer of Al (2 ML) was deposited on the Si surface before the AlN growth was started; the AlN buffer was then grown under nominally nitrogen–rich conditions, that is with a high V/III ratio, to promote metal–polarity. This sample will be referred to as the High V/III Sample. The AlN buffer for the third sample was grown with a two–step process. The first step was under nominally nitrogen–rich conditions, that is with a high V/III ratio, to promote metal–polarity. After roughly 50 nm of AlN growth the V/III ratio was decreased to be slightly metal–rich. This second step, with nominally metal–rich conditions, was chosen to decrease the roughness of the AlN surface. This sample will be referred to as the Two-Step Sample.

For all three samples the growth was paused after the AlN growth, for ~5 min, while the sample cooled to the GaN growth temperature. N–flux was still present during the initial period of this growth interruption. The GaN layer was grown with a nearly stoichiometric V/III ratio and included an AlGaIn/GaN superlattice after ~100 nm of growth.

Sample polarity was monitored during growth by reflection high–energy electron diffraction (RHEED). Cross–sectional lamellae, for scanning transmission electron microscopy (STEM) examination, were prepared from each of the as–grown samples by focused ion beam milling (FIB). The FIB specimen preparation procedure and the STEM imaging conditions have been described previously.¹⁷⁾ All STEM images shown are annular bright field (ABF) images taken along the [11–20] zone axis of the nitrides unless otherwise specified. STEM energy dispersive X–ray spectroscopy (EDS) was also performed. All EDS linescans were taken with the same operating conditions to allow comparison of data from different samples. It should be noted however that, although the elemental concentrations are presented as atomic percent, the EDS data are uncalibrated and only relative comparisons are significant.

3. Results and Discussion

3.1. Low V/III Sample

STEM imaging of the sample with metal–rich growth revealed holes in the Si surface, which persisted to form holes in the GaN layer above them (see Fig. 1a)). Other defects visible in

the GaN layer included vertical inversion domains (IDs) and stacking faults (SFs), identified by atomic imaging. Atomic resolution imaging was also used to establish that the AlN layer was N-polar (Fig. 1b) and c)) and that the GaN layer was predominantly N-polar (Fig. 1e)), apart from Ga-polar inversion domains (Fig. 1d)). Interestingly, IDs were not present in the AlN layer in this sample, but instead formed primarily at the AlN/GaN interface (compare Fig. 1c) and d)) and occasionally on sidewalls of holes in the GaN.

It was not always possible to directly image the polarity of IDs in the samples studied, because many had lateral dimensions from 2 to 20 nm. As shown in Fig. 2a), this is less than the thickness of the FIB lamella resulting in regions of overlapping inverted polarities along the STEM viewing direction, which prevented polarity imaging. Images of an inversion domain boundary (IDB) for a large ID in an adjacent region of the Low V/III Sample are shown in Fig. 2 b–d). The polarity inversion is evident in both the ABF image, Fig. 2b), which shows the change in the N position from below the Ga on the left to above the Ga on the right, and in the high angle annular dark field (HAADF) image, Fig 2c), which shows a shift of the Ga lattice across the IDB. This shift was measured to be ~0.07 nm along the [0001] direction, which is consistent with the 0.064 nm (~ c/8) shift predicted by first-principles calculations of a low-energy IDB structure,²⁴⁾ and with previous STEM HAADF based measurements of the Ga lattice shift across IDBs in GaN, which reported 0.06 nm.^{25,26)} The vertical contrast bands in the GaN in Fig 1a) and in subsequent images (see below) are identified as IDs based on the similarity of their contrast to that of the ID imaged in Fig. 2 and to those in other reports where polarity inversion was directly imaged by STEM.^{10,27)}

As described in an earlier publication, both holes and hillocks formed at the Si/AlN interface under the growth conditions used for the Low V/III Sample.¹⁷⁾ It was also reported previously that voids developed in the GaN layer above hillocks as well as above holes at the Si/AlN interface.¹⁷⁾ Such defects are visible in Fig. 1a). The formation of these defects is almost certainly related to the formation of an Al–Si eutectic during the initial stage of the AlN growth.

