Transmission electron microscopy investigation of AlN growth on Si(111)

D. Litvinov a,*, D. Gerthsen a, R. Vöhringer b, D.Z. Hu b, D.M. Schaadt b,1

a Laboratory for Electron Microscopy and Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), D-76128 Karlsruhe, Germany
b Institute for Applied Physics and CFN, KIT, D-76128 Karlsruhe, Germany

1. Introduction

Group-III nitrides (GaN, AlN, InN and their ternary alloys) are already extensively applied in optoelectronic devices. However, up to now epitaxial growth of these materials is carried out mainly on Al2O3(0001), SiC(0001) or GaN(0001) substrates. The growth of group-III nitrides on silicon has not been extensively pursued although it would be a low-cost alternative compared to growth on the commonly used substrates. It is also attractive due to the large size of Si wafers, good thermal conductivity of Si, and the potential for integration with Si-based devices. The epitaxial growth of nitrides is mainly performed on Si(111), which has the same symmetry as the group-III nitride basal plane. Growth on Si(001) is unfavorable due to the fourfold symmetry of the Si(001) surface leading to two differently aligned domains [1].

Although potentially very attractive, the direct epitaxial growth of GaN or InN on silicon is difficult due to the presence of an amorphous layer at the interface [2], which induces three-dimensional growth and the formation of polycrystalline material. The deposition of an AlN buffer layer significantly improves the crystal quality of GaN or InN [3–5]. Moreover, AlN films are not only interesting as buffer layers but also have considerable potential for high-power, high-temperature and radiation-resistant electronic and optoelectronic applications in the ultraviolet spectral range [6].

Only few detailed studies of the microstructure of AlN grown on Si(111) exist up to now. The transmission electron microscopy (TEM) study by Kaiser et al. [7] is concerned with the microstructure of AlN grown by molecular-beam epitaxy (MBE) on Si(111). They studied the defect types as a function of substrate temperature during growth between 700 °C and 800 °C and for Al/N-flux ratios of about 1 up to large Al-excess. AlN layers grown on Si(111) with high (optimum) quality according to X-ray diffraction rocking curves for the (0002) reflection yield minimum full width at half maximum values for the sample grown at the 900 °C under Al-rich conditions indicating optimum structural quality. However, the discussion of the entity of defects will show that a more differentiated view is required to assess the overall quality of the AlN layers.

2. Experimental

The samples were grown by plasma-assisted MBE in a Riber Compact 21 system with a base pressure of 1 × 10⁻¹⁰ mbar equipped with a solid-source effusion cell for Al and an Oxford...
HD25 radio-frequency plasma source for producing active N₂ at a power of 400 W and nitrogen gas was used with a steady gas flow of 0.5 sccm.

The Si(111) substrates were pre-degreased for 60 min at 130 °C prior to transfer into the growth chamber. The native oxide layer on the substrates was removed by heating up the samples to 900 °C. This was monitored by observing the 7 × 7 surface reconstruction of Si(111) by in-situ reflective high energy electron diffraction (RHEED). AlN layers with approximately 250 nm thicknesses were grown at temperatures between 600 °C and 900 °C with an Al/N₂ ratio which is Al-rich at 700 °C and 800 °C. The Al-rich growth was checked by scanning electron microscopy (SEM) images which yields Al-droplets at the AlN surface.

Five samples were investigated. The first four samples were grown under identical growth conditions apart from Ts which was 600 °C (sample S₆₀₀), 700 °C (sample S₇₀₀), 800 °C (sample S₈₀₀), and 900 °C (sample S₉₀₀). The fifth sample S₉₀₀Al was also grown at 900 °C but with a higher Al-flux than sample S₉₀₀.

The surface morphology of the layers was investigated by SEM using a LEO 1530 Gemini with field emission gun, which is equipped with a Noran Voyager system for energy-dispersive X-ray spectroscopy (EDXS). Further studies of the structural properties of the AlN/Si(111)-heterostructures were carried out by conventional TEM, high-resolution (HR)TEM and scanning TEM (STEM) combined with EDXS. The TEM investigations were performed with a Philips CM 200 FEG/ST electron microscope at 200 kV. Cross-section samples were prepared by standard procedures including grinding, dimpling, polishing and Ar⁺-ion milling as final preparation step. The cross-section samples always contain two pieces of one and the same wafer which are oriented to allow studies along the [1100]- and [1120]-zone axes of the Si-substrate.

