Step-controlled homoepitaxial growth of 4H-SiC on vicinal substrates

Birgit Kallinger[a,*], Patrick Berwian[a], Jochen Friedrich[a], Bernd Thomas[b,1]

[a] *Department of Crystal Growth, Fraunhofer IISB, Schottkystr. 10, 91058 Erlangen, Germany*

[b] *SiCED Electronics Development, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany*

Abstract

A comprehensive study on the step-controlled homoepitaxial growth on the (0001)Si-face of vicinal 4H-SiC substrates was performed in order to establish epitaxial growth on 2° towards $\langle 11\bar{2}0\rangle$ off-cut substrates and 4° towards $\langle 1\bar{1}00\rangle$ off-cut substrates. A standard epitaxial growth process was developed by optimizing the growth temperature T, Si/H ratio and C/Si ratio for growth on 4° towards $\langle 11\bar{2}0\rangle$ off-cut substrates. Thereby, step-controlled epitaxial growth was achieved within a broad operating window. The surface roughness of such epilayers varies typically between rms = 0.5 nm and rms = 2.5 nm and step-controlled growth is conserved even at a growth rate of 27 μm/h. Then, the standard growth process was applied to substrates with different off-cut angles α of 2°, 4° and 8° as well as with different off-cut directions $\langle 11\bar{2}0\rangle$ and $\langle 1\bar{1}00\rangle$. The step-controlled growth was achieved also within a wide range of Si/H ratio and C/Si ratio for growth on 8° and 4°

*Corresponding author; telephone: +49 9131-761-273; fax: +49 9131-761-280

Email address: birgit.kallinger@iisb.fraunhofer.de (Birgit Kallinger)

[1] present address: Dow Corning Semiconductor Solutions, 5300 Eleven Mile Road, Auburn, MI 48611, USA

off-cut substrates, but the process window narrows strongly for growth on 2° off-cut substrates. The epilayers' surface roughness increases with decreasing off-cut angle of the substrate. Epilayers grown on 4° towards $\langle 1\bar{1}00\rangle$ off-cut substrates were significantly smoother than epilayers grown on 4° towards $\langle 11\bar{2}0\rangle$ off-cut substrates. No influence of the substrates' off-cut angle and direction on the growth rate was found. The experimental results of this comprehensive study are discussed globally in consideration of other relevant publications.
Keywords: A1. Surface Roughening, A3. Chemical Vapor Deposition, A3. Hot-wall epitaxy, B1. Silicon Carbide

---

1. Introduction

4H-Silicon Carbide (4H-SiC) is the preferred material for energy-efficient, high voltage power electronic devices due to its outstanding material properties such as the large electronic band gap and high electric breakdown field. For the production of such devices, homoepitaxial layers with good crystalline quality and minimum surface roughness have to be grown at growth rates as high as possible in order to reduce the production costs of epilayers. 4H-SiC homoepitaxial layers are commonly grown by chemical vapor deposition (CVD). Due to the temperature range of CVD growth and the existence of various SiC polytypes, homoepitaxial growth along the $\langle 0001\rangle$ direction of the crystal, i.e. reproducing the polytype of the substrate to the epilayer, is only possible by step-controlled growth [1]. This is achieved by the use of vicinal substrates, i.e. substrates with a certain off-cut angle α towards a distinct (low index) direction. Vicinal substrates provide growth steps al-

ready in the beginning of the epitaxial growth. These growth steps are lying perpendicular to the substrate's off-cut direction, i.e. the step-flow direction coincides with the substrate's off-cut direction [2, 3]. A low index off-cut direction, such as $\langle 11\bar{2}0\rangle$ and $\langle 1\bar{1}00\rangle$, of the substrate leads to the formation of straight growth steps during epitaxial growth [2–4]. CVD growth of 4H-SiC epilayers was originally performed on 8° towards $\langle 11\bar{2}0\rangle$ off-cut substrates because of the resulting low surface roughness of epilayers. By the market launch of 3 inch substrates in 2004, the standard off-cut angle of commercially available substrates was lowered to 4° to reduce the material loss during substrate preparation from the crystal boules; but the surface roughness of epilayers on 4° off-cut substrates increased in comparison to epilayers grown on 8° off-cut substrates [4]. A further reduction of the substrate's off-cut angle to 2° is still under discussion for 150 mm substrates. Therefore, it is of great interest to study the impact of the substrates' off-cut on the step-controlled growth, the surface roughness and the growth rate.

During CVD growth on vicinal substrates, step-controlled growth is conserved as long as heterogeneous nucleation of 2D nuclei on the growth terraces is avoided. Heterogeneous nucleation occurs if the supersaturation on a growth terrace becomes too high, resulting in polycrystalline growth of the epilayer. The transition from step-controlled growth to polycrystalline growth is described in the theory by Burton, Frank and Cabrera [5] (called BCF theory hereafter), which was already adapted to SiC homoepitaxial growth by Matsunami and Kimoto [6]. Based on the BCF theory, the transition criterion between step-controlled and polycrystalline growth can be

written as follows (Equation 1):

$$\lambda \geq w/2 \tag{1}$$

with the diffusion length λ of the reactive species on the growth surface and the terrace width w of growth steps. As long as the reactive species are able to diffuse to a growth step, step-controlled growth takes place. Otherwise, heterogeneous nuclei form on the growth terraces. The diffusion length λ is mainly a function of the process parameters growth temperature T and the mass transport of reactive species to the growth surface, i.e. the concentration of Si-containing precursor in the process gas (Si/H ratio) and the mixture of C- and Si-containing precursors (C/Si ratio) [6].