To investigate this phenomenon further, EDS compositional measurements were made across the AlN layer and interfaces. Figs. 1f–m) are linescans of the Si, Al and Ga concentrations at the locations specified in Fig. 1a). The very high levels of Si in holes in the GaN (Figs. 1i), k) and l)) are clear evidence for Al–Si eutectic formation.⁷⁾ The presence of Ga in a hole in the Si substrate (Fig. 1k)) suggests that in this localized area Si–Ga eutectic formed as well.⁶⁾

Also evident in the scans are increased Si concentrations in localized regions of the AlN/GaN interface away from holes in the Si (see Fig. 1f) and g)). This interfacial increase in Si absent a rapid migration pathway through the AlN is consistent with a Si–Al eutectic layer floating on the surface of the AlN during growth.^{8,10)} The Si from this eutectic layer became buried at the AlN/GaN interface when the Al flux was terminated and the sample was cooled prior to GaN growth. During this growth pause, Al in the eutectic surface layer reacted with the N flux forming stable AlN and leaving Si on the surface. Because relatively

low levels of excess Si were present it was easily buried at the AlN/GaN interface either during the growth pause or when the nominally stoichiometric GaN growth started.

This excess Si is likely responsible for the vertical IDs which formed at the AlN/GaN interface (see Fig. 1 a)). Theoretical calculations have predicted Si will induce polarity inversion of the GaN(0001) surface,^{18,19)} and based on these calculations a structural model for a basal IDB at the AlN(0001)/GaN(0001) interface with Si segregation has been proposed.^{19,20)} The fact that vertical IDs formed only in localized regions of the AlN/GaN interface indicates lateral nonuniformity in the amount of Si at the interface. This may be related to small scale spatial variations in the initial Al flux impinging on the Si substrate or to the formation of Al droplets, which have been frequently observed for Al-rich growth conditions.^{9–12)}

Localized polarity inversion of GaN grown on metal-polar AlN on SiC has been reported previously and attributed to segregation of Si adatoms at the AlN/GaN growth interface.²⁰⁾ Moreover, simulations indicate a monolayer of Si is necessary to induce basal-plane polarity inversion.^{19,20)} As mentioned earlier the EDS data presented here are uncalibrated, so it is not possible to quantify how much Si is present at the AlN/GaN interface. However, in a recent study combining STEM/EDS and atom probe tomography data, it was shown that the EDS detected sub-monolayer concentrations of O and Al in a GaN matrix.²⁸⁾ Since EDS sensitivity to Si is expected to be similar to that for Al, it is reasonable to conclude that there is less than a monolayer of Si at most of the AlN/GaN interface (Fig. 1h), j) and m)) and a monolayer only in regions where the IDs initiated (Fig. 1f) and g)).

The exception to this was in the localized regions above holes in the Si, where large amounts of excess Si were present above the AlN/GaN interface (Fig. 1i), k) and l)). In these areas the larger quantity of Si was not completely incorporated prior to the GaN growth. The excess Si on the surface then reacted with the impinging Ga to form Si-Ga eutectic, which in one instance flowed down through the AlN into the hole in the Si surface (Fig. 1k)). This large excess Si above the AlN/GaN interface and evidence for the Ga-Si eutectic was only found in or near holes in the Si and GaN.

3.2. High V/III Sample

Roughness observed at the Si/AlN interface in the sample grown under nominally nitrogen-rich conditions indicated eutectic formation in this sample as well (Fig. 3 a)). Interestingly Si hillocks were found in this sample, but holes in the Si were absent, which suggests a lower level of eutectic formation compared with that in the Low V/III Sample. This would be expected since less Al was available to react with the Si substrate due to the higher V/III ratio (less metal-rich conditions) used for this sample. In fact, eutectic formation in a sample grown with nominally N-rich conditions is surprising. It may result from the initial 2 ML of Al deposited on the bare Si surface. More likely, due to the expected transients in the N-flux, the eutectic results from the AlN growth initiating with a V/III ratio close to or even slightly less than stoichiometric, and the V/III ratio increasing to above stoichiometric during the growth.