The surface roughness of the layers was studied by atomic force microscopy (AFM) in the contact mode with an instrument from Park Systems using standard Si₃N₄ tips. For the integral evaluation of the crystalline quality we applied XRD using a Bruker D8 system. Rocking curves for the (0002) AlN reflection were acquired for all samples.

### 3. Experimental results

In the following the characteristic structural features of the AlN layers will be presented. Fig. 1 shows SEM images of the surface morphology of all samples on a large and small (insets) scale. On the surface of sample S₆₀₀ (Fig. 1a, overview) large holes marked by arrows are observed. Large droplets are found on the surface of samples S₇₀₀ (Fig. 1b) and S₈₀₀ (Fig. 1c) which consist of Al as determined by EDXS. The number and size of the droplets decrease with increasing substrate temperature leading finally to surfaces for samples S₉₀₀ and S₉₀₀Al (Fig. 1d and e) which are smooth on a large scale. More details of the structural quality of the surfaces are revealed in the high-magnification SEM images in the insets. The surface of sample S₆₀₀ (inset in Fig. 1a) appears to consist of separate small structural features which show often a six-fold symmetry. On the surfaces of samples S₇₀₀ and S₈₀₀ (insets in Fig. 1b and c) terraces with hexagonal faceting occur. Their sizes increase with substrate temperature. The surfaces of the samples grown at 900 °C contain small pits which are marked by arrows. The number of pits decreases with increasing metal flux during AlN growth as demonstrated by the insets in Fig. 1d and e for S₆₀₀ and S₉₀₀Al, respectively.

The results regarding the structural properties of the samples are presented in the following as a function of the growth temperature. Starting with the smallest substrate temperature, Fig. 2 shows TEM cross-section images of S₆₀₀. A (0002)AlN dark-field TEM image close to the [1100]-zone axis of the AlN is presented in Fig. 2a. The pronounced contrast variations in the AlN layer indicate strong lattice distortions which are induced by a high density of defects. The AlN layer consists of small columns elongated along the growth direction with diameters typically below 50 nm. The columns remain sometimes separated from the neighbor columns indicated by arrows in the HRTEM image Fig. 2b, which shows the top region of AlN layer along the [1100]-zone axis. The separation of the AlN columns in
Sample S600 contributes to the large surface roughness. The AlN/Si-interface is depicted in the HRTEM image Fig. 2c taken along the [11–2]AlN-zone axis. The AlN layer consists predominantly of crystallites aligned along the [11–10]AlN-zone axis (marked by 1). However, the small AlN rod marked by 2 is aligned along the [11–20]AlN-zone axis which is rotated by 30° (or equivalently 90° or 120°) with respect to the surrounding grains. Moiré fringes are observed in the AlN layer with a distance of about 1.25 nm in region 3 due to crystallites which are slightly tilted against each other along the electron-beam direction.

Fig. 3a and b shows (contrast-inverted) selected-area electron diffraction (SAED) patterns taken parallel to the [11–2]Si- and [11–10]AlN-zone axes of cross-section TEM specimens which are representative for all samples. The green reflections denote Si and four-index reflections hexagonal AlN. However, AlN crystallites with different orientations (see Fig. 1c) or AlN in the cubic phase may occur. Based on the SAED patterns in Fig. 3a and b, the following epitaxial relationship is derived for AlN/Si(111): (0001)AlN/[11–10]Si with the azimuthal orientation [11–20]AlN/[11–10]Si and [11–10]AlN/777[11–2]Si, denoted as type I domains in the following. Fig. 3c shows the arrangement of the Si- and Al- or N-atoms in the Si(111) and AlN(0001) planes with the corresponding in-plane directions. Fig. 3c demonstrates the large lattice-parameter mismatch between Si with cubic diamond structure and a lattice parameter \( a = 0.543 \text{ nm} \) and AlN with wurtzite structure and lattice parameters \( a = 0.3119 \text{ nm} \) and \( c = 0.4988 \text{ nm} \). An “effective” lattice parameter \( a' = a / \sqrt{2} = 0.384 \text{ nm} \) can be defined for the Si(111) surface. A large tensile strain of \(-19\%\) results from the lattice-parameter mismatch defined by \( f_1 = (a_{\text{AlN}} - a_{\text{Si}}) / a_{\text{Si}} \) in the AlN layer. Fig. 3d will be described in context with Fig. 6.