In contrast to that, the terrace width w is mainly dependent on the off-cut angle α of the substrate:

$$w = \frac{h}{\tan \alpha} \tag{2}$$

with the height of growth steps h. Assuming a microstep height $h = c/4$ = 0.252 nm for 4H-SiC (with lattice parameter c = 1.008 nm [7]), the (theoretical) terrace width w increases strongly with decreasing off-cut angle α of the substrate from $w(8°) = 1.8$ nm to $w(4°) = 3.6$ nm and $w(2°) = 7.2$ nm. But a detailed analysis of the step height and terrace width of epilayers grown on substrates with different off-cut angles revealed [1] that even larger step heights and terrace widths occur as several microsteps can agglomerate to macrosteps, which is known as step bunching. The tendency of forming macrosteps becomes more severe with decreasing off-cut angle of the substrate [4] which suggests that step bunching is driven by the minimization of the surface free energy [8]. In the case of step bunching, the step geometry,

i.e. the h/w ratio according to the substrate's off-cut angle, is conserved. Therefore, the effect of step bunching on the step geometry (h/w = const.) is fundamentally different from the effect of different substrate off-cut angles on the step geometry ($h/w \neq$ const, compare Equation 2).

It is already known [1, 4] that step bunching becomes more pronounced for C-rich growth conditions (increasing C/Si ratio). It was suggested [9] that this kind of step bunching is kinetically driven due to the specific step velocities of microsteps, i.e. faster microsteps are able to catch up to slower growth steps and become pinned.

In summary, the terrace width w depends primarily on the off-cut angle α of the substrate and secondarily on the degree of step bunching. In the case of wide growth terraces, i.e. for growth on substrates with small off-cut angle and/or pronounced step-bunching, the formation probability of heterogeneous nuclei becomes more severe. In order to keep step-controlled growth for a proper polytype reproduction in the epilayer, the process parameters such as growth temperature T, Si/H ratio and C/Si ratio have to be carefully adapted to the terrace width w: a high growth temperature and suitable mass transport (Si/H and C/Si ratios) should be chosen to facilitate the diffusion of reactive species on the growth surface. The rms value of the surface roughness can be used as a measure for step bunching [4, 10].

Very few papers are dealing with homoepitaxial growth on vicinal substrates with different off-cut directions. No significant difference was found for growth on the (0001)Si-face of 8° off-cut substrates with off-cut directions $\langle 11\bar{2}0\rangle$ and $\langle 1\bar{1}00\rangle$ with respect to growth rate [2] and surface roughness [2, 3], i.e. all epilayers were very smooth with typical rms values < 0.25 nm [3] and

rms < 0.8 nm [2], respectively.

The maximum achievable growth rate within step-controlled growth depends also on the process parameters, including growth temperature T, C/Si ratio and Si/H ratio, and the substrate's off-cut angle. The growth temperature T influences the basic chemical reactions such as thermal cracking of precursor molecules and the formation of SiC from reactive Si- and C-containing species on the growth surface, as well as the diffusion of reactive species on the growth surface and the adsorption and desorption rates of reactive species to/from the growth surface. These reactions compete with each other, resulting in three temperature-dependent growth regimes: at very low growth temperatures, polycrystalline growth occurs as the diffusion length of reactive species is too short to reach the growth steps ($\lambda < w/2$). For low growth temperatures, the thermal cracking of precursors as well as the formation of SiC are inefficient. These processes become more efficient with increasing growth temperature, resulting in an increasing growth rate within the kinetically limited growth regime. At medium growth temperatures, the growth rate becomes independent of the growth temperature because growth is no longer limited by reaction rates, but by the transport of species. The growth rate depends mainly on Si/H and C/Si ratios in this transport-limited regime. At higher growth temperatures, the growth rate decreases again with increasing growth temperature as the desorption of reactive species from the growth surface becomes more pronounced, i.e the growth rate is desorption limited.

Within the transport- and desorption-limited growth regimes, the growth rate is proportional to the mass transport to the growth surface, i.e. the C/Si

and the Si/H ratios. At a very small C/Si ratio $\ll 1$, Si droplets form on the growth surface due to the lack of C species. The lack of C species at low C/Si ratios < 1 can reduce the growth rate up to 50% [1, 4]. The growth rate becomes maximum and independent of the C/Si ratio for medium C/Si ≥ 1. At large C/Si ratios $\gg 1$, polycrystalline growth occurs due to the high supersaturation of Si and C species on the growth terraces. Additionally, the C/Si ratio is a very important growth parameter also for the dopant incorporation during epigrowth due to the site-competition effect [11, 12].

The concentration of Si-containing precursor in the process gas, given by the Si/H ratio, is the most important growth parameter with respect to the growth rate in the transport- and desorption-limited growth regimes. Under such growth conditions, the growth rate increases proportionally to the Si/H ratio [1].

The aim of this work is to investigate step-controlled growth on 2° towards $\langle 11\bar{2}0 \rangle$ and 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates. Therefore, a standard growth process was developed for growth on the (0001)Si-face of 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates by investigating certain process parameters, i.e. growth temperature T, C/Si and Si/H ratios. These results are presented in section 3.1. Then, the standard growth process is applied to substrates with different off-cuts in section 3.2.

2. Experimental

2.1. 4H-SiC vicinal substrates

Homoepitaxial 4H-SiC layers were grown on the (0001)Si-face of commercially available 3 inch vicinal substrates with different off-cuts: standard

substrates with 4° off-cut towards $\langle 11\bar{2}0 \rangle$ direction, substrates with 2° or 8° off-cut towards $\langle 11\bar{2}0 \rangle$ direction or 4° off-cut towards $\langle 1\bar{1}00 \rangle$ direction. The Si-face of all substrates was epi-ready polished with a remaining surface roughness $R_a \leq 2$ nm. For each epigrowth series (see below), adjacent substrates cut from one crystal boule were used.

