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Surface morphology of 4H-SiC after thermal oxidation

J. Woerle[1,2], V. Šimonka[3], E. Müller[1], A. Hössinger[4], H. Sigg[1], S. Selberherr[5], J. Weinbub[3], M. Camarda[1], U. Grossner[2]
[1] Paul Scherrer Institute, 5232 Villigen, Switzerland
[2] Advanced Power Semiconductor Laboratory, ETH Zurich, 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
E-mail: judith.woerle@psi.ch

Owing to the continuous efforts in substrate growth and epitaxy, 4H-SiC is nowadays the material of choice for many high-power and high-temperature applications. In order to achieve electronic-grade homoepitaxy of a single polytype, an off-axis growth technique, most commonly with an off-angle of 4° toward the [11-20] direction, is applied. For the (0001)Si-face, these surfaces then exhibit a continuous step pattern with nanometer-sized steps having a height of either 2 or 4 bilayers [1], as well as larger "macrosteps" with several nanometers height [2,3] and faces perpendicular to either the [0001] or [11-2n] direction [4]. When growing a thermal oxide on such step-bunched surfaces, an orientation dependence of the oxide growth rate, commonly explained by the differences in carbon and silicon emission rates during oxidation, is observed [5].

In this study, we use transmission electron microscopy (TEM) and high-resolution (HR) atomic-force microscopy (AFM) to study nano- and macrosteps of off-axis grown 4H-SiC after thermal oxidation and compare measured growth rates of silicon dioxide (SiO_2) for different faces with numerical process technology computer-aided design (TCAD) simulations.

All investigated samples were from the same 4°-off-oriented (0001) 4H-SiC wafer with a 5 µm thick n-type epitaxial layer. After an initial cleaning step, a dry oxidation step at 1050 °C for varying oxidation time, resulting in thicknesses of the oxide between $t_{ox} = 4$ nm and $t_{ox} = 30$ nm, was performed. For the TEM analysis, the lamellas were oriented along [11-20], perpendicular to the step-flow of the epitaxial layer and taken from a region of the sample where isolated macrosteps were present (Fig. 1a). While the terraces of these macrosteps are atomically flat (0001) faces, the surface of the risers have (11-2n) orientation (n = 25-30) [6]. From the TEM image, the oxide thicknesses at the terrace and riser were determined to be 7 nm and 11 nm, respectively.

Parallel to the experimental investigation, the oxidation growth process was simulated using Silvaco's Victory Process simulator. The simulations include calibrated SiC oxidation parameters [7], and a unique three-dimensional interpolation method [8]. The anisotropic interpolation incorporates orientation dependence into the oxidation models according to any known growth rates ([0001] and [11-20] in our case) and thus enables accurate predictions of oxidation behavior for arbitrary crystal structures via a macroscopic process simulation (Fig. 1b).

For the HR-AFM analysis, the SiO_2 layers were subsequently removed after growth by dipping the samples in hydrofluoric acid (HF 10%) in order to expose the SiC surface. All measurements were conducted with a *Bruker MultiMode 8* AFM in tapping mode using probe tips with radii down to 2 nm to enhance lateral resolution. Fig. 2 shows 200 nm large height maps of the 4H-SiC surface of different oxidation times, clearly showing the change in morphology and a smoothing of the step-bunching for increasing oxide thicknesses. A distinct difference in surface faceting is already observed for thermal oxides of only a few nanometers (Fig. 2b). Macrosteps on the other hand, are still present even after prolonged oxidation though also rounded (not shown here, see also [4]).

This work aims to investigate the role of the surface morphology during the initial oxidation process and, in a next step, to investigate its impact on SiC devices. Since the described nanosteps are always present at the 4H-SiC surface, their role during the oxide growth needs to be carefully considered in order to optimize the SiO_2/SiC interface.

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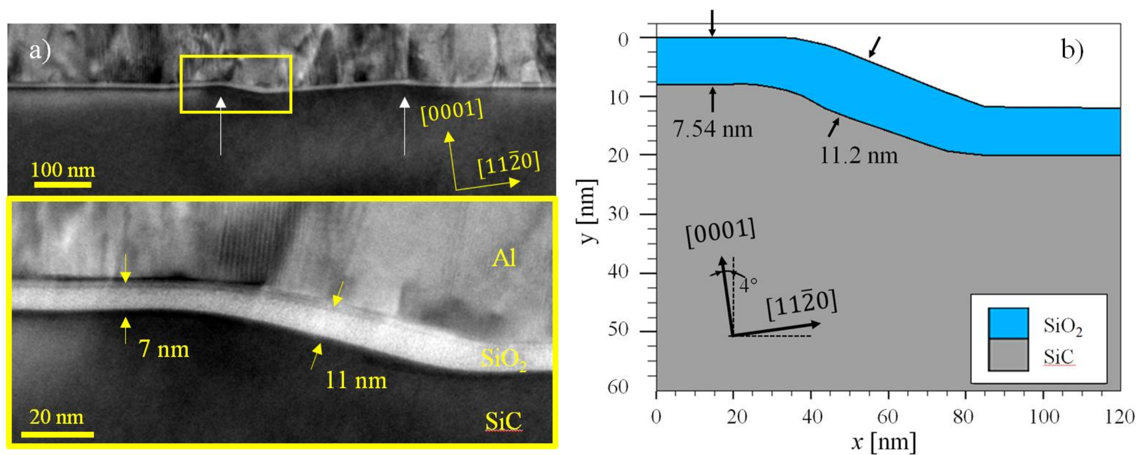

Fig. 1. (a) TEM cross-section of the SiO_2/SiC interface with a macrostep and its characteristic, i.e., double-hill-valley structure, as indicated by the two white arrows. The faces on the left-hand side of the arrows are terraces, the steeper faces on the right-hand side are risers. In the yellow frame below, a close-up image of a single macrostep clearly shows the difference in oxide thicknesses for the terrace and the riser. (b) Results of the oxide growth simulations for this specific surface morphology.

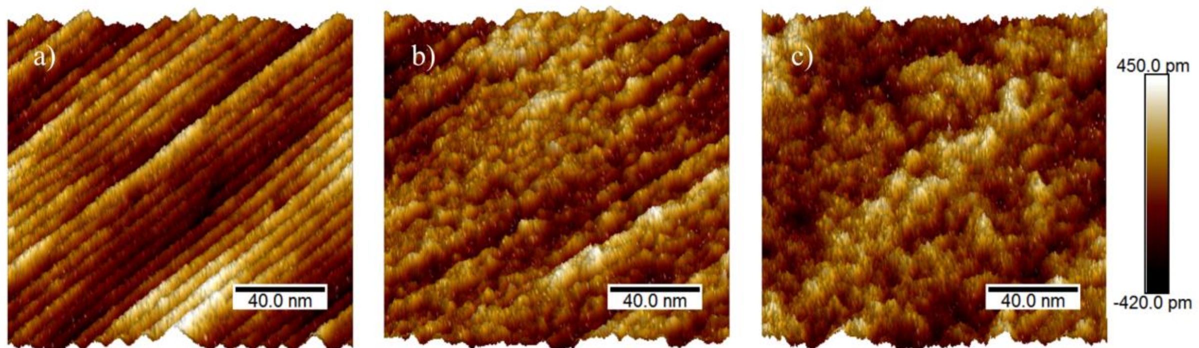

Fig. 2. Height maps of the 4H-SiC surface after oxidation and SiO_2 removal for (a) a non-oxidized reference sample and (b) 10 min and (c) 4 h of thermal oxidation.