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Experimental verification of the model by Klapper for 4H-SiC homoepitaxy on vicinal substrates

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4H-SiC homoepitaxial layers free of basal plane dislocations (BPDs) are urgently needed to overcome the so-called bipolar degradation of high-voltage devices. BPDs being present in substrates are able to either propagate to the epilayer or convert to harmless threading edge dislocations (TEDs) in the epilayer. The model by Klapper predicts the conversion of BPDs to TEDs to be more efficient for growth on vicinal substrates with low off-cut angle. This paper aims to verify the model by Klapper by an extensive variation of epitaxial growth parameters and the substrates' off-cut. It is shown that the off-cut angle is the key parameter for growth of BPD-free epilayers. Furthermore, it is shown that the model also describes adequately the behavior of different types of TEDs, i.e., TED II and TED III dislocations, during epitaxial growth. Therefore, the model by Klapper is verified successfully for 4H-SiC homoepitaxial growth on vicinal substrates. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4829707>]

I. INTRODUCTION

4H silicon carbide (4H-SiC) is the preferred material for energy-efficient power electronic devices due to its outstanding material properties, which is proven by the commercial success of unipolar devices like, e.g., Schottky barrier diodes capable for blocking voltages up to 2 kV. For higher blocking voltages, bipolar devices are needed. But the commercialization of bipolar devices like, e.g., PiN diodes is hindered by the so-called bipolar degradation,¹ which is driven by the formation and expansion of Shockley-type stacking faults within the active volume of the device during device operation. It has been proven² that the generation and expansion of Shockley-type stacking faults occurs due to recombination enhanced dislocation glide (REDG) of Basal Plane Dislocations (BPDs) located within the active volume of the bipolar device, i.e., within the epitaxial layers. Therefore, bipolar degradation can be suppressed by avoiding BPDs within epilayers.³

BPDs are present in 4H-SiC substrates with a typical BPD density in the order of 10^4 cm^{-2} and are able to either propagate to the epitaxial layer or convert to threading edge dislocations (TEDs).^{4–6} It has been reported that converted BPDs, i.e., TEDs in the epilayer, can be inclined about 20° from the crystallographic c-direction of the crystal.^{7,8} Such inclined TEDs are also known as TED II and TED III dislocations and can be identified based on their visibility in x-ray topographs.⁹ Although the BPD conversion mechanism is not fully understood on the microscopic level,⁷ a pertinent model explains the behavior of dislocations at the growth interface based on dislocation

energetics. This model was first invented by Klapper¹⁰ for dislocations in a growing organic crystal and has been applied to semiconducting hexagonal crystals like, e.g., gallium nitride (GaN) by Knoke *et al.*¹¹ and 4H-SiC by Refs. 6, 12, and 13. According to the model by Klapper, the minimization of the dislocation line energy at the growth interface is the driving force for BPD conversion in 4H-SiC homoepitaxial growth on vicinal substrates. It has been shown⁵ that the driving force for BPD conversion becomes much stronger for decreasing off-cut angle α of the vicinal substrate, resulting in lower BPD densities of epilayers grown on 4° off-cut substrates compared to epilayers grown on 8° off-cut substrates. It has also been proven^{6,14,15} that epilayers free of BPDs can be grown on defect selectively etched substrates, which means that a local on-axis condition is provided to BPDs within the vicinity of BPD etch pits. A similar approach to reduce the BPD density in epilayers is to interrupt the epigrowth,¹⁶ i.e., to force the back-etching of the growth interface.

If the minimization of the dislocation line energy at the growth interface is the only reason for BPD conversion during epitaxial growth, growth parameters like, e.g., growth temperature T , mixture of precursor gases (C/Si ratio), and growth rate R are expected having no significant impact on the BPD density of the grown epilayer (at least as long as these growth parameters do not change the geometric conditions at the growth interface). Therefore, the aim of this paper is to verify the model by Klapper by investigating (1) the impact of growth parameters and (2) the impact of the substrate's off-cut angle α and the off-cut direction on the BPD density of epilayers. The model by Klapper is verified for 4H-SiC homoepitaxy if the behavior of all dislocation types during epitaxial growth is described correctly.

