Comparative study of 3C-GaN grown on semi-insulating 3C-SiC/Si(100) substrates

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Abstract. Cubic gallium nitride epitaxial layers grown on differently carbonized silicon substrates were studied by high resolution X-ray diffraction. In the case of cubic GaN layers with equal layer thickness an improvement of the layer quality in terms of full width of the half maximum can be achieved by using higher carbonization temperatures. The higher crystalline quality led to an increase of the residual stress in the grown layer. An increase in the thickness of the cubic Gallium Nitride allows to improve the crystallinity and to reduce the residual stress.

Introduction

Non-polar cubic gallium nitride exhibits prospective properties for the fabrication of low noise high frequency transistors based on two dimensional electron gases. Another advantage of the cubic nitrides is the possibility to achieve normally-off devices without extremely thin AlGaN barrier layers, optoelectronic or spintronic devices in configurations were polarization effects are not desired. Cubic GaN can be grown on GaAs [1-4], Si [4, 5] or SiC [2, 6-8] and other substrates (for example see in [1, 2]) using molecular beam epitaxy (MBE) [1-3, 7] or MOCVD [4, 5]. Most of the studies are carried out on conducting substrates, but an important precondition to fabricate high frequency devices is the growth of 3C-GaN on semi-insulating substrates, for example Si or GaAs. The most promising solution to achieve 3C-GaN growth is the conversion of Si(100) into 3C-SiC(100) silicon carbide offering the possibility of higher growth temperatures compared to GaAs(100) substrates and therefore better 3C-GaN quality [4]. The growth of 3C-GaN on semi-insulating silicon offers cost and processing advantages. The most simple method to form 3C-SiC(100) on Si(100) is the conversion of the Si substrate into silicon carbide by a well designed carbonization process [8, 9]. This study represents a comparative investigation of the 3C-GaN layer quality formed on conducting and semiinsulating Si(100) covered with an ultra thin single crystalline 3C-SiC(100) layer.

Experimental

All 3C-GaN layers were grown in a Riber 32 system by plasma assisted MBE under Ga rich growth conditions leading to a Ga coverage of 1 monolayer. Details of the growth procedure are given in [6]. The 3C-SiC(100)/Si(100) pseudosubstrates were fabricated using carbonization in a rapid thermal chemical vapour deposition reactor (RTP) or alternatively with a CVD based carbonization process under UHV conditions. The process conditions used are given elsewhere in [8] and [9] for the RTP and UHVCVD based carbonization, respectively. The carbonization conditions were chosen to form a 3C-SiC(100) layer with a layer thickness of approximately 3 nm independent on the carbonization method. In case of UHVCVD based carbonisation two different types of 3C-SiC(100) layers were formed, in the first case a conducting (sample AS2) and in the second case an insulating (sample PC490a) 3C-SiC(100) layer.

The morphological and structural properties of the both cubic GaN epitaxial layers and the used pseudosubstrates were investigated by atomic force microscopy (AFM), reflection high energy electron diffraction (RHEED) and ellipsometry. The surface roughness of the samples was determined using a 5x5 μm^2 scan. Additionally, the 3C-GaN layers were studied by high resolution X-ray diffraction (HRXRD) and reciprocal space mapping (*rsm*).

Results and Discussion

The RHEED patterns taken from the three types of carbonized layers show nearly the same features. They consist of large diffuse spots indicating a smooth single crystalline 3C-SiC(100). A typical RHEED is shown in Figs. 1a. The roughness of the conducting 3C-SiC(100) layer formed by UHVCVD carbonization was roughly two times larger than in case of the semi-insulating 3C-SiC(100) layer exhibiting values of 0.54 and 0.28 nm, respectively (Table 1). The RTP carbonization (sample BC7) exhibit a similar value of the surface roughness as the 3C-SiC layer formed in the case of the conducting 3C-SiC UHVCVD layer, namely 0.69 nm. The differences in the surface roughness indicate slightly changed nucleation and growth conditions during the carbonization process depending on the chosen process and the layer properties. Nevertheless, all fabricated pseudosubstrates exhibit a step like surface morphology (Fig. 1b) and single crystalline 3C-SiC(100) structure (Fig. 1a). Independent on the used pseudosubstrate the surface structure after the epitaxial growth exibit a c(2x2)-Ga surface reconstruction on the terraces and three dimensional diffraction features (Fig. 2a) indicating a finite surface roughness which was determined by AFM measurements to be 6 nm. The morphology of the 3C-GaN epitaxial layer showed no remarkable differences in dependence on the used pseudosubstrate as summarized in Table 1. A typical surface morphology of the grown 3C-GaN is shown in Fig. 2b.