2.2. Growth process

Homoepitaxial growth by means of chemical vapor deposition (CVD) was carried out in a horizontal hot wall reactor (EPIGRESS VP508 GFR) equipped with gas foil rotation (GFR) as described in [13]. Silane (SiH_4) and propane (C_3H_8) act as precursors and hydrogen (H_2) as carrier gas. At the beginning of the growth process, the substrate is heated under H_2 atmosphere and in-situ etched under ($H_2 + C_3H_8$) atmosphere. When the desired growth temperature T is reached, the epilayer growth starts by introducing the precursor gases and is stopped by switching off the precursor gas flows. After growth, the substrate cools down under H_2 atmosphere. The parameters growth temperature T, Si/H and C/Si ratio were varied systematically for the use of different vicinal substrates within several growth series. The process pressure and the carrier gas flow were kept constant for all experiments. The total gas flow is considered to be equal to the carrier gas flow as the precursor gas flows are negligibly small compared to the carrier gas flow. The exact growth conditions of all series are summarized in table 1.

In all growth series A-G, the C/Si ratio was varied by adapting the propane flow while keeping the silane flow constant. In series D, the C/Si ratio could not exceed 1.15 due to the flow range of the silane and propane mass flow controllers. All epilayers were intentionally doped with nitrogen

gas (N_2) to obtain n-type epilayers with a net carrier concentration in the order of low 10^{15}cm^{-3}.

2.3. Characterization of epilayers

The epilayer thickness and thickness inhomogeneity was measured by Fourier transformed infrared spectrometry (FTIR) at 9 measurement points, which are regularly distributed across the wafer area. All epilayers were about 10 μm thick with a typical thickness inhomogeneity of σ/mean $\leq$ 12 %. The growth rate R was calculated based on the mean epilayer thickness and the growth duration. The error bars on the growth rate result from the inhomogeneity of the epilayer thickness.

The surface morphology of epilayers was investigated by Atomic Force Microscopy (AFM) on large areas (10 $\times$ 10 μm^2). To determine the surface roughness of epilayers, several small areas (each 1 μm^2) were scanned per epilayer at the wafer center and at half of the wafer radius. A mean rms value as well as its deviation (Δ = max-min) were deduced from these measurements. The deviation Δ from the mean rms value of a sample is displayed as error bars.

3. Results

3.1. Standard growth process on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates

In order to develop a standard growth process on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates, the process parameters such as growth temperature T, C/Si ratio and Si/H ratio were varied systematically. The results of these growth series A-D are presented in the following subsections.

3.1.1. Growth temperature

In series A, the growth temperature T was varied from 1450 °C to 1700 °C in 50 °C steps at fixed C/Si and Si/H ratios of 0.9 and 1.1×10^{-3}, respectively. Polycrystalline growth occurs at the lowest growth temperature T = 1450 °C. Here, the diffusion length λ of the Si- and C-species on the growth surface is too short to reach the growth steps ($\lambda < w/2$) resulting in 2D nucleation on the growth terraces.

For all growth temperatures T > 1450 °C, step-flow growth takes place as can be seen from the surface morphology of the epilayers, shown in figures 1a and 1b. The surface morphology of all these epilayers is characterized by parallel, straight growth steps lying perpendicular to the off-cut direction of the substrates (indicated by arrows in figures 1a and 1b). For growth temperatures T > 1450 °C, the growth species have a sufficiently large diffusion length ($\lambda > w/2$) to reach the growth steps. Therefore, step-flow growth governs the homoepitaxial growth under these growth conditions. The surface roughness of these epilayers, i.e. the rms values obtained from AFM measurements, increases steadily with increasing growth temperature from rms = 1.0 nm (at T = 1500 °C) to rms = 2.0 nm (at T = 1700 °C).

The growth rate depends on the growth temperature T as shown in figure 1c. For low growth temperatures of 1450 °C (polycrystalline growth) and 1500 °C (step-flow growth), the growth rate increases with increasing temperature, i.e. the growth rate is kinetically limited [1]. For growth temperatures of 1550 °C and 1600 °C, the growth rate remains constant at 14.5 μm/h. Within this temperature range, the growth rate is transport limited as the growth rate depends only on the precursor supply. For growth tem-

peratures T $\geq$ 1650 °C, the growth rate decreases again as the desorption rate of growth species from the substrate surface increases with increasing temperature, i.e. the growth rate is desorption limited.

It is known being beneficial for highly supersatured growth [1], i.e. for high precursor gas flows and/or for growth on wide terraces of 4° and 2° off-cut substrates, to work in the desorption limited regime. Therefore, a growth temperature of 1650 °C was chosen for subsequent growth series B-F.

3.1.2. C/Si ratio

In series B, the influence of the C/Si ratio on the growth morphology and the growth rate was investigated for a fixed Si/H ratio of 1.1×10^{-3} at a growth temperature T = 1650 °C. The C/Si ratio was varied in the range between 0.6 and 1.65. For C/Si ratios between 0.6 and 1.5, the epilayers grow in step-flow growth mode and exhibit specular surface morphology. For the C/Si ratio of 1.65, polycrystalline growth occurs instead of step-flow growth due to the high supersaturation on the growth terraces.

The surface roughness of these epilayers increases with increasing C/Si ratio from rms = 0.25 nm (C/Si = 0.6) to rms = 2.25 nm (C/Si = 1.5) as shown in figure 2a, i.e. step-bunching becomes more pronounced for C-rich growth conditions.