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II. EXPERIMENTAL

A. Homoepitaxial growth on vicinal substrates

Homoepitaxial 4H-SiC layers were grown on the (0001)Si-face of commercially available 3 in. vicinal substrates by means of Chemical Vapor Deposition (CVD) in a horizontal hot wall reactor (Epigress VP508GFR) as described in Ref. 17. Several growth series were conducted (see Table I). In series A-E, several growth parameters were varied systematically for the use of standard substrates (4° off-cut towards $\langle 11\bar{2}0 \rangle$). In series A, the growth temperature T was varied from 1500°C to 1650°C in 50 K steps. In series B-D, the growth rate R was successively increased from $7\ \mu\text{m/h}$ to $13\ \mu\text{m/h}$ and $26\ \mu\text{m/h}$ by increasing the Si/H ratio. In these growth series, also the C/Si ratio was varied by adapting the propane flow. In series E, the growth duration t was doubled two times. As the growth rate was kept constant, the epilayer thickness h_f increased from $12.5\ \mu\text{m}$ to $25\ \mu\text{m}$ and $50\ \mu\text{m}$. In series F-H, epitaxial growth was performed under standard conditions on substrates with different off-cuts: 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.

Adjacent substrates cut from one crystal boule were used within each epigrowth series. The epilayer thickness was measured by Fourier transformed infrared spectrometry (FTIR). The growth rate R was calculated based on the epilayer thickness and the growth duration. All epilayers were intentionally doped with nitrogen gas (N_2) to obtain n-type epilayers. The net carrier concentration of all grown epilayers is in the order of low $10^{15}\ \text{cm}^{-3}$ as found by CV measurements.

B. Characterization of epilayers

The dislocation content of substrates and epilayers was investigated by synchrotron x-ray topography (SXRT) and defect selective etching (DSE). SXRT has been used to investigate *ex-situ* the behavior of dislocations by comparing topographs of the substrate and the subsequently grown epilayer. DSE has been applied to study the densities of different dislocation types, especially of rare BPDs, on wafer level.

1. Synchrotron X-ray topography

Dislocations in substrates and epilayers were identified by synchrotron white beam x-ray topography (SXRT) performed at the TOPO-TOMO beam line¹⁸ of the synchrotron light source ANKA in Karlsruhe, Germany. SXRT measurements were performed in back-reflection geometry in order to limit the information depth to about $30\ \mu\text{m}$. Topographs were recorded on high resolution films (Slavich VRP-M).

By using a white beam, several topographs with different diffraction vectors $\vec{g}$ are recorded simultaneously from the measurement point. The topographs were indexed by using the software LauePT¹⁹ in order to identify dislocations based on the $\vec{g} \cdot \vec{b}$ criterion. Further experimental details can be found in Ref. 9.

2. Defect selective etching

The epilayers were defect selectively etched in molten potassium hydroxide (KOH) at 520°C for several minutes. Then, each epilayer surface was investigated by optical light microscopy at 70 measurements points being regularly distributed across one half of each wafer. As all epilayers are n-type with a net carrier concentration of low $10^{15}\ \text{cm}^{-3}$, the etch pits are interpreted as follows:⁹ BPDs are decorated by oval shaped etch pits, TEDs, TED II, and TED III dislocations by small hexagonally shaped etch pits and threading screw dislocations (TSDs) by large hexagonally shaped etch pits, respectively.

Based on the results of these 70 measurement points per epilayer, the mean densities of respective dislocation types and the overall etch pit density (EPD) were determined as well as the respective standard deviations, which are given as error bars in the following figures. The detailed analysis of EPD data revealed that the overall etch pit densities and their lateral distributions across the sample area are comparable within each growth series as adjacent substrates cut from one crystal boule were used. But the overall EPD as well as the lateral EPD distribution differs from series to series. Therefore, relative BPD densities are given (BPD/EPD in %) in the following in order to be able to compare the results of different growth series.

