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Surface Morphology of 4H-SiC After Thermal Oxidation

J. Woerle[1,2,a*], V. Šimonka[3,b], E. Müller[1,c], A. Hössinger[4,d], H. Sigg[1,e], S. Selberherr[5,f], J. Weinbub[3,g], M. Camarda[1,2,h], U. Grossner[2,i]

[1]Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland

[2]Advanced Power Semiconductor Laboratory, ETH Zürich, Physikstrasse 3, 8092 Zurich, Switzerland

[3]Christian Doppler Laboratory for HPTCAD, Institute for Microelectronics, TU Wien, Gußhausstraße 27-29 / E360, 1040 Vienna, Austria

[4]Silvaco Europe Ltd., Compass Point, St Ives, Cambridge PE27 5JL, UK

[5]Institute for Microelectronics, TU Wien, Gußhausstraße 27-29 / E360, 1040 Vienna, Austria

[a]judith.woerle@psi.ch, [b]simonka@iue.tuwien.ac.at, [c]elisabeth.mueller@psi.ch, [d]andreas.hoessinger@silvaco.com, [e]hans.sigg@psi.ch, [f]selberherr@iue.tuwien.ac.at, [g]weinbub@iue.tuwien.ac.at, [h]massimo.camarda@psi.ch, [i]ulrike.grossner@ethz.ch

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Abstract. Step-controlled growth of 4H-SiC epitaxial layers leads to the formation of a step-bunched morphology along the surface with larger macrosteps, composed of smaller microsteps of several Si-C bilayer heights. As thermal oxidation is an orientation-dependent process, a multi-faceted surface is expected to exhibit a different oxidation behavior compared to a perfectly planar surface. In this work, step-bunched surfaces after oxidation are investigated by high-resolution atomic force microscopy (HR-AFM) and transmission electron microscopy (TEM) indicating a morphological change in the early stages of thermal oxidation. An orientation-dependent oxidation model is used to correctly describe variations of the oxide thicknesses at isolated macrosteps.

Introduction

Owing to the continuous efforts in substrate growth and epitaxy, 4H-SiC is nowadays the material of choice for emerging high-power and high-temperature applications. In order to achieve electronic-grade homoepitaxies of a single polytype, an off-axis growth technique is normally applied [1], leading to microsteps along the surface [2]. Even though a range of different off-angles and tilt directions has been reported [3], the most commonly employed off-angle is 4° toward the [11-20] direction. For the (0001) Si-face, the surface exhibits a continuous step pattern with most of the microsteps having a height of either 2 or 4 bilayers [4]. In addition, macrosteps with heights between 2 and 8 nm are observed, resulting from surface rearrangements which occur in order to minimize the surface energy [5].

This peculiar morphology is unfavorable for many reasons: field-crowding at the steps might reduce the blocking voltage and the higher surface roughness can negatively impact the channel mobility in metal-oxide-semiconductor field-effect transistors (MOSFETs) [6,7]. From a process development point of view, it is therefore important to understand the implications of the faceted surface of 4H-SiC on the oxide growth. So far, little is known about the impact of the oxidation process on the micro-faceting of 4H-SiC surfaces. While the non-uniform oxide growth at the macrosteps has already been studied in more detail [8], an accurate prediction of the oxide thicknesses at these morphological features is still missing.

In this study, HR-AFM is used to study the surface morphology of 4H-SiC before and after dry oxidation. An orientation-dependent SiC oxidation model is applied to predict variations of the oxide thicknesses at isolated macrosteps. Finally, the results are compared with TEM thickness measurements.

Sample Preparation

The samples investigated in this study are [11-20] 4° off-oriented Wolfspeed (0001) 4H-SiC wafer. After an initial cleaning step, dry oxidation at 1050 °C for various oxidation times is performed, resulting in thicknesses of the silicon dioxide (SiO_2) between t_{ox} = 4 nm and t_{ox} = 30 nm. On one sample, a SiO_2 layer of t_{ox} = 30 nm is deposited by plasma-enhanced chemical vapor deposition (PECVD). Prior to the HR-AFM analysis, the oxides are stripped again by dipping the samples in hydrofluoric acid (HF 10%).

All measurements are conducted with a Bruker MultiMode 8 AFM in tapping mode with a frequency of 150 kHz. The probe tips used here have radii down to 2 nm to enhance lateral resolution. The scan direction is chosen to be approximately 45 degrees rotated with respect to the step-flow.