Fig. 4a presents a HRTEM image of an undisturbed interface section in sample S700 which was taken along the [11–10]Si-zone axis. However, substrate steps are observed which lead to a disturbed AlN-crystal orientation as exemplified by the HRTEM image Fig. 4b taken along the [11–2]Si-zone axis. Here, the interface contains a step with a height of 3 nm. The diffractogram of this region shown in the inset of Fig. 4b contains two additional reflections 1 and 2 (arrows) that correspond to \{01–10\}AlN reflections indicating that AlN inclusions marked by 1 and 2 with different orientations are present in Fig. 4b. Fig. 4c shows the (0002)AlN-Fourier-filtered image of an enlarged area of Fig. 4b close to the step. Misfit dislocations (labeled by arrows) induce additional (0002) planes of AlN which correspond to a Burgers vector component \( \mathbf{b} = 1/2[0001] \). The formation of the dislocations can be understood by the large mismatch between the Si(111) and AlN(0002) planes which needs to be compensated at the step. The inserted AlN(0002) planes tilts the region on top which leads to Moiré fringes above the step.

Fig. 5 presents cross-section images of sample S800 along the [11–10]Si-zone axis. A high density of threading dislocations oriented along the growth direction is observed in the overview image Fig. 5a. An inclusion with a thickness of 25 nm is observed at the AlN/Si-interface extending to the left-hand side of the arrowed step. The HRTEM image Fig. 5b taken close to the step shows a highly strained region above the inclusion with a thickness of \(-9 \text{ nm} \). The SAED pattern of this region (inset in Fig. 5b) reveals three groups of reflections: unmarked reflections result from AlN, reflections marked with solid circles from Si and additional reflections indicated by dotted circles which are not observed in the standard SAED pattern in Fig. 3a. These reflections can be explained by the presence of pure Al (face-centered cubic structure with \( a_{\text{Al}} = 0.405 \text{ nm} \) in the inclusion in the Si-substrate. EDX spectra (not shown here) confirm the presence of pure Al. The elongation of the AlN reflections is indicative of slight orientation variations and strain which result from the distorted AlN region above the Al-inclusion.

Cross-section images of the same sample (not presented here) show steps with a height of up to 20 nm at the surface of the AlN layer. The distance between the steps amounts up to about...
100 nm which correlates well with the SEM image of sample $S_{900}$ (Fig. 1c).

Fig. 6a presents a HRTEM image of the AlN/Si-interface of sample $S_{900}$ taken along the [11–2]$_{Si}$–zone axis which contains two different orientations in the AlN layer in regions 1 and 2. The diffractogram of the HRTEM image in Fig. 6b shows three groups of reflections that belong to the [11–2]$_{Si}$–zone axis (circles) and AlN along the [1–100]$_{AlN}$ and [11–20]$_{AlN}$–zone axes. The first AlN–zone axis corresponds to the standard type I azimuthal orientation (region 1). Region 2 with [11–20]$_{AlN}$–zone axis is rotated by 30° which will be denoted as type II epitaxial orientation relationship. Fig. 3d schematically shows the atom arrangement in the interface plane in region 2. According to Fig. 3d, the distance $\alpha_{AlN} = 2 \cdot \alpha_{Si} \cdot \cos 30°$ must be compared with the distance $\alpha'_{Si}$ to assess the mismatch $f_{2} = (b_{AlN} - \alpha'_{Si})/\alpha'_{Si}$ which yields a large compressive strain of +40% in the AlN layer. Note that the AlN layer is under tensile strain for the type I orientation relationship in the region 1 and under compressive strain in region 2. Enlarged images of regions 1 (left) and 2 (right) are presented in Fig. 6c after Fourier filtering with the [2–20]$_{Si}$ and [1–120]$_{AlN}$ reflections (region 1) and [220]$_{Si}$ and [–1100]$_{AlN}$ reflections (region 2). All these planes are oriented perpendicular to the interface, which conveniently allows the assessment of mismatch accommodation by the concept of domain matching epitaxy proposed by Narayan and Larson [9] as discussed in Chapter 4. We count 45 (11–20) AlN planes and 36 Si(1–10) planes for the type I orientation relationship in the region 1 (left image of Fig. 6c) which corresponds to a ratio of 5:4. In the rotated type II domain (right image of Fig. 6c) 35 Si(1–10) planes and 25 AlN (1100) planes yields a 5:7 ratio. Additional (1–120)$_{AlN}$ planes in region 1 and (2–20)$_{Si}$ planes in region 2 are marked by arrows.