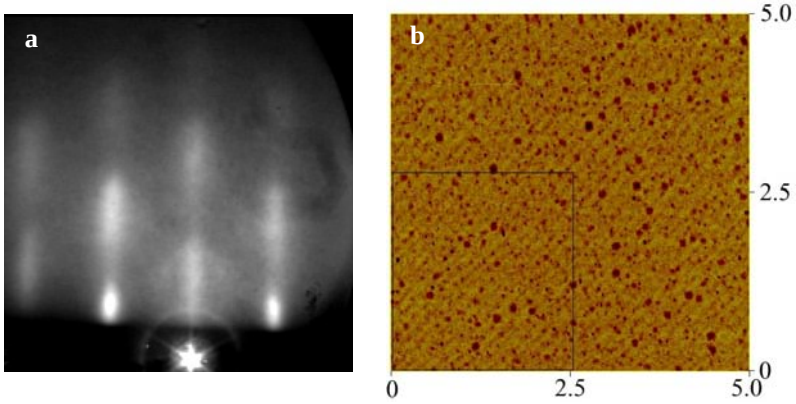

Fig. 1: Typical RHEED (a) and AFM (b) pattern taken from the carbonized silicon sample 1716 (BC7).

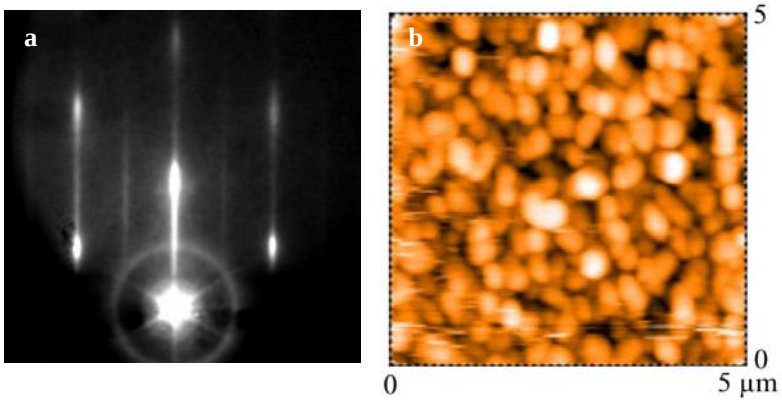

Fig. 2: Typical RHEED (a) and AFM (b) pattern taken from a 3C-GaN layer grown on 3C-SiC/Si(100) wafer

XRD rocking curve and *rsm* measurements of the symmetric (002) and asymmetric (224) X-ray diffraction ~~a~~ revealed a dependence of the crystallographic layer properties reflected by the full width of the half maximum (FWHM). The results are summarized in Table 1. The FWHM in the RTP case (sample 1716 (BC7)) was found to be approximately 15% narrower then in the UHVCVD cases. Thus the defect density is not improved by an improved surface roughness and it seems to be, that a well defined rough surface morphology of the initial pseudosubstrate can be beneficial to improve the growth of cubic GaN on 3C-SiC(100)/Si(100) and to accelerate the dislocation annihilation. Another parameter which might positively affect the nucleation and growth condition is the higher carbonisation temperature used in the RTP case (1280°C compared to 1000°C in the UHVCVD technique) which may lead to a denser silicon carbide lattice. Beside the design of the

properties of the pseudosubstrate with respect to the surface morphology and the crystallinity, the thickness of the grown layer can be used to reduce the dislocation density and to improve the quality of the epitaxial layer. In the present case this can be concluded by comparing the FWHMs and the *rsm's* of the samples 1707 (PC490a) and 1715 (PC490a). This two epitaxial layers differ only in their thickness. The *rsm* of the 620 nm thick epitaxial layer (sample 1715 (PC490a)) shows the typical features of the thinner epitaxial layers a nearly symmetric diffraction spot consiting of a streak along [001] due to the crystal truncation rod (CTR) and two additional streaks along two different directions (Fig. 3). The measured angle between these two remaining streaks and the surface normal, i.e. the CTR, was determined to be approximately 54° which corresponds to the angle between the (111) and (100) plane (54.74°). Thus, this streaks originate from stacking faults and their associated partial dislocations in the {111} planes. In the thinner epitaxial layers the defects are nearly evenly distributed in the different {111} plane whereas in case of the thicker 3C-GaN layer one direction is very weakly present. This means that the defect elimination occurs along a certain direction and led to assymetries in the defect distribution.