Microsteps after Oxidation

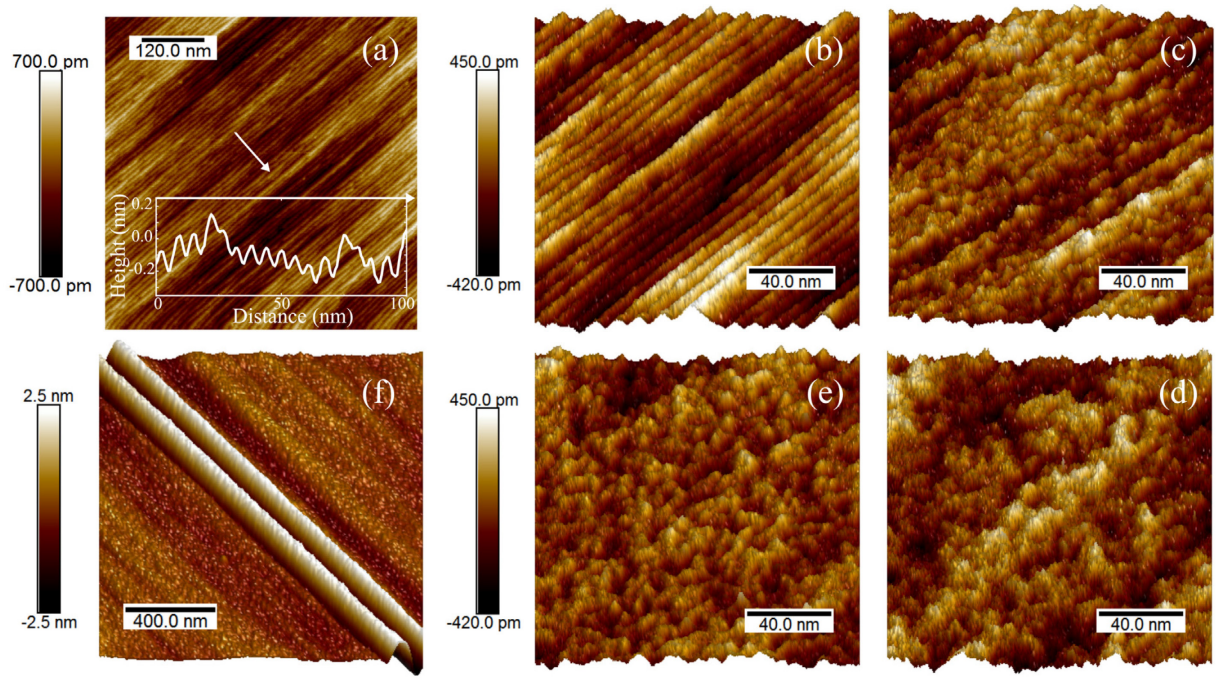

Fig. 1 (a) shows a height scan taken before thermal oxidation. The depicted area is free of isolated macrosteps but exhibits the previously described micro-faceting with an average terrace width of 6 to 7 nm. Even though the physical height of the microsteps cannot be resolved by the AFM tip, the distance between adjacent steps suggests that steps of two-bilayer height (i.e. 2.52 Å) are dominant.
Fig. 1: (a) AFM scan of (0001) 4H-SiC prior to oxidation. The inset shows a typical height profile perpendicular to the step flow with an average periodicity of 6 nm. Note that due to the large radius of the tip, the height of the steps cannot be accurately resolved. (b-e) Height maps after oxidation and SiO_2 removal for (b) a non-oxidized reference sample and (c) 10 min, (d) 4 h and (e) 24 h thermal oxidation at 1050°C. (f) Periodic and isolated macrosteps of several nanometers height are preserved even after 24 hours of oxidation.

After oxidation, all oxidized samples (together with a non-oxidized reference sample) are etched with HF for 2 minutes and re-measured. Fig. 1 (b-e) show 200 nm large height maps of the 4H-SiC surface after different oxidation times, clearly indicating a change in morphology and a smoothing of the step-bunching for increasing oxidation times. A distinct difference in surface faceting is already observed for thermal oxides of only a few nanometers (Fig. 1 (c)), while the sample with the PECVD-deposited and stripped SiO_2 maintained the original surface morphology (not shown here). The surface roughness (R_q) of the investigated samples shows a slightly decreasing trend for increasing oxidation time, reducing from R_q = 0.13 nm for the non-oxidized sample to R_q = 0.10 nm for the sample with t_{ox} = 30 nm.

Macrosteps on the other hand, are still present even after prolonged oxidation (Fig. 1 (f)), though also rounded. Watanabe et al. explain the smoothing of these steps by the differences in oxide thickness between terrace and riser and, related to this, different amounts of oxygen molecules diffusing through the SiO_2 layer, leading to the observed rounding of the edges [8].

Oxidation at Isolated Macrosteps

In order to assess how strongly the oxide thickness at the macrosteps is differing from the average thickness, TEM is used to measure the thickness of the SiO_2 layer and to compare it with macroscopic process simulations.