Fig. 7 displays HRTEM images of sample $S_{900Al}$ along the [–110]$_{Si}$–zone axis from two regions taken with different magnifications. Several types of defects can be identified in the AlN layer: threading dislocations (an example being marked by D in Fig. 7a) and a high concentration of stacking faults (especially in regions marked by SF$_{w}$ and SF$_{s}$), which are oriented parallel or inclined with respect to the AlN/Si-interface (Fig. 7a and b). Diffractograms of the lower and upper parts of the AlN layer are shown as inset in Fig. 7b. AlN in the wurtzite structure is found in the 30 nm thick layer above the Si substrate which is oriented along the expected [11–20]–zone axis and contains stacking faults oriented parallel to AlN/Si-interface (e.g. in region SF$_{w}$). The AlN on top is crystallized in the sphalerite structure. It is oriented along the [110]–zone axis and contains numerous stacking faults SF$_{s}$, which are inclined with respect to AlN/Si-interface.

The cross-section images of $S_{900}$ and $S_{900Al}$ presented in Fig. 8a and b illustrate the effect of the Al-flux on the growth mode and surface quality of the AlN layer. A smooth surface is achieved for sample $S_{900Al}$ (Fig. 8b) along sections with a width of up to several 100 nm whereas pits are found on the surface of $S_{900}$ (Fig. 8a) in accordance with Fig. 1d (inset). Different contrast of columnar regions in the AlN layer of $S_{900}$ can be associated with columnar growth despite the high substrate temperature. Pits are typically formed at the boundaries between different columns as marked by the arrows in Fig. 8a.

Table 1 summarizes the observed structural features of all investigated samples. Inversion domains with diameters of about

![Fig. 3. Diffraction patterns of AlN/Si(111) cross-section samples along the (a) [−110]$_{Si}$ and (b) [11–2]$_{Si}$–zone axes. (c,d) Arrangement of Si– and Al– or N– atoms in the interface plane with corresponding directions for AlN and Si: (c) for the standard azimuthal orientation and (d) for the second azimuthal orientation rotated by 30° with respect to the standard orientation.](image-url)
10 nm are found in samples $S_{800}$ and $S_{900}$ (images not shown here) where the polarity along the [0001] direction is reversed. The existence of inversion domains in group-III nitrides can be inferred from dark-field TEM images taken with imaging vectors $g = \pm (0002)$ as described e.g. in Ref. [10] for GaN on Al$_2$O$_3$(0001) and in Ref. [7] for AlN/Si(111). Table 1 also lists the FWHM of the (0002) XRD rocking curves which contain integral information on orientation variations and defect densities. The FWHM decreases with increasing substrate temperature reaching an optimum value for sample $S_{900Al}$ (918 arcsec) which is the smallest value for the growth of AlN on Si(111) reported in literature so far [8]. However, the quality of the AlN layers grown on Al$_2$O$_3$(0001) substrates ($\sim$56 arcsec FWHM of the (0002) XRD, see Ref. [11]) still exceeds significantly the quality of AlN layers on Si(111). The root mean square (RMS) roughness values of the sample surfaces with an area of $2 \mu m \times 2 \mu m$ are also added in Table 1. The RMS values were calculated from AFM images in regions without Al-droplets on the surface (for samples $S_{700}$ and $S_{800}$). The roughness of the AlN layer is minimal for samples grown at 900 °C.