TABLE I. Substrate properties and process parameters for all epigrowth series. The growth duration t was adapted to the growth rate R in order to obtain $10\ \mu\text{m}$ thick epilayers except for series E.

Series	Substrate off-cut		Epigrowth parameters			
	Angle α [$^\circ$]	Direction	C/Si ratio	Growth rate R [$\mu\text{m/h}$]	Temperature T [$^\circ\text{C}$]	Layer thickness h_f [μm]
A)	4	$\langle 11\bar{2}0 \rangle$	0.9	≈ 13	1500–1650	10
B)	4	$\langle 11\bar{2}0 \rangle$	0.6–1.5	13	1650	10
C)	4	$\langle 11\bar{2}0 \rangle$	0.6–1.5	7	1650	10
D)	4	$\langle 11\bar{2}0 \rangle$	0.6–1.15	26	1650	10
E)	4	$\langle 11\bar{2}0 \rangle$	0.9	13	1650	12.5 and 25 and 50
F)	8	$\langle 11\bar{2}0 \rangle$	0.6–1.5	7 and 13	1650	10
G)	2	$\langle 11\bar{2}0 \rangle$	0.75 and 0.9	7 and 13	1650	10
H)	4	$\langle 1\bar{1}00 \rangle$	0.6 – 1.5	14.5	1600	10

III. RESULTS

First, the basic dislocation behavior of different dislocation types is investigated by a comparative x-ray topography study. Then, the impact of the substrate's off-cut and of several process parameters on the BPD density of epilayers is studied by defect selective etching of epilayers.

A. Behavior of dislocations during epigrowth

In order to study the behavior of dislocations during epitaxial growth, topographs were recorded from bare substrates and from epilayers subsequently grown on these substrates. Topographs of a bare substrate and the corresponding epilayer are shown in Figures 1(a) and 1(b), respectively, which were recorded at the same sample position. In Figure 1(a), the intersection points of BPDs at the substrate's surface are marked by triangles, TSDs are marked by squares. In the corresponding topograph of the epilayer (Figure 1(b)), TSDs are found at the same positions as in the substrate, indicating that TSDs propagate to the epilayer without any change to the dislocation line direction. Contrary to that, TEDs are found in the epilayer (marked by circles) at the former intersection points of BPDs at the substrate's surface. This experimental observation proves that substrate-BPDs are able to convert to TEDs in the epilayer.

Moreover, the behavior of different TED-types during epigrowth was investigated. Different types of TEDs, i.e., TED, TED II, and TED III dislocations, can only be distinguished based on their visibility in SXRT topographs and their black/white contrast.⁹ All types of TEDs are assumed to have an a-type Burgers vector. The dislocation line of TEDs is exactly oriented along the $\langle 0001 \rangle$ direction, whereas the dislocation line of TED II and TED III dislocations can deviate up to 20° from the c-axis.

FIG. 1. Comparison of topographs from substrate ((a) and (c)) and subsequently grown epilayers ((b) and (d)). All topographs were recorded in back-reflection geometry with given diffraction vector $\vec{g} = 10\bar{1}9$. Exemplary dislocations are marked: TSD: square, TED: circle, TED II: broken triangle, TED III: broken circle, and BPD's intersection point at the surface: triangles. The dislocations were identified by comparison of several topographs with different diffraction vectors (not shown here).

In the substrate (Figure 1(c)), TEDs and TED III dislocations (marked by broken circles) are found besides TSDs and BPDs. By comparing the corresponding epilayer topograph (Figure 1(d)) to the substrate's topograph, it is found that TEDs can either propagate to the epilayer or convert to TED II dislocations (marked by broken triangles) and that TED III dislocations from the substrate can either thread in the epilayer or convert to TED II dislocations during epitaxial growth. All substrate TSDs are found to continue to the epilayer.

A detailed quantitative analysis of these topographs reveals that each dislocation in the substrate can be correlated to a dislocation in the epilayer, i.e., the dislocation density remains constant during epitaxial growth.