The impact of the C/Si ratio on the growth rate R is shown in figure 3. For the lowest C/Si ratio of 0.6, the growth rate is about 5% smaller than for C/Si ratios in the range from 0.75 to 1.2 due to the lack of C-species at low C/Si ratios.

3.1.3. Si/H ratio

In series B, C and D, the Si/H ratio is varied from 0.6 $\times 10^{-3}$ (series C) to 1.1 $\times 10^{-3}$ (series B) and 2.2 $\times 10^{-3}$ (series D) as well as the C/Si ratio from 0.6 to 1.5 (for series D: C/Si $\leq$ 1.15), respectively. All these epilayers were grown in step-flow growth mode at T = 1650 °C and exhibit specular surfaces. The resulting rms values of the epilayers' surface roughness of series B, C and D are plotted versus the C/Si ratio in figure 2a. For each C/Si ratio, the rms values obtained from epilayers grown at different Si/H ratios fit within experimental deviation, i.e. the Si/H ratio plays a minor role for the epilayer surface roughness. For increasing C/Si ratio, the rms values of the surface roughness increase linearly, i.e. the C/Si ratio is the dominating factor with regard to the surface roughness.

The influence of the Si/H ratio on the growth rate R is shown in figure 2b for three different C/Si ratios. The growth rate R increases linearly with the Si/H ratio and the C/Si ratio has a much smaller impact on the growth rate (for same Si/H ratio). These results show clearly, that the growth rate is mainly determined by the mass transport of Si-containing species to the growth interface at a growth temperature of 1650 °C. On 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates, step-controlled growth is conserved even at a growth rate of 27 μm/h.

3.2. Growth studies on different vicinal substrates

The standard growth process for 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates (series B) is now applied to substrates with different off-cuts (series E1 and F1 for 8° and 2° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates and series G for 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates, respectively). In order to investigate the influence

of the substrate's off-cut angle α on the growth rate R, the Si/H ratio as well as the C/Si ratio is varied in series E2 and F2 for 8° and 2° towards $\langle 11\bar{2}0\rangle$ off-cut substrates, respectively.

3.2.1. Growth on 8° towards $\langle 11\bar{2}0\rangle$ off-cut substrates

In series E1, the standard growth process originally developed for 4°C off-cut substrates is applied to 8° towards $\langle 11\bar{2}0\rangle$ off-cut substrates. All epilayers of series E1 are grown in step-flow growth mode and exhibit specular, smooth surfaces. The surface morphology of these epilayers on 8° off-cut substrates is characterized by microsteps as shown in figure 4a. The surface roughness of these epilayers increases slightly from rms = 0.3 nm (C/Si = 0.6) to rms = 0.6 nm (C/Si = 1.5) with increasing C/Si ratio.

In series E2, the Si/H ratio is varied while keeping C/Si = 0.75. The growth rate changes from R = 7 μm/h (Si/H = 0.6 $\times 10^{-3}$) to R = 27 μm/h (Si/H = 2.2 $\times 10^{-3}$). Smooth epilayers with specular surfaces are obtained as can be seen from low rms values $<$ 0.5 nm, i.e. step-flow growth is governed by microsteps even at a high growth rate of 27 μm/h. The growth rates observed for growth on 8° off-cut substrates (series E1 and E2) fit very well the results of comparable series B-D on 4° off-cut substrates.

3.2.2. Growth on 2° towards $\langle 11\bar{2}0\rangle$ off-cut substrates

In series F1, the standard growth process is applied to 2° towards $\langle 11\bar{2}0\rangle$ off-cut substrates. At C/Si = 0.75, the epilayer is grown in step-flow mode (as can be seen in figure 4b) and exhibits a specular surface across the whole wafer area. Most of the growth steps are straight, but some are wavy. This could be due to beginning growth instabilities because of the high supersat-

uration. At higher C/Si = 0.9, step-flow growth takes place at the center of the wafer, but instable growth occurs at the wafer edge. For C/Si = 0.9, the supersaturation on the growth terraces is too high, i.e. the growth species can no longer reach the growth steps ($\lambda < w/2$) and 2D nucleation happens on the large growth terraces of 2° off-cut substrates. Therefore, the C/Si ratio is not further increased for growth on 2° off-cut substrates.

The surface roughness of these epilayers increases from rms = 1.2 nm to rms = 1.7 nm with increasing C/Si ratio of 0.75 and 0.9, respectively, i.e. step-bunching becomes more pronounced for C-rich growth conditions on 2° off-cut substrates.

In series F2, a lower Si/H ratio of 0.6×10^{-3} is applied than in series F1. The two epilayers grown at C/Si ratio of 0.75 and 0.9 are grown in step-flow growth mode and exhibit specular surfaces across the whole wafer area. Lowering the mass transport, i.e. the Si/H as well as the C/Si ratio, stabilizes the step-flow growth mode on the 2° off-cut substrate, but lowers the growth rate from R = 13 μm/h (series F1) to R = 7 μm/h in series F2. These growth rates obtained on 2° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates fit very well the results on 4° and 8° off-cut substrates (compare series B-E).

3.2.3. Growth on 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates

In order to investigate the influence of the off-cut direction on the epilayer morphology and the growth rate, the standard epigrowth process (series B) is applied to 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates (series G). In contrast to all other epigrowth series (series B-F: T = 1650°C), a lower growth temperature T = 1600°C was applied in series G in order to investigate step-flow growth also in the transport limited regime. To be able to compare the growth re-

sults obtained on 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates with the results on standard substrates, growth on both types of substrates is conducted simultaneously (two half substrates with different off-cut directions are used in some experiments, called dual seed experiments hereafter).