4. Discussion

In the following we discuss the structural features of the investigated AlN/Si(111) heterostructures and their dependence on the substrate temperature during growth.

4.1. Surface properties

The surface properties of the AlN layers are shown in Figs. 1 and 8 and RMS roughness values are listed in Table 1. For $T_s = 600$ °C columnar growth occurs which leads to a rough layer surface with an RMS roughness of 52.7 nm (Table 1). Large Al-droplets are observed at $T_s = 700$ °C and $T_s = 800$ °C indicating excess Al on the growth surface. The increase of $T_s$ and Al-rich conditions lead to a lateral enlargement of the growth columns which is visualized by the size of the hexagonal features in the insets of Fig. 1b and c. Cross-section TEM images of $S_{700}$ and $S_{800}$ (not shown here) show smooth surfaces along the surface regions of the hexagonal structures. However, RMS roughness values based on AFM images for samples $S_{700}$ and $S_{800}$ (67.0 nm and 63.3 nm correspondingly, see Table 1) are slightly larger than for sample $S_{900}$. This can be attributed to height difference between the hexagonal structures on the surfaces of samples $S_{700}$ and $S_{800}$.
The appearance of the surface morphology changes considerably for the samples grown at 900 °C which contain pits (insets Fig. 1d and e) with a density that depends on the Al-flux. Moreover, Al-droplets are not observed anymore for $S_{900}$ and $S_{900Al}$ and minimum RMS roughness values are achieved (26.2.0 nm and 27.5 nm correspondingly, see Table 1). The lack of Al-droplets is related to the reduction of the Al/N-atom ratio at the growth surface due to increasing Al-desorption at this high temperature. This even applies to $S_{900Al}$ which was grown with an increased Al-flux. Fig. 8a demonstrates that the pits are formed at contact regions between different columnar crystallites. The effective reduction of the Al/N-atom ratio on the growth surface due to increasing Al-desorption at this high temperature. This even applies to $S_{900Al}$. Which was grown with an increased Al-flux. Fig. 8a demonstrates that the pits are formed at contact regions between different columnar crystallites. The effective reduction of the Al/N-atom ratio on the growth surface due to increasing Al-desorption at this high temperature.

4.2. Dislocations and inversion domain boundaries

All AlN layers contain treading dislocations which are mainly oriented perpendicular to the AlN/Si-interface. They are partially formed at boundaries between different AlN columns which is particularly obvious at low growth temperature (Fig. 2a and b). Other threading dislocations originate at the AlN/Si-interface (Figs. 5a and 7a) as threading segments of misfit dislocations. In sample $S_{900Al}$ we observe a reduced dislocation density but instead stacking faults with a high concentration (see Fig. 7). The reduction of the dislocation density can be attributed to the suppression of columnar growth and dislocations formation at boundaries between slightly misoriented columns which is consistent with a minimum value of the FWHM of (0002) XRD rocking curves for this sample.

4.3. Stacking faults and formation of cubic AlN crystallites

Apart from sample $S_{600}$, inclusions of the metastable cubic sphalerite phase are found in all samples. For sample $S_{700}$ only small regions of cubic AlN are observed close to the AlN/Si-interface (images not shown here). The number density and size of cubic inclusions increases with the growth temperature. For samples grown at 900 °C (e.g. Fig. 7 for sample $S_{900Al}$) large sphalerite crystallites with numerous stacking faults are observed. Calleja et al. [12] describe the formation of cubic inclusions in an AlN buffer layer between Si and GaN, which is correlated with N-deficient AlN. Schupp et al. [13] report about plasma-assisted MBE growth of cubic AlN on 3C-SiC(001) substrates which is observed for Al-coverages below 1 ML on the growth surface. Accordingly, the formation of the metastable sphalerite phase in our AlN films can be explained by the reduction of the Al/N-atom ratio on the growth surface with
increasing substrate temperature as already discussed in context with the surface properties. The increase of the stacking fault density is correlated with increasing volume fractions of the cubic AlN. It can be understood by the transformation mechanism between cubic and wurtzite structures requiring the formation and movement of partial dislocation which is always associated with the formation of stacking faults as outlined in e.g. Ref. [14].