B. BPD density in epilayers

The influence of several process parameters as well as the substrate's off-cut on the BPD density of epilayers was studied by a systematic parameter variation. The relative BPD densities are given (BPD/EPD in %) in the following in order to be able to compare the results of different growth series.

1. Influence of process parameters on the BPD density of epilayers

In order to study the influence of the process parameters growth temperature T , growth rate R and C/Si ratio, as well as growth duration t , on the BPD density of epilayers, about 20 epilayers were grown on standard substrates, i.e., with 4° off-cut towards $\langle 11\bar{2}0 \rangle$ direction. The experimental results are displayed in Figure 2.

In series A, the growth temperature T was varied from 1500°C to 1650°C . The relative BPD densities of these epilayers together with the arithmetic mean value of this series are given in Figure 2(a) as data points and trendline, respectively. The experimental data hardly deviate from the mean value. Hence, no significant impact of the growth temperature T on the BPD density of epilayers was found.

In Figure 2(b), the relative BPD densities of epilayers grown at different growth rates of $7\ \mu\text{m/h}$, $13\ \mu\text{m/h}$, and $26\ \mu\text{m/h}$ and C/Si ratios from 0.6 to 1.50 are given (series B-D, compare Table I). A trendline is given as broken line for the data of series B. It can be seen from Figure 2(b) that the relative BPD density typically amounts to less than 0.3%, regardless of the applied growth rate and C/Si ratio. The lowest BPD densities are found in epilayers grown at C/Si ratios of 0.75 and 0.9.

In Figure 2(c), the relative BPD density of epilayers is shown in dependence of the epilayer thickness h_f (and growth duration t , series E). The BPD density is decreasing with increasing growth duration or epilayer thickness. The thickest epilayer with $h_f = 50\ \mu\text{m}$ is free of BPDs within experimental accuracy, i.e., no BPD etch pit was found at 70 measurement points.

2. Influence of the substrate's off-cut on the BPD density of epilayers

The relative BPD densities of about 20 epilayers grown on substrates with different off-cuts are displayed in Figure 3

FIG. 2. Influence of epitaxial growth parameters on the relative BPD densities (given as BPD/EPD in %) of epilayers grown on standard substrates. (a) Influence of growth temperature T . (b) Influence of C/Si and different growth rates R . The broken line is a trendline to series B. (c) Influence of the epilayer thickness or growth duration, respectively.

FIG. 3. Influence of the substrate's off-cut on the relative BPD densities (given as BPD/EPD in %) of epilayers grown at different C/Si ratios. The broken lines are trendlines. (a) Relative BPD densities of epilayers grown on 8° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates. (b) Relative BPD densities of epilayers grown on 4° towards $\langle 11\bar{2}0 \rangle$ and $\langle 1\bar{1}00 \rangle$ off-cut substrates. (c) Relative BPD densities of epilayers grown on 2° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates.

in dependence of the applied C/Si ratio. All epilayers were grown under standard conditions (compare Table I).

The relative BPD densities of epilayers grown on 8° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates are displayed in Figure 3(a). The BPD density of these epilayers varies between 4% and 7% of EPD with a local minimum at C/Si = 0.9.

In Figure 3(b), the relative BPD densities of epilayers grown on 4° off-cut substrates with different off-cut directions are shown. The relative BPD densities of epilayers grown on 4° off-cut substrates with different off-cut direction fit qualitatively and quantitatively very well, proving that the off-cut direction of the substrate has no impact on the BPD density of epilayers. The epilayers grown on 4° off-cut substrates have low BPD densities of $\leq 0.5\%$ of EPD and epilayers nearly free of BPDs can be grown at moderate C/Si ratios of 0.75 to 1.05, i.e., very few BPD etch pits were found at 70 measurement points per epilayer.

In Figure 3(c), the relative BPD densities of epilayers grown on 2° towards $\langle 11\bar{2}0 \rangle$ off-cut substrates are shown. The process window for stable step-flow growth on such substrates is narrowed to C/Si ratios of 0.75 and 0.9.¹⁷ Therefore, no more than two epilayers could be grown. A low BPD density of 0.25% of EPD was found for the epilayer grown at C/Si = 0.9. For the epilayer grown at C/Si = 0.75, no BPD etch pit was found at 70 measurement points, i.e., the epilayer is free of BPDs within experimental accuracy.