This transient related scenario is consistent with RHEED images of this sample taken during growth. As shown in Fig. 4a), the RHEED pattern for the first part of the AlN growth was streaky, consistent with a smooth surface obtained under Al-rich conditions which promote N-polar growth.¹²⁾ As the growth continued the RHEED transitioned to a 2x surface reconstruction (Fig. 3b)), which became clearer with longer growth time but was not recorded, indicative of N-rich conditions and Al-polar growth.¹²⁾

This scenario explains the initial N-polarity of the AlN found at the Si interface in this sample (Fig. 3 c)) and its subsequent reversal to metal-polarity (as the nitrogen flux increases). This inversion occurs via lateral inversion domain boundaries (Figs. 3 a) c) and d)) after the period of growth during which the N-flux is expected to be increasing.

As can be seen in Fig. 3 a) the inversion was spatially nonuniform. In some areas the inversion boundary was planar, consistent with a basal plane inversion boundary.^{29,30)} In other regions the IDB had a diffuse appearance, similar to inversion boundaries observed in Mg doped GaN,^{30–33)} and consistent with the IDBs lying in $\{h, h, -2h, l\}$ planes.³⁰⁾ These IDBs appear sharp and jagged when imaged along $[1-100]$ but diffuse along $[11-20]$, the imaging direction used here.³⁰⁾ A flat section of the basal plane inversion boundary, along with vertical IDs which nucleated on it, is shown in Fig. 3 b). In this sample vertical IDs were found to nucleate only on planar sections of the lateral IDB.

Similar to many of the vertical IDs in the Low V/III Sample the small lateral dimensions of these IDs (less than the lamella thickness) precluded direct imaging of the polarity reversal, but the STEM contrast is consistent with that of IDs in this and other studies.^{10,27)} These IDs propagate from the AlN into the GaN (see Fig. 2 a) and b)). In the GaN some of the IDs terminated on a stacking fault slightly above the AlGaN superlattice (near the center of Fig. 2 a)). Termination of IDs at SFs has been reported previously for N-polar IDs in a Ga-polar GaN matrix, along with a model for the termination mechanism which involves reducing the ID area until it is eliminated.³⁴⁾ This differs from the current observation of an abrupt planar termination of the IDs at the SF. An EDS linescan (not shown) was taken vertically across the SF in Fig. 2 a), but no compositional variations were identified across the defect.

EDS linescans across the AlN layer of the High V/III Sample revealed an increase in Si with a concomitant decrease in Al at the lateral inversion boundary (Fig. 3). Where the inversion boundary is planar, the compositional changes were sharp (Fig. 3 b) and c)). The compositional changes were broader in the diffuse, or jagged, regions of the boundary (Fig. 3 d) and e)). It is unclear what caused the nonuniformity of the N- to Al-polarity inversion in the AlN layer (i.e. planar vs diffuse IDBs). However, it is similar to the spatial nonuniformity in the AlN/GaN interface in the Low V/III Sample, where vertical inversion domains formed only locally in a few areas, and it is likely related to variations in the amount of Si present.

Si induced inversion of polarity along the $\langle 0001 \rangle$ direction has been reported for both basal plane^{19,20)} and non-basal plane boundaries in GaN.²¹⁾ As described above, inversion on the basal plane was reported to require a monolayer of Si.¹⁹⁾ For inversion on the non-basal plane facets, 1 to 2 ML of Si was reportedly required.²¹⁾ Since the non-basal boundaries,

which have a diffuse appearance, have a larger effective surface area relative to the basal-plane boundaries, they would be expected to require a higher concentration of Si to promote their inversion. Thus, a lower concentration of Si may be responsible for inversion via a planar boundary. A lower Si concentration at the basal plane boundaries is also consistent with the formation of vertical inversion domains at these boundaries, since the inversion would not be expected to occur if insufficient Si were present (i.e. less than a ML). The resulting un-inverted regions form the vertical inversion domains. This is the opposite of the behavior observed in the Low V/III Sample, where polarity inversion in the GaN layer was induced by excess Si at the AlN/GaN interface.

Little or no increase in Si was observed at the AlN/GaN interface in the High V/III Sample, suggesting most or all of the Si floating on the AlN surface during growth was incorporated into the lateral inversion boundaries in the AlN layer.

