# Geometrical Aspects of Three-Dimensional Silicon Carbide Oxidation Growth Rate Modeling

Vito Šimonka[*], Georg Nawratil[□], Andreas Hössinger[#], Josef Weinbub[*], Siegfried Selberherr[+]
[*]Christian Doppler Laboratory for High Performance TCAD at the
[+]Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Wien, Austria
[□]Institute of Discrete Mathematics and Geometry, TU Wien, Wiedner Hauptstraße 8-10, 1040 Wien, Austria
[#]Silvaco Europe Ltd., Compass Point, St Ives, Cambridge, PE27 5JL, United Kingdom
*Email: simonka@iue.tuwien.ac.at*

## 1. Introduction

We investigate geometrical aspects of silicon carbide (SiC) and propose a direction dependent interpolation method for computing oxidation growth rates for three-dimensional simulations. Additionally, we analyze the temperature dependence of SiC oxidation for different crystal directions. Our approach is an essential step for highly accurate three-dimensional oxide growth simulations.

SiC is a wide bandgap semiconductor and has superior physical properties for power device applications, such as approximately three times wider bandgap, ten times larger electrical break-down field, and three times higher thermal conductivity, compared to silicon [1,2]. Therefore, SiC devices (e.g. MOSFETs) can better operate under high pressure, high frequency, and high temperature environments.

However, thermal oxidation of SiC is considerably more complicated compared to the oxidation of silicon [2]. There are one-dimensional oxidation models available [1,2,3,4], where the most popular one is the Deal-Grove model [3] and the more accurate Massoud empirical relation [1]. Due to their one-dimensional nature those models cannot correctly predict oxidation growth for three-dimensional SiC structures. Our approach extends these models by incorporating crystal direction dependence into the oxidation growth rate modeling.

## 2. Geometry of SiC

In this work we focus on the 4H-SiC polytype as it has been recognized as the most promising material for electronic high power, high frequency, and high temperature applications [3]. Geometrical aspects of SiC must be described mathematically in order to calculate growth rate variations for different crystal directions. We thus propose an interpolation method to convert an arbitrary crystal direction into a growth rate of oxidation according to known growth rates [1]. For fixed points of oxidation growth rate values we use the (0001), (10-10), (11-20), and (000-1) direction, which have been examined experimentally [1,3] and correspond to the Si-, m-, a-, and C-plane, respectively (Fig. 1). The parametric expression of the interpolation method is:

$$\begin{aligned} x &= \left(k_y + \left(k_x - k_y\right)\cos^2(3t)\right)\cos(t)\cos(u), \\ y &= \left(k_y + \left(k_x - k_y\right)\cos^2(3t)\right)\sin(t)\cos(u), \\ z &= k_z^+ \sin(u) \quad \text{for} \quad u \geq 0, \\ z &= k_z^- \sin(u) \quad \text{for} \quad u < 0, \end{aligned} \tag{2}$$

where $t \in [0, 2\pi]$ and $u \in [-\pi/2, \pi/2]$ are arbitrary parametric variables and $k_{x,y,z}$ are known growth rates in $x$, $y$, and $z$ direction, respectively. The positive and negative $z$ coordinates are calculated separately, as the oxide growth on top $k_z^+$ and bottom $k_z^-$ of the crystal are different. The proposed growth rate surface is then given by a non-linear interpolation between the known growth rate values and follows the geometry of SiC, i.e. the planes tangent to the growth rate surface at $k_{Si}$, $k_m$, $k_a$, and $k_C$ are parallel to the corresponding atomic planes. It consists of a symmetric star shape in x-y plane and a tangent-continuous union of two half-ellipses in $z$ direction (Fig. 2). The SiC oxidation growth rate surface is shown in Fig. 4 and Fig. 5, and its intersection curves with the x-y and x-z planes are shown in Fig. 3.