For all epilayers grown, the majority of BPD etch pits and dislocation lines of BPDs are oriented along the step-flow direction of the epilayer.

IV. DISCUSSION

The influence of process parameters and the substrates' off-cut on the epilayers' BPD density was investigated extensively. First, the results of these growth series will be compared in order to identify the main influencing factor for the BPD density of epilayers. Then, the model by Klapper will be verified by comparison of the theoretical predictions to the experimental results.

A. Determination of the main influencing factors on the BPD density of epilayers

In series A, the influence of the growth temperature T on the BPD density of epilayers was investigated. As the growth temperature T has no significant impact on the epilayer's BPD density, no thermally activated process is involved in the BPD-TED conversion.

In series B-D, the influence of the growth rate R on the BPD density of epilayers was studied. Similar BPD densities were found for epilayers grown at different growth rates R (for same C/Si ratio), indicating that the growth rate R and hence, the step velocity, has no significant impact on the BPD density of epilayers.

In series E, it has been found that the BPD density of epilayers decreases with increasing growth duration/epilayer thickness. This result proves that all substrate BPDs can be converted during epigrowth.

The influence of the C/Si ratio on the epilayers' BPD density was investigated in series B-D and F-H. For all growth series, a similar trend of the BPD density in dependence of the C/Si ratio was found: The BPD density shows a local minimum at $C/Si \approx 1$ and slightly higher BPD densities at lower and higher C/Si ratios. It was already reported^{5,17} that step-bunching becomes more severe for increasing C/Si ratio, i.e., there might exist an optimum step geometry at $C/Si \approx 1$ for BPD-TED conversion.

The influence of the substrate's off-cut direction on the epilayer's BPD density was studied in series B and H for 4° off-cut substrates. The BPD densities of these two growth series are very similar, indicating that the substrate's off-cut direction has no significant impact on the epilayer's BPD density. This result agrees to those of other groups^{20,21} for epigrowth on 8° off-cut substrates with different off-cut directions. Moreover, in series B and H, epigrowth was conducted at different growth temperatures of 1650°C and 1600°C , respectively, but resulting in very similar BPD densities of the epilayers. This observation supports the result of series A that the growth temperature T has no significant influence on the epilayer's BPD density.

In series B, F, G, and H, the impact of the substrates' off-cut angle α on the epilayers' BPD density was studied. The BPD densities of epilayers grown on 8° off-cut substrates are about 10 times higher than those on 4° off-cut substrates, and a BPD-free epilayer was grown on a 2° off-cut substrate. Hence, the off-cut angle α of the substrate has a strong impact on the BPD density of epilayers, i.e., a lower off-cut angle α of the substrate results in a significantly lower BPD density in the epilayer.

This might be due to the geometric conditions at the growth interface according to the model by Klapper or to the step velocity. The step velocity ν_a can be calculated from the growth rate R and the off-cut angle α of the substrate according to Eq. (1)

$$\nu_a = R/\sin \alpha. \quad (1)$$

The step velocity ν_a increases strongly with decreasing off-cut angle α for a fixed growth rate R or with the growth rate R for a fixed off-cut angle α of the substrate. The latter case has been investigated in series B, C, D, and H for growth on 4° off-cut substrates with the result that the step velocity has no impact on the BPD conversion. This means in turn that the different BPD densities of epilayers grown on substrates with different off-cut angles cannot be attributed to the different step velocities but to the different geometric conditions at the growth interface.

Therefore, the off-cut angle α of the substrate is the main influencing factor for the BPD density of epilayers among all investigated process parameters and substrate properties.

