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Investigation of the structure of 2H-AlN films on Si(001) substrates

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Abstract. By conventional transmission electron microscopy (CTEM) investigations on 2H-AlN films grown by plasma-assisted molecular beam epitaxy (MBE) on Si(001) the influence of the off-axis angle of the substrate surface on the film structure was studied. Three types of Si(001) substrates were used: on-axis, ~1°, and ~5° off-axis Si(001) substrates. The AlN layer on an exact oriented Si(001) substrates consists of 3 AlN film domains: two main film domains, AlN_1 and AlN_2, and a small domain AlN_3 at substrate surface defects. Their c-axis orientations are parallel to the c-axis of the substrate: $[0001]AlN_{1,2,3}\|[001]Si$. The a-axes of AlN_1 and AlN_2 rotated by 30° to each other: $[11\bar{2}0]AlN_1\|[01\bar{1}0]AlN_2\|[1\bar{1}0]Si$ [3]. The a-axis orientation of AlN_3 is $[01\bar{1}0]AlN_3\|[100]Si$. In 2H-AlN films grown on off-axis Si(001) substrates (~1° and ~5°) the ratio between the AlN_1 and AlN_2 film domains changes dramatically as far as a single domain film structure consisting of only AlN_1 is reached. The AlN c-axes of all domains on the off-axis substrates are not parallel to the Si c-axis but tilted by the off-axis angle of the Si(001) substrate (~1° respectively ~5°), i.e. [0001]AlN is parallel to the Si(001) substrate surface orientation.

Introduction

Aluminium nitride (AlN) is a promising material as a wide band-gap, high temperature, radiant resistant semiconductor. It exists in the thermodynamically stable wurtzite phase (basal plane lattice parameter a = 0.3112nm [1]) but also in the zincblende polytype [2]. Wurtzite AlN (2H-AlN) deposited on commonly used silicon (Si) (001) substrates (lattice parameter a = 0.54307nm) is a good solution as a template substrate for III-nitride electronic and optoelectronic devices. The successful AlN film epitaxy on Si(001) would allow to integrate the group III-nitride technology into the mature silicon technology. Especially the growth of single domain AlN films on Si (001) is a challenging task for heteroepitaxy due to the mismatch in the lattice parameters and the different crystallographic symmetry of the hexagonal closed-packed (0001)AlN lattice plane (six-fold symmetry) and the (001)Si substrate surface plane (four-fold symmetry).

Experimental

AlN films were grown in a home-made plasma-assisted molecular-beam epitaxy (PAMBE) system equipped with a radio-frequency plasma source for activated nitrogen supply and using thermally evaporated aluminium. Three different Si(001) substrate surfaces were prepared: A) on-axis (±0.5°) (for details [3]), and off-axis substrates with B) about 1° (±0.5°) , and C) about 5° (±0.5°) tilt of the substrate surface orientation towards [110]Si (for details [4]). Thin plan-view (pv) and cross-sectional (xs) foils for conventional transmission electron microscopy (CTEM) investigations were prepared using standard techniques. For the CTEM studies a JEOL JEM 3010 at 300kV was used. Plan-view specimen of the 2H-AlN/Si(001) heterosystem were examined in [0001]AlN zone axis and the cross-section specimen in $[1\bar{1}0]$Si zone axis orientation.

2H-AlN on on-axis Si (001) substrate

Fig.1 shows CTEM images of a AlN film grown on an exact (±0.5°) oriented Si(001) substrate in plan-view (pv) orientation. In the diffraction pattern (DP) inserted in the upper right corner of the bright-field (BF) image (Fig.1a) the reflexes indicate an unusual 12-fold symmetry. The dark-field (DF) images in Fig.1b and 1c, where 1b was taken with the reflection marked by a square, and 1c with the reflection marked by a cycle, explain this phenomenon as two usual 6-fold symmetrical reflex systems of hexagonal 2H-AlN in c-axis viewing direction. Therefore the AlN film consists of two main film domains with a 30° rotation of their a-axes orientations to each other. The ratio of these domains in the entire film is approximately 1:1. At some areas of the film (see DF image in Fig.1d) the DP shows a third weak 6-fold symmetrical spot system in addition (marked by a triangle in the inserted DP in Fig.1d). The a-axes of the third 2H-AlN domain have a 15° rotation with respect to the two main domains. In cross-sectional (xs) view (Fig.2) we can determine the crystallographic orientation between the AlN film and the Si(001) substrate.