## 3. Growth Rates of Oxidation

We have obtained the growth rates of Si-, a-, and C-plane from experimentally measured data [1] and approximated the growth rate for the m-plane linearly based on published oxide thicknesses [5].

As the oxidation of SiC strongly depends on the temperature we use an Arrhenius plot to analyze the effect of temperature on the growth rates. Fig. 6 shows Arrhenius plots of the growth rates for all four SiC planes. These plots allow to directly obtain fixed growth rate values for different oxidation temperatures.

## 4. Summary

We have proposed an interpolation method for oxidation rates based on the SiC geometry, which converts an arbitrary crystal direction into a growth rate value. This allows to calculate SiC oxidation growth rates in three dimensions according to four known growth rate values. These vary with oxidation temperature and can be calculated with provided Arrhenius plots.

The authors wish to thank Y. Hijikata for providing experimental data. The financial support by the *Austrian Federal Ministry of Science, Research and Economy* and the *National Foundation for Research, Technology and Development* is gratefully acknowledged.

**References**

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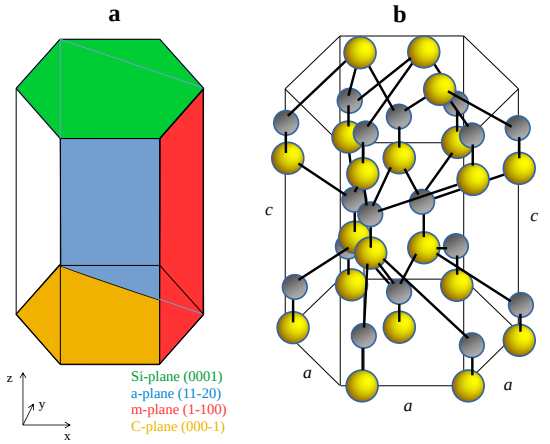


**Fig.1:** *A schematic illustration of* ***a)*** *atomic planes of a hexagonal structure and* ***b)*** *atomistic view of a 4H-SiC polytype with sequence ABAC. Green, blue, red, and orange shapes show the Si-, a-, m-, and C- plane, respectively. Yellow spheres show the Si atoms, gray spheres C atoms, a is crystal dimension, and c is the crystal height.*

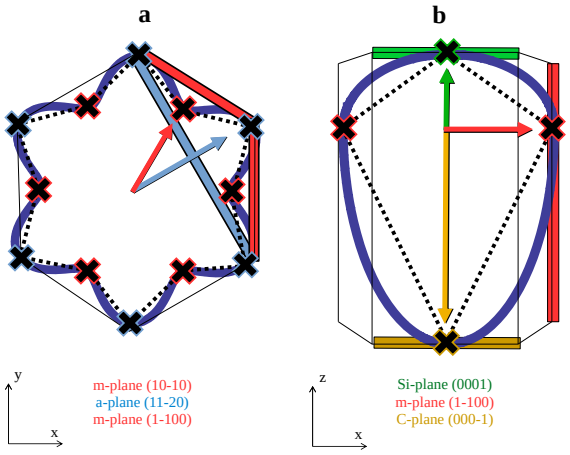


**Fig.2:** *Schematic representation of the two-dimensional interpolation in the* ***a)*** *x-y and* ***b)*** *x-z plane. A linear (black dotted) and a non-linear (dark blue line) interpolation is used according to known growth rate values (black crosses) of Si- (green), m- (red), a- (blue), and C-plane (orange square). Colored arrows present directions towards the atomic planes.*