B. Verification of model by Klapper

The model by Klapper^{6,10,12,13} is based on the specific dislocation line energies at the growth interface W . Therefore, the dislocation line energies E in the crystal

volume of all dislocation types have to be determined first. Then, the specific dislocation line energies W at the growth interface are to be calculated and compared to experimental results. The model of Klapper is only valid for 4H-SiC homoepitaxy if the behavior of all dislocation types, i.e., threading dislocations as well as BPDs, at the growth interface is described correctly.

1. Dislocation types and their line energies in crystal volume

The SXRT study in Sec. III A revealed the occurrence of several dislocation types in substrates and epilayers as summarized in Table II.

BPDs have an a-type Burgers vector $\vec{b}$ and a line vector $\vec{l}$ within the (0001) plane. Therefore, BPDs occur in edge, mixed, and screw configuration. Epilayer-BPDs are often oriented along the step-flow direction as found in this study and by Ohno *et al.*¹² The preferred orientation of epilayer-BPDs will be discussed in Sec. IV B 2.

All kinds of TEDs have an a-type Burgers vector $\vec{b}$. As TEDs propagate exactly along the c-direction of the crystal, i.e., $\vec{l} = \langle 0001 \rangle$, they are edge dislocations. TED II and TED III dislocations are interpreted having an a-type Burgers vector $\vec{b}$ and a line vector $\vec{l}$ inclined from the c-direction by several degrees, i.e., they are mixed-type dislocations with a large edge component. If they lie on pyramidal glide planes $\{1101\}$, the angle θ between the $\langle 0001 \rangle$ direction and line vector $\vec{l}$ amounts to 14.8° , which is in reasonable agreement to the angle of 20° reported by Wu⁸ and Chung *et al.*⁷ Further details about the interpretation of TED II and TED III dislocations can be found in Ref. 9.

TSDs are always screw dislocations. Therefore, no glide plane can be assigned for this dislocation type.

The dislocation line energies E in the crystal volume are now calculated based on Eq. (2)²²

$$E(\vec{b}, \vec{l}, c_{ij}) = \frac{K(\vec{b}, \vec{l}, c_{ij}) \cdot b^2}{4\pi} \cdot \ln \frac{R}{r} \quad (2)$$

with $\vec{l}$: line vector of dislocation, $\vec{b}$: Burgers vector of dislocation, c_{ij} : elastic constants of 4H-SiC as given in Ref. 23, K : energy factor, and R, r : outer and inner radii of dislocation strain field, respectively. The term $\ln \frac{R}{r}$ can be neglected as the radii R and r are difficult to determine and the term gives a small and constant factor to E .²⁴

TABLE II. Properties of dislocation types as reported in Sec. III A: Burgers vector $\vec{b}$, line vector $\vec{l}$, glide plane, and presence in substrate and epilayers.

Dislocation	$\vec{b}$	$\vec{l}$	Glide plane	Substrate	Epilayer
BPD	$\frac{1}{3}\langle 11\bar{2}0 \rangle$	$\vec{l} \in \langle 0001 \rangle$	(0001)	x	x
TED	$\frac{1}{3}\langle 11\bar{2}0 \rangle$	$\langle 0001 \rangle$	$\{1\bar{1}00\}$	x	x
TED II	$\frac{1}{3}\langle 11\bar{2}0 \rangle$	$\approx \langle 0001 \rangle$	$\{1\bar{1}01\}$	...	x
TED III	$\frac{1}{3}\langle 11\bar{2}0 \rangle$	$\approx \langle 0001 \rangle$	$\{1\bar{1}01\}$	x	x
TSD	$\langle 0001 \rangle$	$\langle 0001 \rangle$	n. def.	x	x

FIG. 4. Dislocation line energies E within the crystal volume as a function of the angle θ between Burgers vector $\vec{b}$ and line vector $\vec{l}$. Line energies are calculated based on a numerical solution for dislocations with $\vec{b} = a$ on different glide planes. The data points represent the results of Ohno *et al.*,¹² which were obtained by an analytical approach being valid for basal plane and prismatic plane glide systems.