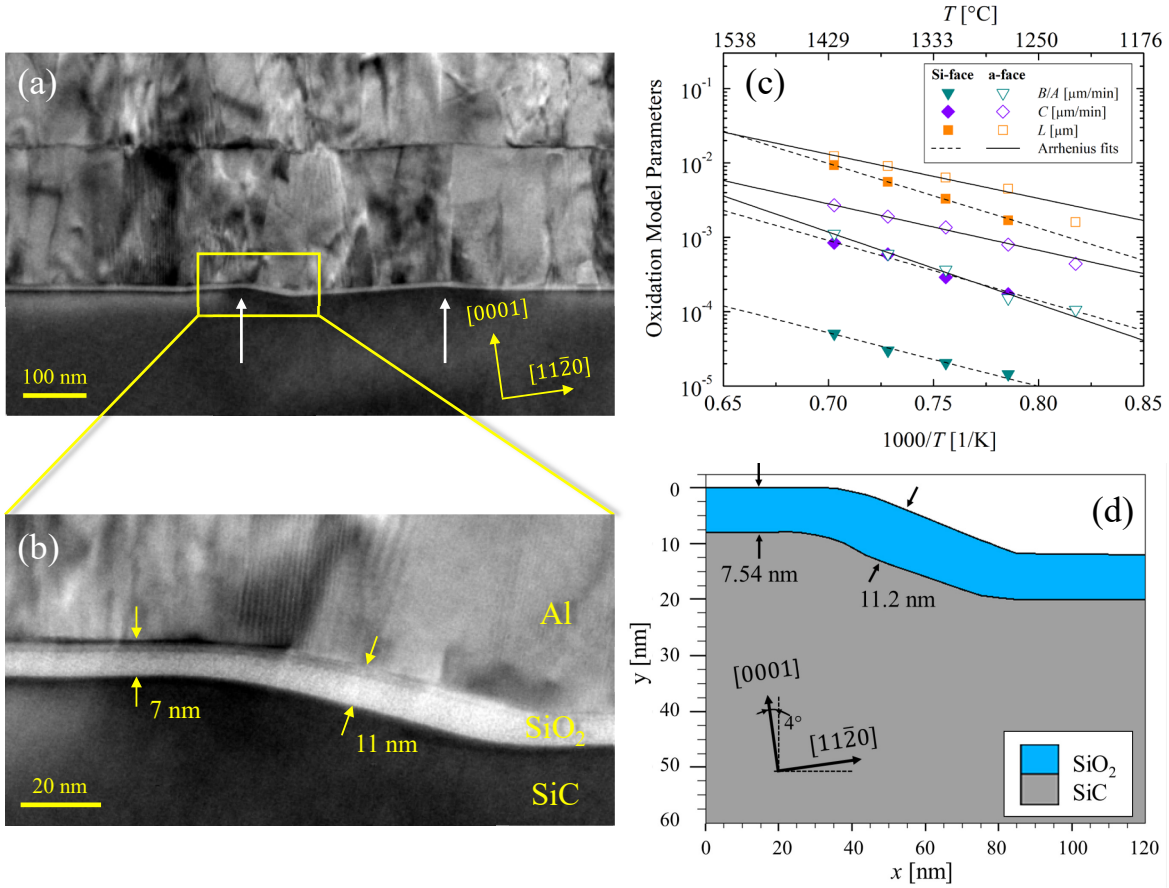

Fig. 2: (a) TEM cross-section of the SiO_2/SiC interface with a macrostep and its characteristic, i.e., double-hill-valley structure, as indicated by the two white arrows. The faces on the left-hand side of the arrows are terraces, the steeper faces on the right-hand side are risers. (b) The close-up image of a single macrostep clearly shows the difference in oxide thicknesses for the terrace and the riser. (c) Temperature-dependent oxidation model parameters used to predict the oxide growth for different crystal faces. (d) Results of the oxide growth simulations for this specific surface morphology, showing an excellent overlap with the measured oxide thicknesses from (a) and (b).

TEM Analysis. For the TEM analysis, one sample is oxidized for 4 hours (a twin sample of the one shown in Fig. 1. (d)) and a 500 nm thick aluminum film is deposited on the SiO_2 layer before the focused ion-beam (FIB) treatment. The TEM lamella is oriented along [11-20], perpendicular to the step-flow of the epitaxial layer and taken from a region of the sample where isolated macrosteps are present (Fig. 2 (a,b)). While the terraces of these macrosteps are atomically flat (0001) faces, the surface of the risers have (11-2n) orientation (n = 25-30) [9]. From the TEM image, the oxide thicknesses at the terrace and riser are determined to be 7 nm and 11 nm, respectively.

Orientation-Dependent Oxidation Model. Parallel to the described experiment, the oxidation growth process is simulated using Silvaco's Victory Process simulator. The simulations include calibrated SiC oxidation parameters [10], shown in Fig. 2 (c), and a unique three-dimensional interpolation method [11]. The anisotropic interpolation incorporates orientation dependence into the oxidation models according to any known growth rates ([0001] and [11-20] in this case) and thus enables accurate prediction of oxidation of arbitrary crystal structures. Fig. 2 (d) shows that the results from simulations are in excellent agreement with results from the TEM analysis.

Summary

The aim of this work was to deepen the understanding of morphological changes during the initial oxidation process and to investigate its impact on SiC device processing. Already after a few minutes of oxidation, no micro-faceting was observed anymore. Even after various cleaning and oxide-etch attempts, the initial morphology could not be recovered. Macrosteps, on the other hand, were still present even after extended oxidation times and experimental results showed strong deviations of the oxide thickness in vicinity of these morphological features. A direction-dependent SiC oxidation model was employed to accurately predict the variations in oxide thicknesses.

Acknowledgments

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