

MBE growth of cubic AlN on 3C-SiC substrate

Thorsten Schupp^{*1}, Georg Rossbach², Pascal Schley², Rüdiger Goldhahn², Marcus Röppischer³, Norbert Esser³, Christoph Cobet³, Klaus Lischka¹, and Donat Josef As^{**1}

¹Department of Physics, University of Paderborn, Warburger Str. 100, 33095 Paderborn, Germany

²Institut für Physik, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany

³Department Berlin, ISAS – Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin, Germany

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* Corresponding author: e-mail tschupp@mail.uni-paderborn.de, Phone: +49 5251 60 5831, Fax: +49 5251 60 5843

** e-mail d.as@uni-paderborn.de

We present our recent results on the growth of cubic AlN (001) layers by plasma assisted molecular beam epitaxy (PAMBE) using freestanding 3C-SiC (001) substrate. For high-quality c-AlN layers reflection high-electron energy diffraction (RHEED) patterns in all azimuths show RHEED patterns of the cubic lattice, hexagonal reflections are absent. High-resolution X-ray diffraction (HRXRD) measurements confirm the cubic structure of the c-AlN layers with a lattice parameter

of 4.373 Å. Atomic force microscopy (AFM) scans show an atomically smooth surface with a roughness of 0.2 nm RMS. Ellipsometry studies yield the dielectric function (DF) of c-AlN from 1 to 10 eV. The direct gap is determined with 5.93 eV at room temperature, while the indirect one is below 5.3 eV (onset of adsorption). The high-energy part of the DF is dominated by two transitions at 7.20 and 7.95 eV attributed to critical points of the band structure.

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1 Introduction AlN is a group III nitride wide-bandgap semiconductor. It has a large thermal conductivity comparable to copper, a hardness close to sapphire and a high-chemical stability. The metastable cubic (c-) phase of AlN has no polarization electrical fields in growth direction known from hexagonal AlN [1]. With these properties, c-AlN in combination with other group III nitrides like c-GaN and c-InN is suitable for fast high-power electronic and photonic devices [2]. Until recently c-AlN layers had considerable surface roughness, leading to short-circuits and broadening of confined electronic states of low dimensional structures [3, 4]. However, it was demonstrated that the structural and optical properties for c-InN and GaN layers were considerably improved by growing on freestanding 3C-SiC substrate [5, 6]. We report on the plasma assisted molecular beam epitaxy (PAMBE) growth of atomically flat c-AlN layers on freestanding 3C-SiC substrate.

2 Experimental Pseudomorphically strained and relaxed c-AlN layers were grown on freestanding 3C-SiC (001) substrates by PAMBE in a Riber 32 growth chamber.

Ga and Al were evaporated from Riber effusion cells, activated N was supplied by an Oxford Instruments RF plasma source.

The c-AlN nucleation on the 3C-SiC substrate was done under one monolayer (ML) of Al surface coverage. The substrate temperature was 730 °C. The beam flux for Al was $2 \times 10^{14} \text{ cm}^{-2} \text{ s}^{-1}$. The growth was monitored *in situ* by reflection high-electron energy diffraction (RHEED). RHEED specular spot intensity oscillations (RHEED oscillations) have revealed a growth rate of 150 nm h^{-1} [7].

3 Results and discussion

3.1 Growth of cubic AlN The growth procedure started with a deoxidation of the substrate. A RHEED pattern of the unprepared 3C-SiC (001) surface is shown in Fig. 1(a). Surface oxides lead to blurred reflections of the cubic lattice, three-dimensional islands on the surface cause disc shape reflections due to an electron transmission component [7]. After a cleaning process, the RHEED pattern of the 3C-SiC surface in Fig. 1(b) shows long thin streaks indicating a two dimensional oxide free surface with a (2×4) reconstruction and Kikuchi lines. More details concerning the cleaning

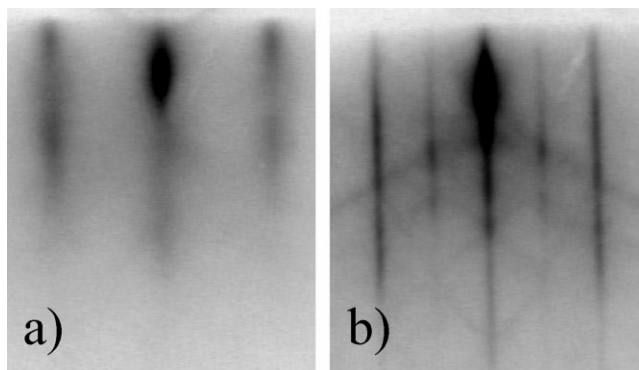


Figure 1 RHEED patterns observed during the cleaning process of the 3C-SiC substrate with Al flashes. (a) $[-110]$ azimuth of the 3C-SiC substrate before Al flashes and (b) $[-110]$ azimuth of the 3C-SiC substrate after Al flashes.

process can be found in Ref. [8]. Because of its metastable nature, exposing a c-AlN surface to nitrogen leads to the formation of hexagonal clusters. Growing Al rich c-AlN with 1 ML Al surface coverage can prevent hexagonal condensation. A model linking the Al surface coverage and RHEED intensity has been developed to maintain 1 ML Al coverage [8, 9].