It has been shown¹¹ that the energy factor K of a dislocation in a hexagonal crystal lattice needs to be calculated based on a numerical solution, especially for dislocations on pyramidal glide planes. The numerical solution ANACALC of Head *et al.*²⁵ was used in the current implementation DISDI by J. Douin. The calculated dislocation line energies in the crystal volume E are shown for dislocations with a-type Burgers vector in Figure 4. It can be seen that the current results for the basal plane and prismatic glide systems fit those of Ohno *et al.*,¹² which were calculated by an analytical solution. The line energies of TED II and TED III dislocations can only be obtained by the numerical solution and are found to be slightly smaller than $E(\text{TED})$. Therefore, it has been proven that the existence of TED II and TED III dislocations in the crystal volume is energetically possible.

The dislocation line energy E of TSDs amounts to $E(\text{TSD}) = 75 \times 10^{-18} \text{ J/nm}$ (not shown in Figure 4) and is about 10 times higher than the line energies of dislocations with a-type Burgers vector.

2. Behavior of dislocations at the growth interface

According to the model by Klapper, the specific dislocation line energy W at the growth interface determines the behavior of a dislocation during growth as each dislocation tends to minimize its specific line energy by minimizing the angle between the growth normal n_s and the line vector $\vec{l}$ or, in other words, the length of the dislocation line within the growing epilayer. The geometric conditions at the growth interface are shown in Figure 5(a) for BPDs and threading dislocations: Pure threading dislocations, i.e., TEDs and TSDs with their line vectors being exactly oriented along $\langle 0001 \rangle$, include the angle α to the growth normal n_s , which is the off-cut angle α of the substrate. Contrary to threading dislocations, BPDs include a larger angle between the growth normal and their line vector of $\angle(n_s, \vec{l}) = (90^\circ - \alpha)$. The specific dislocation line energy W at the growth interface can be calculated according to Eq. (3)

$$W = \frac{E \cdot h_f}{\cos \angle(n_s, \vec{l})}. \quad (3)$$

FIG. 5. Geometrical model of dislocation behavior during epitaxial growth. (a) cross-sectional view showing two possibilities of a substrate-BPD: I. A substrate-BPD (BPD_{sub} , solid line) propagates to the epilayer (BPD_{epi} , dashed line). The epi-BPD has a long dislocation line and a large angle $\beta = (90^\circ - \alpha)$ between its dislocation line and the surface normal n_s . II. A substrate-BPD converts to an epi-TED (TED_{epi} , dashed line) with a short dislocation line and a small angle α between its dislocation line and the surface normal n_s . The angle α is equal to the off-cut angle of the substrate. The epilayer thickness is named h_f . (b) Top-view onto growth steps and preferential line orientation of BPD: a BPD close to the growth surface tends to minimize its angle γ between dislocation line direction and step-flow direction according to the model by Zhang and Sudarshan.¹³

The results of these calculations are given in Figure 6(a), i.e., the specific line energies W of TEDs and BPDs are plotted versus the off-cut angle α of the substrate. The specific line energy of TEDs hardly changes for different off-cut angles, but the specific line energy of BPDs increases strongly for decreasing off-cut angle α of the substrate. Therefore, a substrate BPD can minimize its specific line energy by conversion to a TED at the growth interface. This driving force becomes much stronger for decreasing off-cut angle α of the substrate, i.e., epilayers grown on substrates with a small off-cut angle α are expected to contain less BPDs than epilayers grown on substrates with a large off-cut angle, e.g., $\alpha = 8^\circ$. Our best experimental results with respect to the BPD density of epilayers are given in Figure 6(b) in dependence of the substrate's off-cut angle α . The BPD etch pit density of epilayers significantly decreases with decreasing off-cut angle α of the substrate. To compare the BPD etch pit densities for epilayers grown on substrates with different off-cut angles α , one has to consider as well that for a fixed true BPD density ρ (as dislocation line length per unit volume) the number of BPDs intersecting the surface has to decrease with decreasing off-cut angle α of the substrate due to geometrical reasons.²⁶ The expected decrease of the BPD etch pit density is given by means of a conversion factor,²⁶ which is proportional to $\sin \alpha$, as dotted line in Figure 6(b). However, our experiments showed a much stronger decrease of BPD etch pit density with reduced off-cut angle α of the substrate than the expected decrease by geometrical reasons. This must be caused by a drastic reduction of the true BPD density ρ , which is only explicable by the Klapper model.