All epilayers grown at C/Si ratio between 0.6 and 1.35 are grown in step-flow growth mode as can be seen from the exemplary surface scan in figure 4c. The straight growth steps are lying parallel to each other and perpendicular to the off-cut direction $\langle 1\bar{1}00 \rangle$ (as indicated by arrow in figure 4c), i.e. the step-flow direction coincides with the off-cut direction of the substrate. At C/Si = 1.5, polycrystalline growth occurs, indicating a slightly smaller operating window with regard to the C/Si ratio for growth on 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates than for 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates.

The surface roughness of these epilayers increases steadily with increasing C/Si ratio from rms = 0.4 nm (C/Si = 0.6) to rms = 0.9 (C/Si = 1.35), indicating that step-bunching becomes more pronounced for C-rich growth conditions as observed for $\langle 11\bar{2}0 \rangle$ off-cut substrates. The epilayers grown on 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrates are significantly smoother than those on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates, i.e. for a dual seed experiment at C/Si = 0.9, the rms value of the epilayer on a standard substrate amounts to rms = 1.0 nm, but only to rms = 0.6 nm for the epilayer on a 4° towards $\langle 1\bar{1}00 \rangle$ off-cut substrate.

4. Discussion

4.1. Comparison of epilayers' surface roughness

The influence of growth parameters on the growth morphology and the epilayers' surface roughness was investigated in series A-D for growth on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates. The surface roughness of these epilayers varies from rms = 0.5 nm to rms = 2.5 nm, which is the characteristic range of surface roughness for epitaxial growth on standard substrates. Among the investigated process parameters, the C/Si ratio has the strongest impact on the surface roughness of epilayers. The rms values range from rms = 0.5 nm (C/Si = 0.6) to rms = 2.25 nm (C/Si = 1.5), which is in good qualitative and quantitative agreement to the results of Chen and Capano [4].

The impact of the substrate's off-cut on the surface roughness of epilayers is shown for different C/Si ratios in figure 5. For all epigrowth series on different vicinal substrates, the rms value of the surface roughness increases with increasing C/Si ratio, i.e. step-bunching becomes generally more pronounced for C-rich growth conditions due to specific step velocities of microsteps (kinetically driven step bunching) [9]. These experimental results fit very well those of other groups [2–4].

Although the epilayers' surface roughness increases with increasing C/Si ratio for all kinds of substrates, the quantitative analysis of rms data reveals significant differences between epilayers grown on substrates with different off-cuts: For decreasing off-cut angles α of substrates with off-cut direction $\langle 11\bar{2}0 \rangle$, the rms values generally increase. For example, the surface morphology of all epilayers grown on 8° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates is characterized by microsteps, resulting in a very low surface roughness of rms < 0.5

nm irrespective of the growth rate. This finding agrees well to the results of other groups [2, 3]. For use of 4° towards $\langle 11\bar{2}0\rangle$ off-cut substrates, the epilayer grown at C/Si = 0.6 is quite smooth with rms $<$ 0.5 nm, which is comparable to epilayers grown on 8° off-cut substrates. But the rms values of 4° off-cut epilayers show a steep increase with increasing C/Si ratio as macrosteps occur instead of microsteps. An even stronger increase of the epilayers' rms values with increasing C/Si ratio is observed for growth on 2° off-cut substrates. In summary, the trend lines to the rms values for epilayers grown on substrates with different off-cut angles become steeper with decreasing off-cut angle α, i.e. step-bunching becomes more pronounced for decreasing off-cut angle α of the substrate as reported by Chen and Capano [4].

For epilayers grown on 4° off-cut substrates with different off-cut directions $\langle 11\bar{2}0\rangle$ and $\langle 1\bar{1}00\rangle$, the epilayers' surface roughness differs significantly as proven in dual-seed experiments. Epilayers grown on 4° towards $\langle 1\bar{1}00\rangle$ off-cut substrates are significantly smoother than those on 4° towards $\langle 11\bar{2}0\rangle$ off-cut substrates. Therefore, step-bunching is less pronounced for the $\langle 1\bar{1}00\rangle$ step-flow direction. No such difference was found in epigrowth studies on 8° towards $\langle 1\bar{1}00\rangle$ off-cut substrates [2, 3].

For growth of smooth epilayers, a low C/Si ratio as well as a large off-cut angle of the substrate should be chosen. If 4° off-cut substrates are to be used, the $\langle 1\bar{1}00\rangle$ off-cut direction is preferable for growth of smooth epilayers.

4.2. Growth rate on vicinal substrates

Within the transport- and desorption-limited growth regimes, the growth rate R is mainly determined by the mass transport to the growth surface,

i.e. the Si/H and the C/Si ratio. As shown in figure 2b, the Si/H ratio has a larger impact on the growth rate R than the C/Si ratio.

Moreover, the influence of the substrate's off-cut angle α on the growth rate is investigated for series B-F. The growth rate R is plotted versus the substrate's off-cut angle for different Si/H ratios in figure 6. It can be seen that substrate's off-cut angles from $\alpha = 2°$ up to 8° do not influence the growth rate R.