At the initial growth process, a transition from a 2D to a 3D surface was observed. This is concluded by comparing the RHEED pattern of the substrate in Fig. 1(b) with the RHEED pattern after the deposition of 6 ML of c-AlN in Fig. 2(a). Long streaks are transformed into spotty reflections originating from an electron transmission component through islands on the surface. A second roughness transition was observed after growth of about 20 ML, transforming the surface back to an atomically smooth 2D state, as can be seen in Fig. 2(b). After a smooth surface was established, growth interruptions of 30 s were applied every 20 atomic layers. RHEED oscillations were observed, where every oscillation indicates the growth of one atomic layer. The growth rate was determined to be 0.2 ML s^{-1} . After the growth of 142 nm (650 ML) c-AlN the RHEED pattern as seen in Fig. 2(c) still indicated a smooth 2D surface. Using this method c-AlN layers up to 300 nm thickness have been grown. All azimuths show RHEED patterns of the cubic lattice, hexagonal reflections are absent.

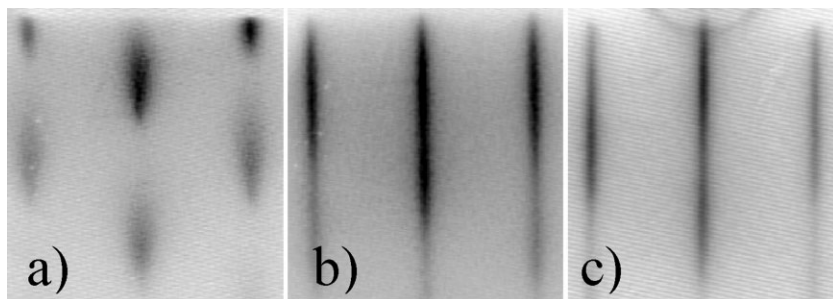


Figure 2 RHEED images of the c-AlN surface during the initial growth process. (a) after the growth of 6 ML, (b) after the growth of 30 ML and (c) after the growth of 650 ML.

3.2 High-resolution X-ray diffraction The cubic structure of the AlN layer is clearly shown by high-resolution-X-ray diffraction (HRXRD) measurements. In Fig. 3, the HRXRD (113) reciprocal space map of a 300 nm c-AlN (001) layer on 3C-SiC (001) can be seen. Number 3 indicates the position of the 3C-SiC Bragg peak, number 1 indicates the position of the c-AlN reflection. The elliptic shape originates from a mosaic structure caused by strain relaxation [10]. The main axis of the ellipse (Fig. 3 number 4) is perpendicular to the reciprocal lattice vector. A small shift of the c-AlN peak along the main axis can be interpreted as tilt of the c-AlN layer versus the substrate. Taking into account the tilt the position of the c-AlN reflection is at Fig. 3 number 2. From reciprocal space maps of c-AlN layers with a thickness between 40 and 200 nm (not shown here) we find that layers below 90 nm are pseudomorphically strained, layers above 120 nm are relaxed. The c-AlN lattice parameter in growth direction extracted from Fig. 3 is $4.373 \pm 0.002 \text{ \AA}$.

3.3 Atomic force microscopy The high-surface quality of the c-AlN layers is verified with atomic force microscopy (AFM). The AFM image of the c-AlN layer in Fig. 4(a) shows an atomically smooth surface with a roughness of 0.2 nm RMS. The respective line scan in Fig. 4(b) depicts a peak-to-valley height of only one lattice constant over a lateral extension of ~ 2000 lattice constants.

3.4 Ellipsometry A commercial ellipsometer was employed for recording the ellipsometric parameters Ψ and Δ under different angles of incidence (Φ : 60, 67 and 74°) in the photon ($\hbar\omega$) energy range from 1 to 6.4 eV. A homemade construction attached to the Berlin Electron Storage Ring for Synchrotron Radiation (BESSY II) allowed measurements of Ψ and Δ under $\Phi = 67.5^\circ$ from 5 to 10 eV with the set-up described in Ref. [11]. The dielectric function (DF) is obtained by a multilayer fitting procedure similar to the approach presented in Ref. [12]. No assumption was made concerning the shape of the DF, i.e. the real (ϵ_1) and imaginary parts (ϵ_2) of the DF were separately fitted for all photon energies.