4.4. Interface properties and orientation relationship between AlN and Si(111)

The dominant type I orientation relationship for AlN/Si(111) is $(0001)_{\text{AlN}}/[(11\overline{1})_{\text{Si}}$ with the azimuthal orientation $[11–20]_{\text{AlN}}[-110]_{\text{Si}}$ and $[11–100]_{\text{AlN}}[11–2]_{\text{Si}}$ in agreement with previous studies, e.g. [7,15]. However, all samples contain type II domains with $[11–20]_{\text{AlN}}[11–2]_{\text{Si}}$ and $[11–100]_{\text{AlN}}[−110]_{\text{Si}}$ (Figs. 6 and 3d) corresponding to a rotation of 30° (or equivalently 90° or 120°) with respect to the type I orientation. A two-domain film structure was reported in Ref. [8] for AlN grown on Si(001) with a 30° rotation between neighboring domains which is related to the different symmetries of the Si(001) substrate and any possible AlN plane. A two-domain structure for 25 nm-thin AlN layers grown on Si(111) was found by Bourret et al. [15]. They noted that the type I orientation relationship is favored for deposition temperatures above 650 °C and a Si(111) substrate with 7 × 7 reconstruction while higher type II fractions are observed for an unreconstructed Si-substrate surface. The two-domain structure on a Si(111) substrate is on first view less plausible because the substrate symmetry matches with the symmetry of the AlN(0001) plane. To understand the two-domain structure the amount and sign of the lattice-parameter mismatch has to be considered. The mismatch in the standard orientation is −19% between Si(111) and AlN(0001) with AlN under tensile stress. In contrast, the AlN layer is under compressive stress in the type II orientation with a mismatch +40%. One reason for the two-domain structure may be the opposite sign of stress. Second, domain matching according to Ref. [9] can be considered, which is appropriate for large misfit systems with $f > 7\%–8\%$. Here it is proposed that the decisive factor is the match of $m$ crystal planes of the film with lattice-plane distances $d_f$ with $n$ crystal planes of the substrate with lattice-plane distances $d_s$. The deviation from the matching determines the residual strain $\varepsilon_i = (md_f/n) - 1$. According to Fig. 6c we calculate $\varepsilon_i = 0.0165$ for the type I azimuthal orientation (region 1) with $m = 5 (11–20)_{\text{AlN}}$ and $n = 4 (2–20)_{\text{Si}}$ planes ($d_f = 0.15615$ nm and $d_s = 0.19201$ nm). For the type II orientation (region 2) we obtain $\varepsilon_i = 0.0061$ with $m = 5 (1100)_{\text{AlN}}$ planes and $n = 7 (2–20)_{\text{Si}}$ planes ($d_f = 0.27046$ nm and $d_s = 0.19201$ nm). Thus, the smaller residual strain can explain the formation of type II domains despite the huge lattice parameter mismatch.

Regions with perfect epitaxial quality (e.g. Fig. 4a) occur in all samples. Steps at the AlN/Si-interface are observed to be nucleation sources for crystallites with tilted orientation, e.g. at the 3 nm-high step shown in Fig. 4b. Another example is the crystallite with type II orientation in Fig. 6a which is observed to be formed at a step.

4.5. Al-inclusions in the Si-substrate

Crystallites consisting of pure Al are observed in the Si-substrate for the samples grown at 700 °C and 800 °C (Fig. 5b). These regions are particularly large in sample $S_{900}$ with a thickness up to 25 nm. Al-crystallites were also detected by Kaiser et al. [7] after AlN deposition on Si(111) at 800 °C and 900 °C under high Al-rich conditions. They explained the Al-crystallite formation by the existence of a low-temperature eutectic transformation which takes place in the Si-Al binary system below 577 °C [16]. Al-excess on the Si-substrate surface leads first to the dissolution of Si in Al above the transformation temperature. After growth, an eutectic transformation occurs during cool down at 577 °C [16] with the separation of the melt into the solid Al- and Si-phases.