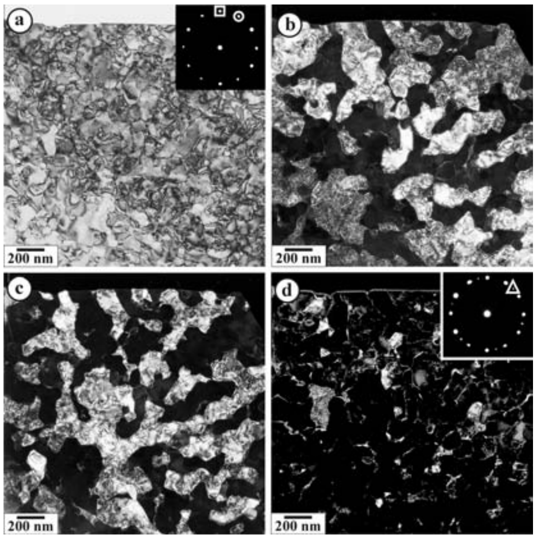

Figure 1 pv-CTEM images of the AlN film grown on on-axis Si(001) substrate. **(a)** BF image with the inserted DP. **(b)-(d)** DF images taken with the reflexes marked by a square (b), by a cycle (c), and by a triangle(d)

The xs-CTEM images were taken in the $[1\bar{1}0]$Si zone axis. Additionally to the Si reflections, the DP in Fig.2b shows the $[11\bar{2}0]AlN_1$ and the $[01\bar{1}0]AlN_2$ zone axis orientation at the same time, which confirmed the existence of two main domains. This can be explained by two completely identical symmetry fittings of the 6-fold (0001)AlN lattice plane on the 4-fold (001)Si plane. The reflections (0002)AlN and (002)Si are in one row (see Fig.2b). That means, the c-axes of AlN_1 and AlN_2 are parallel to the Si (001) surface orientation, i.e. in case of this on-axis substrate: [0001]AlN ‖ [001]Si. In Fig.2c the DF image was taken by a reflection of the AlN_1 domain (marked by a square) and the DF image in Fig.2d by a reflection (encycled) of the AlN_2 domain. This corresponds to the pv DF images in Fig.1b and 1c. Figs.2c and 2d are also nearly complementary except small AlN crystals in the film at the film substrate interface which can be seen in Fig.2e. This DF image was taken after a 15° tilt of the TEM specimen along the interface. That is equal to a third domain (AlN_3) with an a-axis orientation of $[01\bar{1}0]AlN_3$ ‖ [100]Si where the AlN_3 c-axis is parallel to the Si substrate c-axis as was the case for AlN_1 and AlN_2. The existence of the AlN_3 film domain is caused by irregularities at the Si substrate