5. Conclusions

A comprehensive study on the CVD growth on the (0001)Si-face of 4H-SiC vicinal substrates was performed. The influence of different process parameters and substrate off-cuts on the step-flow growth and on the growth rate was investigated. On 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates, step-controlled growth takes places for growth temperatures T >1450 °C. Three temperature-dependent growth regimes were identified, and the influence of the mass transport on the growth rate was investigated for the transport- and desorption-limited growth regimes. For a growth temperature of T=1650 °C, the Si/H ratio mainly determines the growth rate on all vicinal substrates. Growth rates up to 27 μm/h were achieved on 8° and 4° off-cut substrates. The C/Si ratio has a minor impact on the growth rate, but it is the main influencing factor for the surface roughness of epilayers. The epilayers' surface roughness increases strongly with increasing C/Si ratio, i.e. step bunching becomes more pronounced under C-rich growth conditions. The epilayers' surface roughness also depends on the substrates' off-cut: For the decreasing off-cut angle α, the surface roughness strongly increases. For growth on 4° off-cut substrates,

significantly smoother epilayers were grown on $\langle 1\bar{1}00 \rangle$ off-cut substrates than on $\langle 11\bar{2}0 \rangle$ off-cut substrates.

The operating window for step-controlled growth on 2° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates is quite narrow with respect to applicable Si/H and C/Si ratios. Further work is needed to determine the limits of step-controlled epigrowth on 2° off-cut substrates more precisely and to optimize the step-controlled epigrowth with respect to defect density and other aspects of epitaxial growth.

6. Acknowledgments

This work was part of the KoSiC project funded by the Bavarian Research Foundation (BFS) under contract number AZ-720-06. The SiCrystal AG, especially Dr. Gerd Trachta and Sabine Storm, are gratefully acknowledged for provision of the substrates with different off-cuts.

[1] H. Matsunami, T. Kimoto, Materials Science and Engineering R 20 (1997) 125–166.

[2] B. Landini, G. Brandes, Applied Physics Letters 74 (1999) 2632–2634.

[3] H. Tsuchida, I. Kamata, S. Izumi, T. Tawara, K. Izumi, Materials Science Forum 457-460 (2004) 229–232.

[4] W. Chen, M. Capano, Journal of Applied Physics 98 (2005) 114907.

[5] W. Burton, N. Cabrera, F. Frank, Philosophical Transactions of the Royal Society London, Series A 243 (1951) 299–358.

[6] H. Matsunami, T. Kimoto, Journal of Applied Physics 75 (1994) 850–859.

[7] B. Kallinger, P. Berwian, J. Friedrich, G. Müller, A.-D. Weber, E. Volz, G. Trachta, E. Spiecker, B. Thomas, Journal of Crystal Growth 349 (2012) 43–49.

[8] C. Herring, Phys. Rev. 82 (1951) 87–93.

[9] A. Danilewsky, K. Benz, T. Nishinaga, J. Crystal Growth 99 (1990) 1281–1286.

[10] T. Kimoto, A. Itoh, H. Matsunami, T. Okano, Journal of Applied Physics 81 (1997) 3494.

[11] D. Larkin, P. Neudeck, J. Powell, L. Matus, Applied Physics Letters 65 (1994) 1659–1661.

[12] T. Kimoto, A. Itoh, H. Matsunami, Applied Physics Letters 67 (1995) 2385–2387.

[13] C. Hecht, B. Thomas, W. Bartsch, Materials Science Forum 527-529 (2006) 239–242.

Table 1: Substrate properties and process parameters for all epigrowth series.

Series	substrate off-cut		epigrowth parameters		
	angle α	direction	C/Si ratio	Si/H ratio $[\times 10^{-3}]$	temperature [°C]
A)	4	$\langle 11\bar{2}0\rangle$	0.9	1.1	1450-1700
B)	4	$\langle 11\bar{2}0\rangle$	0.6 - 1.65	1.1	1650
C)	4	$\langle 11\bar{2}0\rangle$	0.6 - 1.5	0.6	1650
D)	4	$\langle 11\bar{2}0\rangle$	0.6 - 1.15	2.2	1650
E1)	8	$\langle 11\bar{2}0\rangle$	0.6 - 1.5	1.1	1650
E2)	8	$\langle 11\bar{2}0\rangle$	0.75	0.6 & 2.2	1650
F1)	2	$\langle 11\bar{2}0\rangle$	0.75 & 0.9	1.1	1650
F2)	2	$\langle 11\bar{2}0\rangle$	0.75 & 0.9	0.6	1650
G)	4	$\langle 1\bar{1}00\rangle$	0.6 - 1.5	1.1	1600