An indicator for Al-excess on the growth surface is the presence of Al-droplets on the surface of the AlN layer at 700 °C and 800 °C. The lack of Al-inclusions at 600 °C and 900 °C is therefore consistent with the lack of Al-droplets (as indication of low Al-coverage at the growth surface) at these growth temperatures. The large size of the

![Fig. 8. Cross-section images taken along the [−110]$_{\text{Si}}$-zone axis: (a) HRTEM image of sample $S_{900}$ and (b) $[0002]_{\text{AlN}}$ dark-field TEM image of sample $S_{900AL}$.](image-url)
Al-inclusions at 800 °C can be understood by the large superheating above 577 °C which leads to comparably large melt volume fractions. Phase separation during cool down can also explain the thin, highly defective AlN layer on top of the Al-crystallite (Fig. 5b) as a result of stress during solidification of the AlSi melt.

5. Conclusions

In this study, the microstructure of epitaxial AlN layers on Si(111) substrates was investigated by different electron microscopic techniques and (0002) XRD rocking curves. The layers were grown by plasma-assisted gas source MBE at substrate temperatures between 600 °C and 900 °C under metal-rich conditions. The dominant epitaxial relationship between AlN and Si(111) is \((0001)_{\text{AlN}} \parallel (111)_{\text{Si}}, (11 \,-20)_{\text{AlN}} || (11 \,-100)_{\text{Si}}, (11 \,-21)_{\text{Si}}\). However, domains with the azimuthal orientation \([1 \,-20]_{\text{AlN}} || (11 \,-21)_{\text{Si}}\) and \([1 \,-100]_{\text{AlN}} || (11 \,-10)_{\text{Si}}\) are found in all samples which corresponds to a \(30°\) rotation with respect to the main azimuthal orientation. The formation of a two-domain structure can be understood by the opposite sign of the lattice-parameter mismatch in the two domains and the concept of domain matching epitaxy.

The observed types and densities of defects depend strongly on the growth temperature. The microstructure of the AlN layer grown at 600 °C is dominated by columnar growth, a rough surface and high dislocation density. A smoothing of the layer surfaces is observed for growth temperatures of 700 °C and 800 °C but Al-droplets are formed due to excess Al on the growth surface. The latter also causes pure Al-inclusions at the AlN/Si-interface due to the dissolution of Si by Al and an eutectic transformation during cool down with the separation of the melt into the solid Al- and Si-phases. The density and size of droplets decrease with the growth temperature. The microstructure is optimized at 900 °C with respect to dislocation density, lack of Al-droplets and Al-inclusions in the Si-substrate. These effects can be understood by Al-desorption and corresponding reduction of the local Al/N-ratio on the growth surface which leads on the other hand to the formation of sphalerite AlN inclusions in combination with a high stacking fault density. A high density of small pits is observed on the surface of the AlN layer grown at 900 °C, which can be reduced by increasing the Al-flux at this temperature. The crystalline quality of the AlN layers has to be evaluated with respect to the desired application. Minimum dislocation densities and a smooth surface are obtained for the sample grown at 900 °C under Al-rich conditions. Layers grown at 900 °C contain on the other hand a significant fraction of sphalerite inclusions and stacking faults which are not present at low growth temperatures.

High growth temperatures and an even higher Al/N-ratio can be expected to be beneficial for further microstructure improvement of AlN on Si(111). In this context it is important to note that the nominal Al/N-ratio, determined by the Al-source temperature, N2-flux and operation conditions of the rf-plasma source, has to be distinguished from the real Al/N-atom ratio on the growth surface. The latter is strongly affected by the substrate temperature and resulting Al-desorption. An increase of the Al/N-atom ratio on the growth surface at high substrate temperatures can be expected to suppress the nucleation of sphalerite AlN (and corresponding stacking fault formation) which was associated with N-deficient AlN. Moreover, the surface quality may be further improved by the reduction of the pit density. However, the Al/N-ratio should on the other hand not exceed values where Al-droplet formation occurs as an indication of a significant Al-excess on the growth surface because this would lead to the undesirable formation of Al-inclusions at the AlN/substrate interface.

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