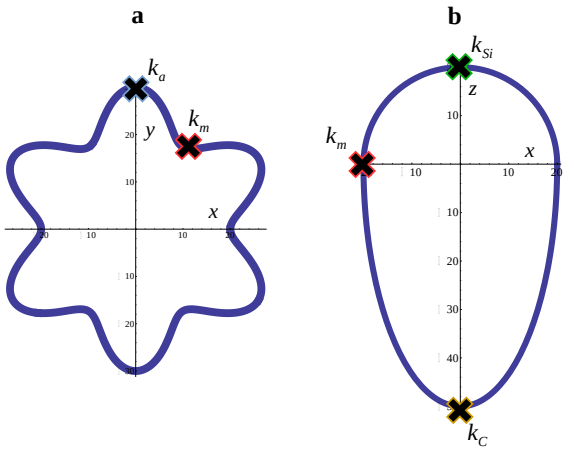


**Fig.3:** *Two-dimensional* ***a)*** *x-y and* ***b)*** *x-z plots of 4H-SiC oxidation growth rates. Non-linear interpolation of growth rates is performed with the proposed method according to the known growth rate values (black crosses).*

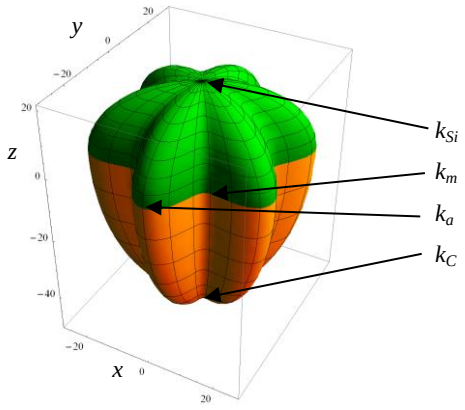


**Fig.4:** *Three-dimensional parametric plot of 4H-SiC oxidation growth rates. An arbitrary direction growth rate is calculated according to the four known growth rates ($k_{Si}$, $k_m$, $k_a$, and $k_C$) shown with black arrows. The surface color shows calculations for positive (green) and negative (orange) z direction.*

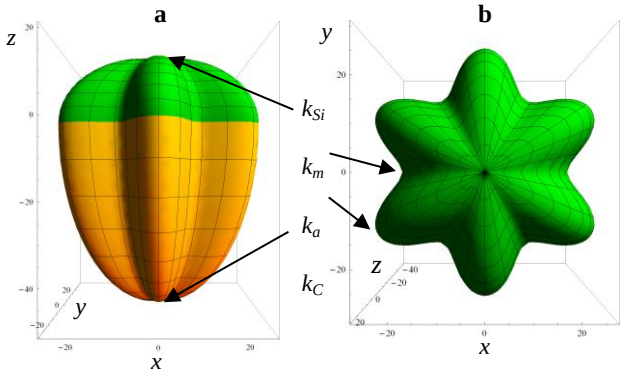


**Fig.5:** *Three-dimensional parametric plot of 4H-SiC oxidation growth rates from* ***a)*** *side and* ***b)*** *top view. The four fixed points for the calculations are shown with black arrows. The surface color shows calculations for positive (green) and negative (orange) z direction.*

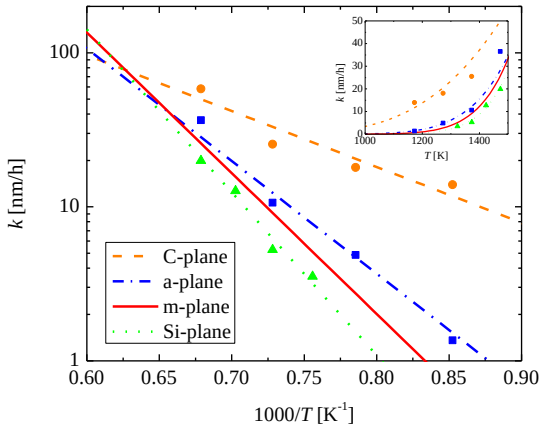


**Fig.6:** *Arrhenius plots of 4H-SiC oxidation growth rates versus oxidation temperature for the Si- (green), m- (red), a- (blue, and C-plane (orange). Experimental data for the Si-, a- and C- plane (symbols) were obtained from [1].*