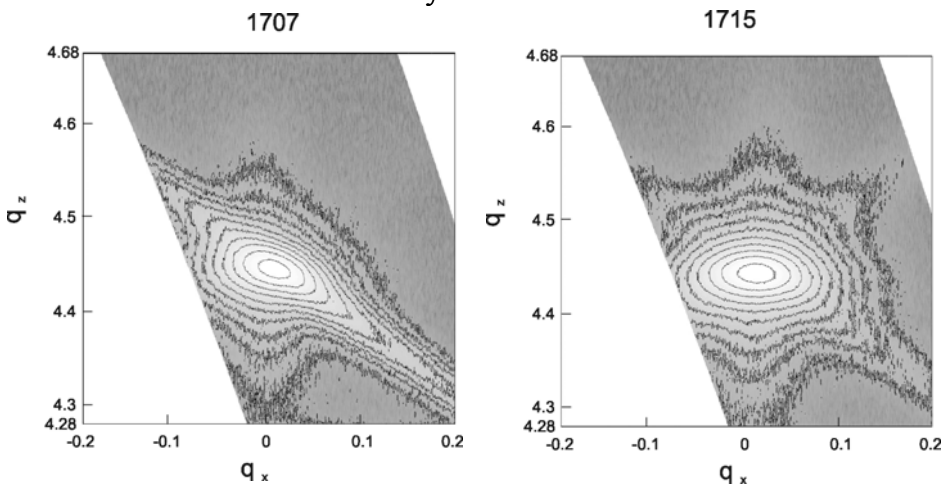

Fig. 3: Reciprocal space maps of the symmetric (002) diffraction peak in case of a 1050 nm (1707) and 630 nm (1715) thick 3C-GaN epitaxial layer.

Surface roughness, epitaxial layer thickness and full width of the half maximum (FWHM) of the (200) and (224) diffraction peaks and the *in plane* and *out of plane strain* Table 1

	1707 (PC490a)	1715 (PC490a)	1716 (BC7)	1717 (AS2)
Substrate roughness, nm	0.28	0.28	0.69	0.54
$FWHM_{200}$	0.78°	0.87°	0.71°	0.82°
$FWHM_{224}$	0.50°	0.68°	0.56°	0.57°
$\varepsilon_{\parallel}$	0.00316	0.00581	0.00622	0.00337
$\varepsilon_{\perp}$	-0.00211	-0.00265	-0.01196	-0.00146
Epilayer roughness, nm	11.0	6.0	6.0	6.0
Epilayer thickness, nm	1050	630	610	620

The unstrained lattice constant was assumed to be $a_{GaN} = 4.5027$ nm [10]

The analysis of the symmetric (002) and asymmetric (224) diffraction peaks revealed that all layers are biaxial strained with a tensile *in plane* strain. Furthermore, the reduced FWHMs and therefore, the improved crystallographic properties of the grown layers is accompanied by an increased residual strain in the 3C-GaN epitaxial layer. This residual strain can be lowered if the layer thickness is increased as evident from the data of the *in plane* and *out of plane* strain, i.e. $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$, respectively. The residual tensile strain results from the misfit of the lattice constants and the thermal mismatch between GaN/SiC and Si.

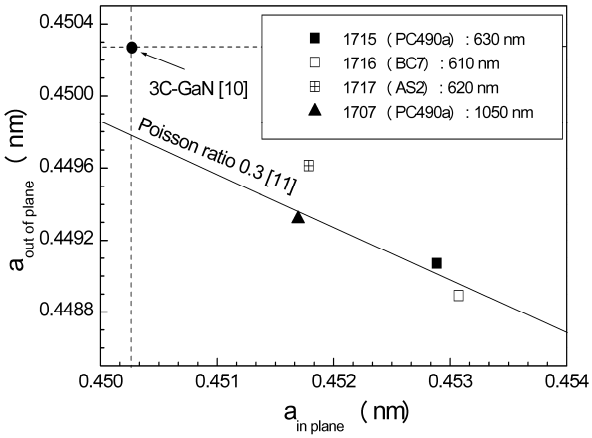

Fig. 4: Coupling of the *in plane* and *out of plane* lattice constants measured by HRXRD.

The interrelationship between the *in plane* and *out of plane* lattice constants is shown in Fig. 4. For biaxial strained layers the lattice distortions in vertical and lateral direction are coupled by the Poisson ratio and have to follow a linear relation ship between the strained and unstrained values. None of the samples follows this rule and on all samples a hydrostatic pressure is present resulting in a decreasing effective volume of the 3C-GaN. This might be due to an increased defect density in the layer, originating from the interface, and a substantial concentration of nitrogen vacancies. Investigations about its origin are in progress.

Summary

The influence of differently prepared 3C-SiC(100) pseudo-substrates on the crystalline properties of 3C-GaN was investigated. An improved epitaxial layer was achieved using higher carbonization temperatures and a slightly rougher morphology. The improvement of the crystallinity is accompanied with an increase of the residual strain.

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