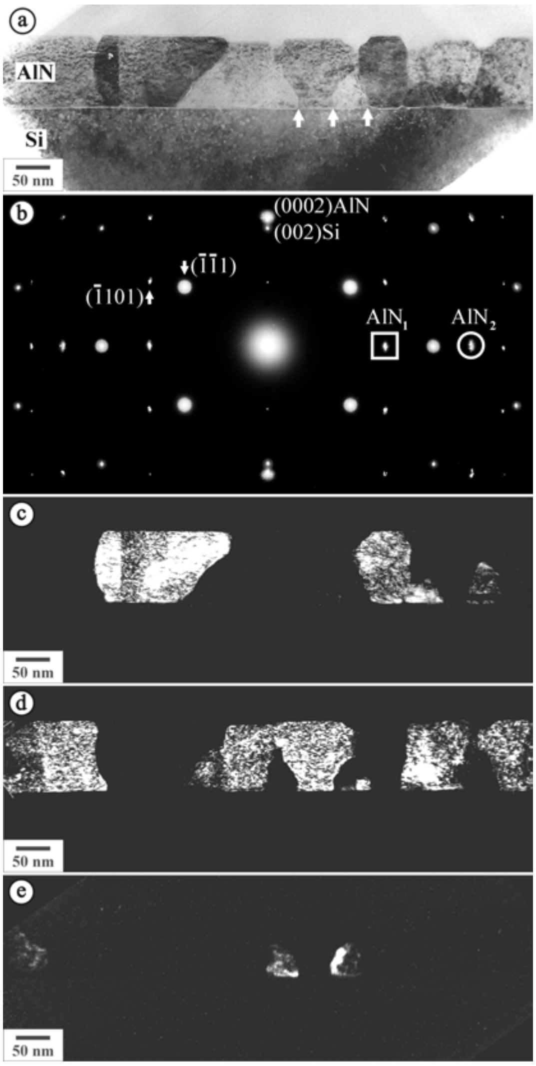

Figure 2 xs-CTEM images in $[1\bar{1}0]$Si viewing direction of the AlN film grown on on-axis Si(001). **(a)** BF image, **(b)** DP, **(c)**,**(d)** DF images taken with the reflexes marked by a square (c) and by a cycle (d), (e) DF image after a 15° tilt along the film substrate interface.

surface (arrowed in the BF image, Fig.2a) which are likely to be caused by Si diffusion on the substrate surface.

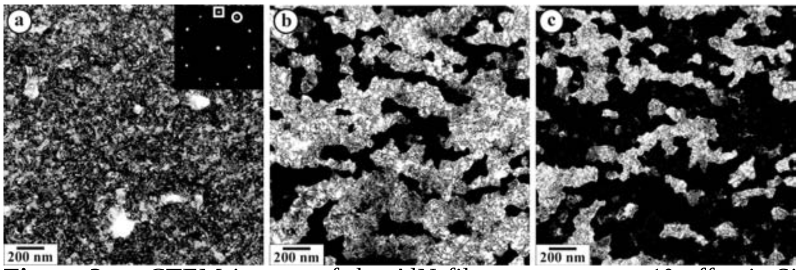

Figure 3 pv-CTEM images of the AlN film grown on a ~1° off-axis Si (001) substrate. **(a)** BF image (inserted DP), **(b)**,**(c)** DF images taken with the reflections marked by a square (b) and by a cycle (c)

2H-AlN on ~1° off-axis Si(001)

Fig.3 shows the pv CTEM images of a AlN film grown on a ~1° (±0.5°, tilted towards [110]Si) off-axis Si(001) substrate surface. The DP inserted in the BF image in Fig.3a indicates two reflex systems with 6-fold symmetries but with different spot intensities. The DF image in Fig.3b was taken with the reflex of the more intensive system marked by a square in the DP, and Fig.3c taken with a weak reflex marked by the cycle. The AlN film consists of the same two film domains like in the on-axis case, but the ratio is approximately 2:1.