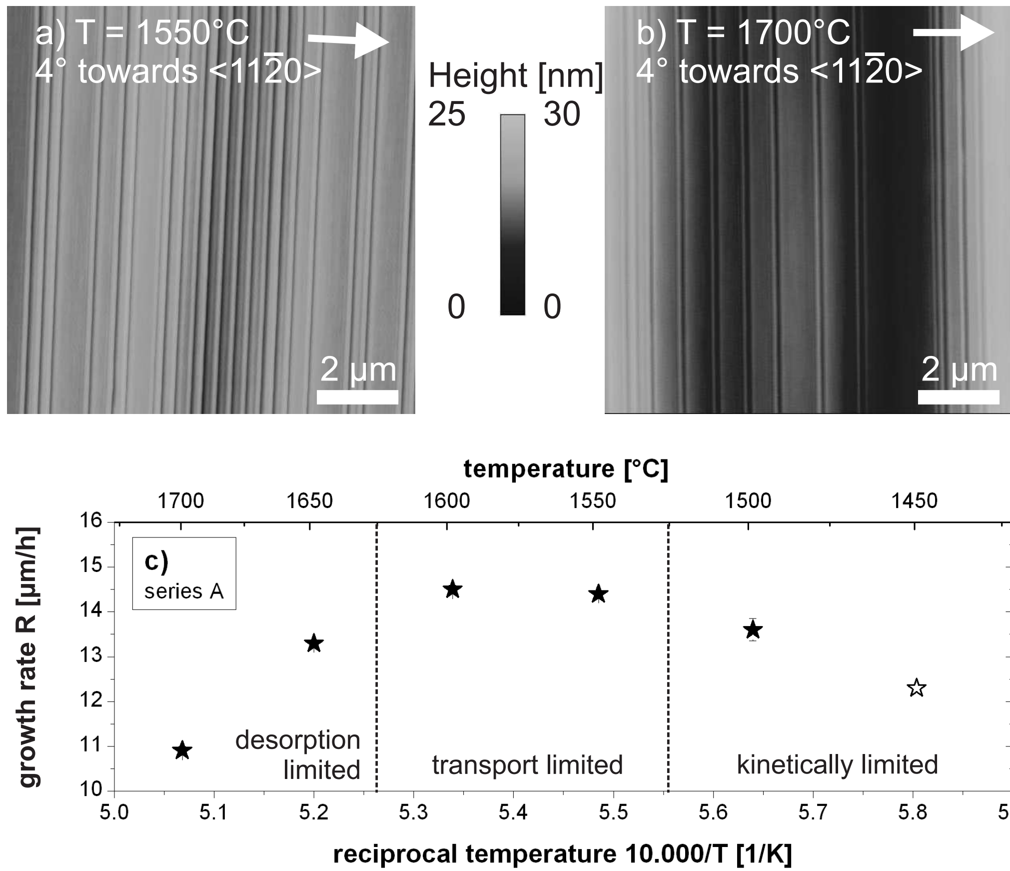

Figure 1: Influence of the growth temperature T on the surface morphology and growth rate. Top: AFM images of epilayers' surface morphologies grown on 4° towards $\langle 11\bar{2}0\rangle$ off-cut substrates at T = 1550 °C (a) and T = 1700 °C (b). The off-cut direction of the substrates is indicated by arrows. Bottom, c: Growth rate R plotted versus the reciprocal growth temperature. Open star: polycrystalline growth, closed stars: step-controlled growth mode.

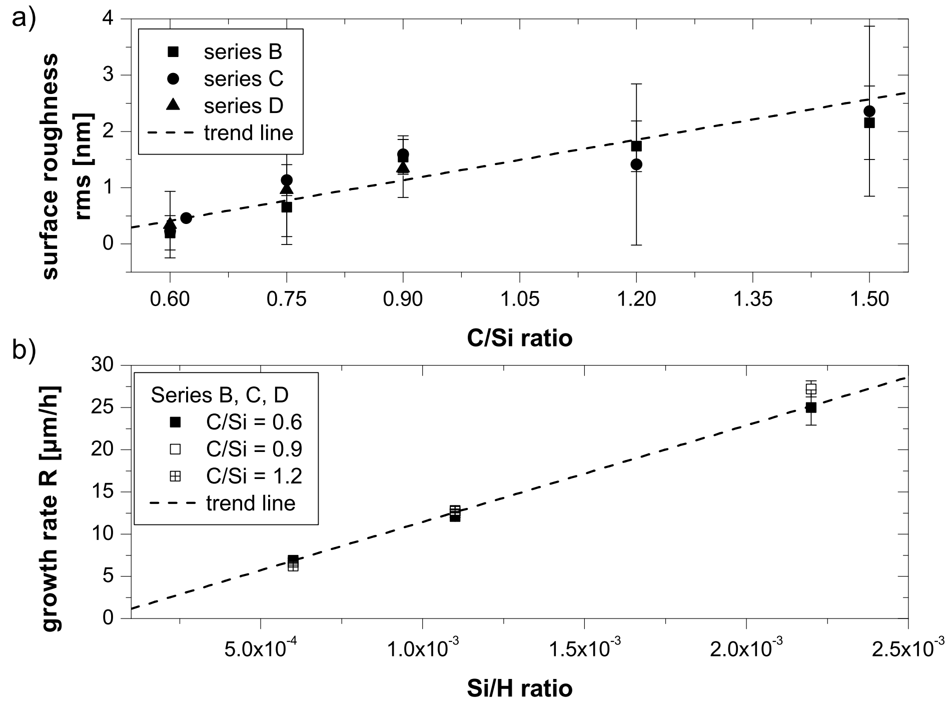

Figure 2: Influence of the Si/H and C/Si ratio on the surface roughness and the growth rate of epilayers grown on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates (series B, C and D): a) rms values characterizing the surface roughness plotted versus the C/Si ratio for different Si/H ratios of 1.1×10^{-3} (series B), 0.6×10^{-3} (series C) and 2.2×10^{-3} (series D). b) Growth rate R plotted versus the Si/H ratio for different C/Si ratios of 0.6, 0.9 and 1.2.

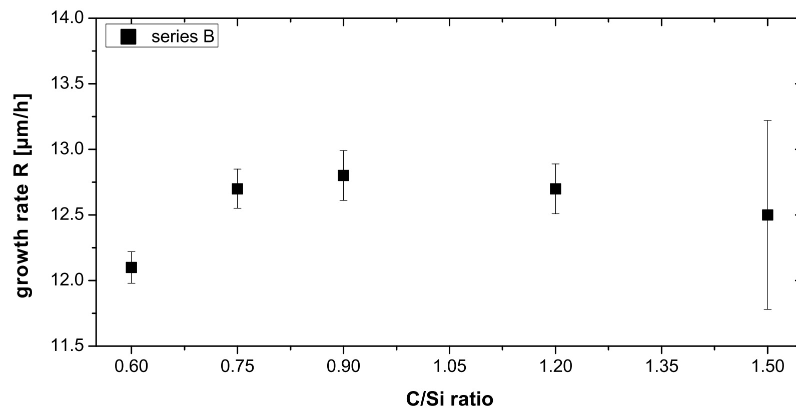

Figure 3: Influence of the C/Si ratio on the growth rate R of epilayers deposited on 4° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates (series B).