The line vectors of remaining BPDs in epilayers are preferably oriented along the step-flow direction. Zhang and Sudarshan have shown¹³ that there exists a secondary minimum of the dislocation line energy W during growth with respect to the angle γ between the dislocation line vector and the step-flow direction. This is a useful extension of the basic model by Klapper and fits our own results.

It has been shown in Sec. III A that different types of TEDs can convert to each other. This is possible as TEDs, TED II, and TED III dislocations have an a-type Burgers vector and conversion is due to the change in the dislocation

FIG. 6. Comparison of theoretical model and experimental results on BPD density in epilayers: (a) specific dislocation line energies W at the growth interface in dependence of the substrate's off-cut angle α . (b) Best experimental results with regard to BPD density in epilayers in dependence on substrate's off-cut angle α . The dotted line is an exponential fit to the experimental data, the broken line displays the conversion factor²⁶ for BPD etch pit densities to true BPD densities ρ .

line direction. As the line vector of TED II and TED III dislocations deviates about 20° from the $\langle 0001 \rangle$ direction, their specific line energies W during growth can be calculated with the angle $\angle(n_s, \vec{l}) = (\alpha \pm 20^\circ)$. The specific dislocation line energies of TED II and TED III dislocations are also plotted in Figure 6. As $W(\text{TED II})$ and $W(\text{TED III})$ hardly deviates from $W(\text{TED})$, there is no significant difference in the driving force for conversion of a BPD to one of these TED types. Therefore, all types of TEDs can be present in the epilayer. Moreover, these kinds of TED dislocations can easily convert to each other. A small perturbation at the growth interface as, e.g., a locally different step geometry might be sufficient to trigger the conversion among TED dislocation types.

C. Reasons for remaining epilayer-BPDs

The model by Klapper describes the principal behavior of dislocation at the growth interface, i.e., the thermodynamics of dislocation behavior. The driving force for BPD conversion becomes larger for a decreasing off-cut angle of the substrate, but BPDs are able to propagate to the epilayer even for epigrowth on substrates with small off-cut angles of 4° and 2° . Moreover, the BPD density in epilayers differs for growth on substrates with a certain off-cut angle, i.e., within each growth series, and also the epilayer thickness or growth duration has a positive influence on the BPD density in the epilayer. Therefore, other influencing factors on the dislocation behavior at the growth interface cannot be neglected like, e.g., interactions with growth steps. BPDs at the growth interface might get pinned at growth steps preventing the BPD conversion. Such interactions between BPDs and growth steps are known, e.g., for BPD multiplication based on the Hopping Frank-Read source mechanism.²⁷

V. CONCLUSIONS

The model by Klapper is verified for all dislocation types in 4H-SiC homoepitaxy by an extensive experimental

study. The dislocation line energies E of all dislocation types are calculated by a numerical approach to cope with the symmetry of the hexagonal crystal lattice. The conversion of substrate-BPDs to TED-types in the epitaxial layer is due to the minimization of the dislocation line energy W at the growth interface, which mainly depends on the substrate's off-cut angle α . It is shown that BPD-free homoepitaxial layers can be grown on low off-cut substrates without additional effort. Other epitaxial growth parameters like, e.g., the C/Si ratio are not crucial for BPD conversion but need to be optimized also with respect to other epilayer properties like, e.g., the surface morphology and doping level. TED II and TED III dislocations exist in 4H-SiC material and are interpreted having an a-type Burgers vector and a dislocation line vector inclined up to 20° from $\langle 0001 \rangle$. These different types of TEDs can convert to each other as their dislocation line energies W at the growth interface are quite similar. Therefore, the model by Klapper describes adequately the behavior of all dislocations types during 4H-SiC homoepitaxial growth on vicinal substrates.

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