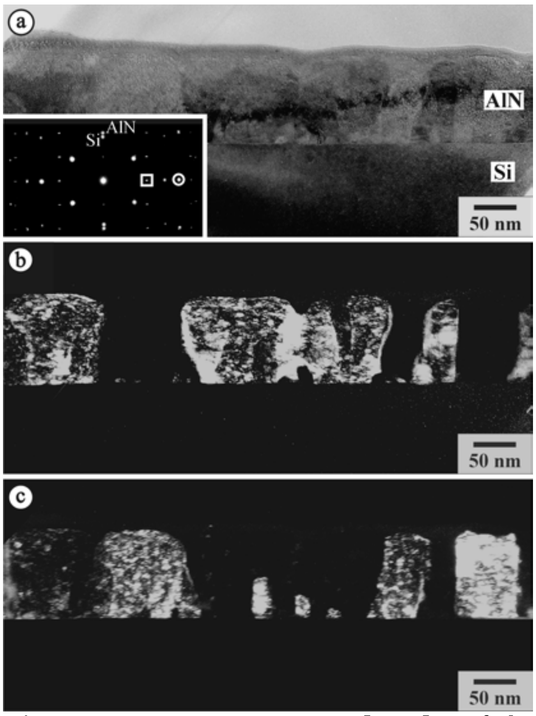

Figure 4 xs-CTEM images in [1 1 0]Si of the AlN film grown on a ~1° off-axis Si (001) substrate. **(a)** BF image with inserted DP, **(b)**,**(c)** DF images of the two AlN film domains

Fig.4 shows the corresponding xs-CTEM images in the $[1\bar{1}0]$Si zone axis orientation. In the DP (inserted in the BF image, Fig.4a) again the $[11\bar{2}0]$AlN$_1$ and the $[01\bar{1}0]$AlN$_2$ zone axis orientation can be indicated. The c-axes orientation (marked with “AlN” and “Si” in the DP in Fig.4a) are tilted towards each other by the off-axis angle (~1°) of the Si(001) substrate, i.e. the film c-axis is parallel to the substrate surface orientation. In Fig.4b the DF image was taken by a reflection of the AlN$_1$ domain (marked by a square in the DP) and the DF image in Fig.4c by a reflex of the AlN$_2$ domain (encycled). Fig.4b and 4c as well as Fig.3b and 3c are complementary. No AlN$_3$ orientation were revealed.

2H-AlN on ~5° off-axis Si(001)

The pv CTEM images in Fig.5 show an almost single domain structure of the AlN film grown on an off-axis Si(001) substrate surface, which has a surface orientation tilted ~5° (±0.5°) towards [110]Si. The DP inserted in the BF image in Fig. 5a indicates a single 6-fold symmetry of the AlN film. The DF image in Fig.5b was taken with the AlN reflex marked by a square in the DP. This AlN domain contributes to the entire film by approximately 95%. The other film parts have a 30° a-axis rotation which can be seen in the DP inserted in Fig.5c. This DF image was taken by the reflection marked by the a cycle in the DP in Fig.5c.

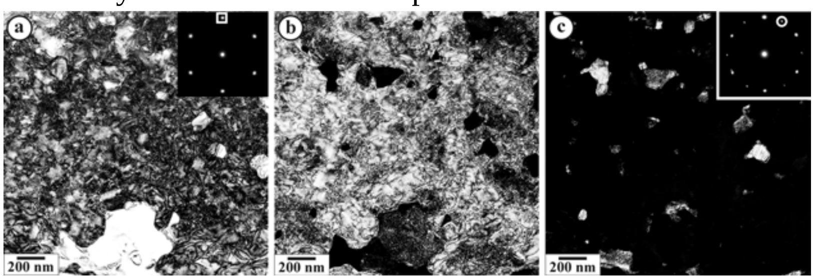

Figure 5 pv-CTEM images of the AlN film grown on a 5° (towards [110]Si) tilted Si (001) substrate surface. **(a)** BF image with the inserted DP, **(b)** DF image taken with the reflection marked by a square, **(c)** DF image taken with the encycled reflection in the inserted DP

The xs CTEM images in Fig.6 determine the crystallographic orientation of the main film domain in respect to the substrate. The BF image in Fig.6a and the DP in Fig.6b prove the existence of one main AlN$_1$ film domain