3.3. Two-Step High V/III Sample

Similar to the High V/III Sample, hillocks but not voids were observed at the Si surface in the Two-Step Sample, as described in an earlier publication (see Fig 5 c) in ref 17). It is interesting that while both holes and hillocks were observed at the Si(111)/AlN interface of the sample grown with a low V/III ratio, only hillocks were found in the samples grown with nominally high V/III ratios. Because a relatively small fraction of the entire sample can be examined by STEM, it is possible holes were present in these samples. However, if they are present they have a much lower density than holes in the Low V/III Sample which occurred with a linear density of ~1 hole per 500 nm. Since less free Al is expected to be present during the nominally nitrogen-rich, high V/III growths, this suggests the voids in the Low V/III Sample formed due to the increased Al and associated Al-Si eutectic phase formed at the growth interface at the beginning of growth. Formation of Si hillocks appears to require less excess Al and/or eutectic formation.

Polarity imaging revealed that the AlN in the Two-Step Sample inverted from N- to Al-polarity close to the Si interface (Figs. 5 b) and c)). Remarkably, as Figs. 5 d) and e) illustrate, once the inversion to metal-polarity occurred it persisted for the remainder of the growth, regardless of the subsequent change in the growth conditions part way through the AlN layer from high to low V/III.

The fact that the initial inversion, from N- to Al-polarity, took place earlier in the growth for this sample than for the High V/III Sample is likely due to a higher effective V/III ratio for this sample relative to that for the High V/III Sample. While this is not evident from the fluxes reported in Table 1, the fluxes have large uncertainties (see Table 1 footnote). A higher effective V/III ratio for the Two-Step Sample is consistent with the RHEED measurements taken during the growth, which revealed initially streaky patterns suggesting metal-rich growth for the High V/III Sample (Fig. 4a)) and initially spotty patterns characteristic of N-rich growth for the Two-Step Sample (Fig. 4c)).¹²⁾

It is interesting that the inversion domain boundary at which the polarity reverses in the Two-Step Sample was not clearly visible as it was in the High V/III Sample (compare Fig. 5 a) and Fig. 3 a)). This lack of contrast may result from an absence of Si at the IDB. EDS

linescans across the AlN in the Two-Step Sample reveal little variation in the Si level throughout the layer. There was a small peak in the Si $\sim 1/3$ from the bottom of the AlN layer in Fig. 5 f), which is probably due to Si segregation at the threading dislocation visible in the STEM image, Fig. 5 a).¹³⁾ Excess Si was also present above the Si/AlN interface in Fig. 5 g), which is likely due to a hillock on the Si surface. A slight increase in Si was also found in some regions of the AlN/GaN interface (see Figs. 5 f) and i)). This is similar to the Low V/III Sample which had Si segregation at the AlN/GaN interface. Also similar to the Low V/III Sample, the Si concentration remains low throughout the AlN layer. Thus, the same mechanism is likely responsible for the increased Si at the AlN/GaN interface, that is Si that floated on the AlN surface in an Si/Al eutectic phase, precipitated out when the Al flux was removed and the excess Al on the surface was converted to AlN.

However, the Two-Step Sample differs from the Low V/III Sample in that it contains no vertical IDs, despite the presence of Si at the Al/GaN interface. This is probably because there is a lower concentration of Si at the interface of the Two-Step Sample, which was not sufficient to induce a polarity inversion (i.e. it was less than a monolayer),¹⁹⁾ which is consistent with less free Al and less eutectic phase forming during the initial nitrogen-rich, high V/III step of this growth.

4. Summary

Evidence of Al-Si eutectic formation and subsequent interfacial segregation of Si was found in three samples grown under different conditions. The eutectic formed correlated with the growth conditions used, with more highly Al-rich conditions (low V/III) producing larger amounts of eutectic and subsequently higher levels of Si incorporation. Although the quantity of eutectic formed, and the concentration and location of the Si precipitation varied, all three samples can be described by the following model. Under metal-rich conditions excess Al reacts with the Si substrate to form an Al-Si eutectic layer on the surface of the growing AlN film. When the film growth is converted to nitrogen-rich, through planned or uncontrolled flux changes, the Si from this layer is incorporated into the film and can induce inversion of the polarity from nitrogen to metal-polar. In two of the samples the presence of small regions with narrow, vertical inversion domains are indicative of lateral inhomogeneity in the Si concentration. Further experiments are underway to check these hypotheses.