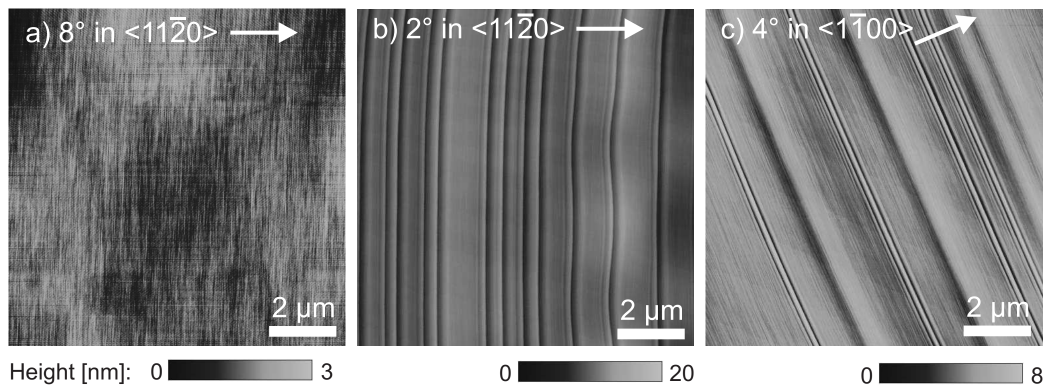

Figure 4: Surface morphologies of epilayers grown on substrates with different off-cuts as indicated in the figures (same process parameters for epigrowth, especially C/Si = 0.75). The arrows indicate the off-cut direction of the substrates.

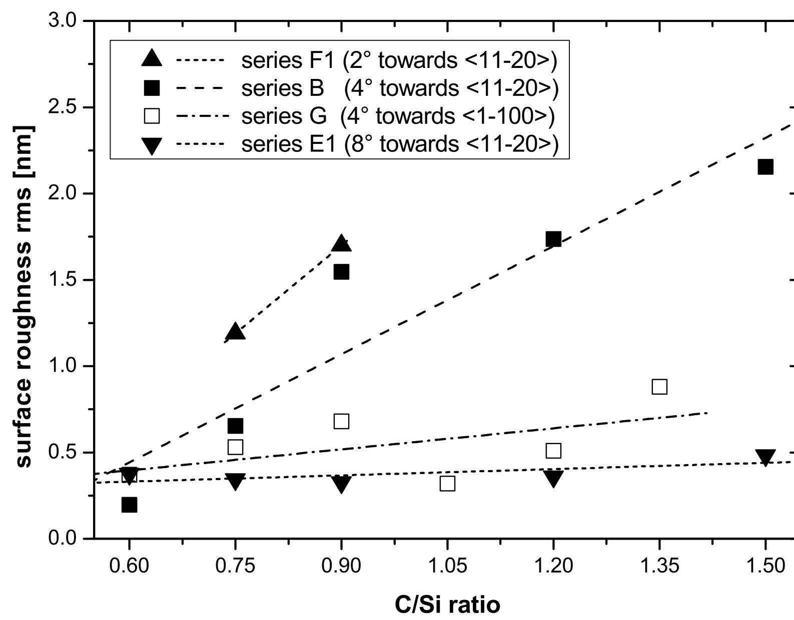

Figure 5: Surface roughness (rms) plotted versus C/Si ratio for different off-cuts of vicinal substrates. For each growth series, trend lines are given instead of error bars to highlight the general trends of results. The rms values of each sample deviate about 30 % from the given mean rms value.

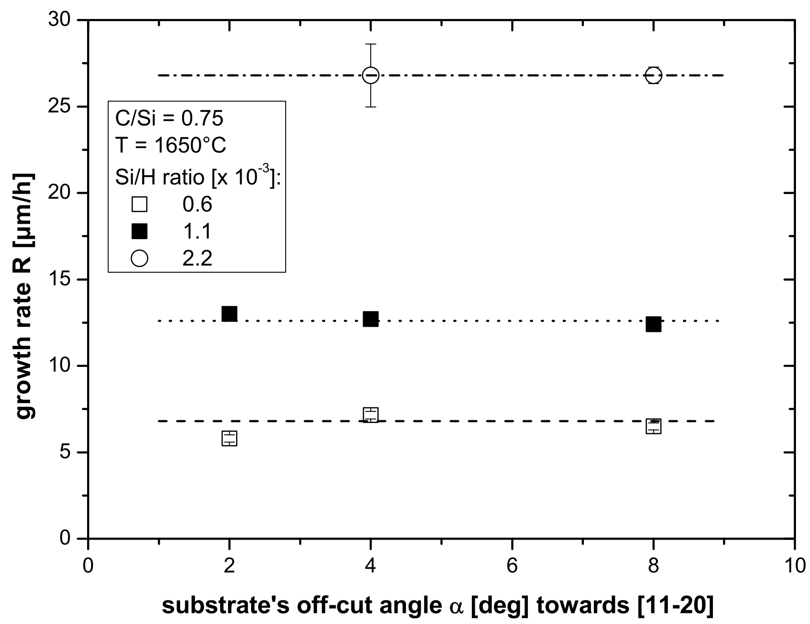

Figure 6: Growth rate R plotted versus the off-cut angle α of vicinal substrates (off-cut direction: $\langle 11\bar{2}0\rangle$) for different Si/H ratios.