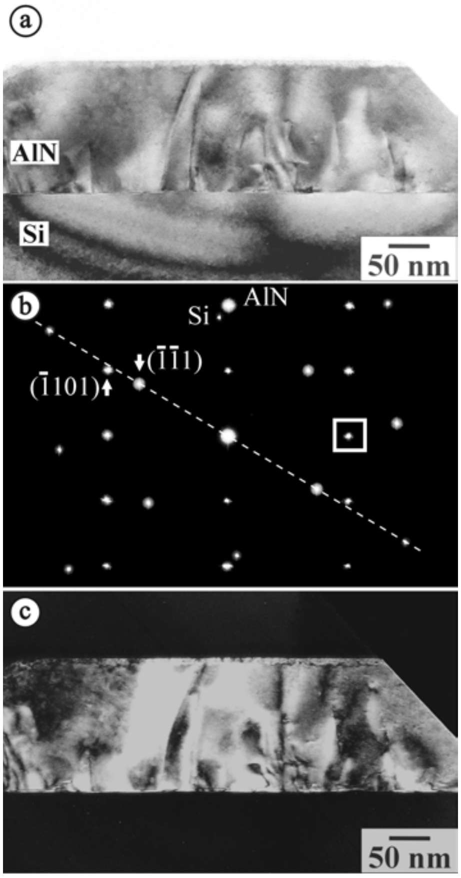

Figure 6 xs-CTEM images in [1$\bar{1}$0]Si of the AlN film grown on a ~5° off-axis Si (001) substrate. **(a)** BF image, **(b)** DP, **(c)** DF image taken with an AlN reflection (marked by a square)

with an a-axis orientation of [11$\bar{2}$0]AlN_1 ∥ [1$\bar{1}$0]Si. The AlN c-axis (marked with "AlN" in the DP) shows a ~5° tilted to Si c-axis (marked by "Si) which is equal to the off-axis angle of the substrate. The AlN film c-axis is again parallel to the substrate surface orientation. The DF image in Fig.6c, which was taken by a AlN_1 reflection marked by a square, confirms the single domain structure of the 2H-AlN film.

The preferred appearance of the AlN_1 domain over AlN_2 may be explained crystallographically in the following way. The tilt of the Si(001) substrate surface towards the [110]Si direction leads to a better fit of the film domain with the [11$\bar{2}$0]AlN_1 ∥ [1$\bar{1}$0]Si orientation. The substrate surface lattice vector in [110] projection (cosine of the off-axis angle) is shortened compared to the on-axis case. While increasing the off-axis angle the resulting lattice mismatch between the AlN_1 domain and the Si in [110] direction is being decreased in contrast to the AlN_2 domain, where the similar mismatch in [1$\bar{1}$0] projection remains unchanged. By comparison of the DP of the on-axis case in Fig.2b and the DP in Fig.6b it is possible to see that in the off-axis case the ($\bar{1}$101)AlN reflection (arrowed) is aligned with the ($\bar{1}\bar{1}$1)Si reflection (arrowed) which may now has caused a less strained state of the film. It is suggested that an off-axis angle of 6.64° leads to a complete single domain 2H-AlN film structure as that is the value at which the ($\bar{1}$101)AlN and the ($\bar{1}\bar{1}$1)Si reflections are aligned along a symmetry line as marked.

Summary

The influence of the off-axis angle of the Si(001) substrate surface on the heteroepitaxial 2H-AlN film structure were studied by CTEM techniques. On on-axis substrate surfaces three AlN film domains were found: AlN_1 and AlN_2 with [11$\bar{2}$0]AlN_1 ∥ [01$\bar{1}$0]AlN_2 ∥ [1$\bar{1}$0]Si, and AlN_3 with [01$\bar{1}$0]AlN_3 ∥ [100]Si. The c-axis orientation of all 3 film domains are parallel to the c-axis of the substrate: [0001]$AlN_{1,2,3}$ ∥ [001]Si. Using off-axis Si(001) substrates slightly tilted by about 1°, it has been shown that only one of the three film domain orientation (AlN_1) is preferred. Using off-axis Si(001) substrates tilted as far as about 5° towards [110]Si, the 2H-AlN films show an almost single domain (AlN_1) film structure.

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