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Fig. 1.

a) STEM ABF image of the GaN/AlN/Si structure of the Low V/III Sample showing holes in the Si substrate surface, which propagate to form holes in the GaN layer; also shown are SFs and IDs in the GaN layer, and the locations of: b–e) high-resolution images of the nitride polarity, and f–m) EDS linescans of the Si, Al and Ga distributions. Interdiffusion of Si into the GaN layer is visible in i) k) and l). Also visible in k) is Ga in a hole in the Si substrate. Si segregation at the AlN/GaN interface is visible in f) and g) where IDs are present in the GaN layer as seen in a).

Fig. 2.

a) Schematic of a FIB lamella cross-section, showing IDs with lateral dimensions less than the lamella thickness; when viewed in the STEM the overlap of regions with opposite polarities precludes polarity imaging. b) Atomic resolution STEM ABF image of an IDB in the Low V/III Sample; on the left the N atoms are below the Ga atoms in the Ga-polar ID, on the right the N atoms are above the Ga atoms in the N-polar material. c) HAADF STEM image of the same area shown in b) with the expected shift in the Ga lattice across the IDB (see text). d) Lower magnification STEM image of the area where b) and c) were taken, showing that the Ga-polar ID is large and probably as thick as the TEM lamella; narrower IDs, for which the polarity could not be imaged, are visible to the right of the IDB imaged.

Fig. 3.

a) STEM image of the GaN/AlN/Si structure of the High V/III Sample showing the lateral inversion boundary in the AlN layer, which is flat in one region (see also b)), but otherwise has a diffuse appearance (see explanation in text); also shown are SFs and IDs in the GaN layer, and the locations of higher resolution images b–d) and EDS linescans e–h). b) Higher resolution image of vertical inversion domains which initiated at a planar section of the lateral inversion boundary in a). c) and d) Atomic-resolution images of the nitride polarity just above the Si substrate and in the GaN layer (N-polar and Ga-polar respectively). e) and f) EDS linescans taken across the planar section of the lateral AlN polarity inversion boundary, showing a sharp increase in Si and associated decrease in Al at the IDB. g) and h) EDS linescans across diffuse regions of the lateral AlN polarity inversion boundary, showing broader increases and decreases in Si and Al respectively.

Fig. 4. RHEED images taken during AlN growths. a) Streaky pattern from the High V/III Sample taken after 5 min of AlN growth indicated a smooth surface and metal-rich, N-polar growth. b) After 7 min a 2X reconstruction appeared, consistent with N-rich conditions and Al-polar growth. c) Spotty RHEED pattern from the Two-Step Sample after 5 min of AlN growth indicated N-rich growth.

Fig. 5.

a) STEM image of the GaN/AlN/Si structure of the 2 Step High V/III Sample showing the locations of higher resolution images b–e) and EDS line scans f–i). Atomic resolution STEM images showing: b) N–polarity of the AlN layer just above the Si substrate, c) Al–polarity only slightly higher in the AlN layer, c) Al–polarity near the top of the AlN layer, and d) Ga–polarity in the GaN layer. f–i) EDS line scans across the AlN layer. A small increase in

Si and associated decrease in Al approximately a third of the way into the AlN layer in f) are probably associated with Si segregation at the threading dislocation visible in a). A higher level of Si just above the Si substrate in g) is probably due to a hillock on the Si surface. A slight increase in the Si concentration is also visible at the AlN/GaN interface in some of the scans.

Table 1.

Specimen growth conditions.

Sample	AlN						GaN			
	Al pre	step	Tsub (°C)	N ¹ Flux (nm/hr)	Al ² Flux (nm/hr)	Time (min)	Tsub (°C)	N ¹ Flux (nm/hr)	Ga ³ Flux (nm/hr)	Time (min)
Low V/III	no		805	152	218	6	675	213	204	84
High V/III	yes		805	260	131	12	675	205	186	84
2 Step High V/III	no	1	805	247	168	15	675	227	225	84
		2	805	228	237	20				

¹ Measured at equilibrium, uncertainty 35 %.² Uncertainty 20 %.³ Uncertainty 6 %.