Figure 5(a) and (b) summarize typical results of the fitting procedure for one of the c-AlN films (layer thickness here was 100 nm). The spectral dependence shows similarities to the recently reported results for the hexagonal

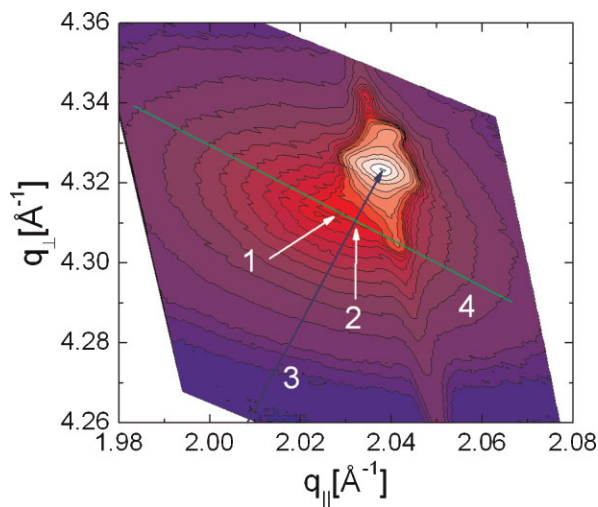


Figure 3 (online colour at: www.pss-a.com) HRXRD reciprocal space map of the (113) reflections of c-AlN and 3C-SiC. (1) Position of the c-AlN peak, (2) position of c-AlN peak after tilt correction, (3) reciprocal lattice vector of 3C-SiC reflection, and (4) axis for tilt correction perpendicular to (3).

counterpart [13], however, the characteristic energies E_0 , E_1 and E_2 differ appreciably.

The imaginary part of the DF exhibits a sharp onset at 5.88 eV which defines the direct excitonic band gap. Adopting the exciton binding energy of 50 meV for the hexagonal AlN [14], we determine the direct band gap (E_0) at the Γ point of the Brillouin zone with 5.93 eV. This result is in excellent agreement to the calculated quasi-particle band gap of 5.86 eV if the lattice polarizability is taken into account [14]. For comparison, previous studies of mixed phase AlN yielded for the zinc-blende compound 5.74 eV [15]. The pronounced absorption tail below 5.88 eV in Fig. 5b is attributed to phonon-assisted indirect absorption. The imaginary part differs appreciably from zero only above 5.3 eV, i.e. this energy defines the upper limit of the indirect band gap. A slightly lower value might be possible as well, but ellipsometry is not sensitive enough in the case of low absorption. Finally, the E_1 and E_2 transition energies at room temperature amount to 7.20 and 7.95 eV, respectively. More results on the optical characterization will be published elsewhere [13].

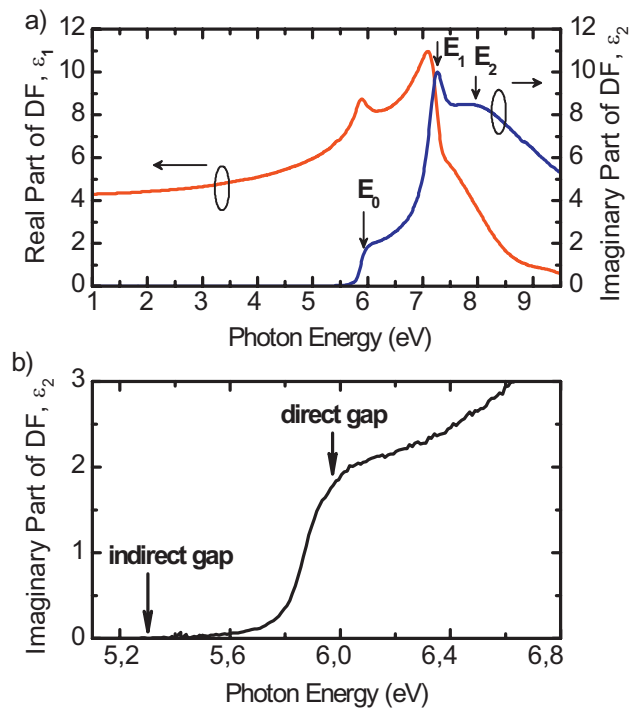


Figure 5 (a) (online colour at: www.pss-a.com) Real and imaginary part of the DF for c-AlN from 1 to 10 eV. (b) Magnification of the behaviour around the absorption edge.

4 Conclusion Atomically smooth c-AlN layers on 3C-SiC substrate have been grown by PAMBE. AFM scans and RHEED patterns verified the smooth surface. HRXRD measurements confirmed the cubic structure of the c-AlN layers with a lattice parameter of 4.373 Å.

Finally, we determined the DF of c-AlN over a large spectral range yielding the direct and indirect band-gap energies at 5.93 eV and about 5.3 eV, respectively.

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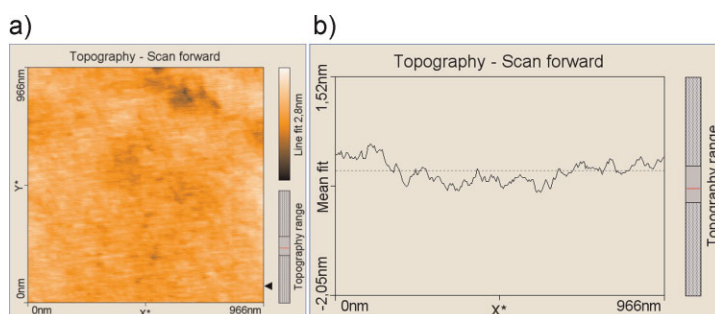


Figure 4 (online colour at: www.pss-a.com) AFM images: (a) $1 \times 1 \mu\text{m}^2$ area of the c-AlN layer with a roughness of 0.2 nm RMS, (b) line scan of Fig. 4(a).

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