Direction Dependent Three-Dimensional Silicon Carbide Oxidation Growth Rate Calculations

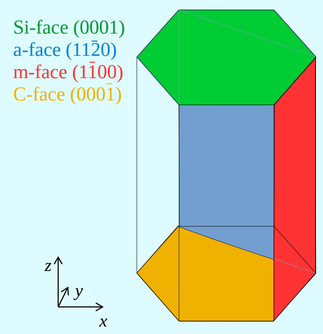
Vito Šimonka*, Georg Nawratil‡, Andreas Hössinger§, Josef Weinbub*, and Siegfried Selberherr†

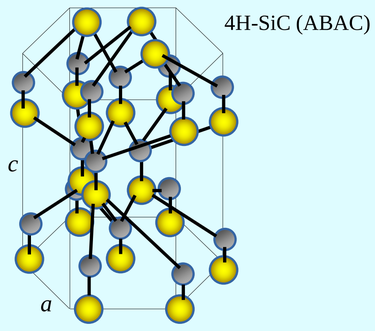
* Christian Doppler Laboratory for High Performance TCAD at the
†Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Wien, Austria
‡Institute of Discrete Mathematics and Geometry, TU Wien, Wiedner Hauptstraße 8-10, 1040 Wien, Austria
§Silvaco Europe Ltd., Compass Point, St Ives, Cambridge, PE27 5JL, United Kingdom

simonka@iue.tuwien.ac.at

Introduction

- We propose a direction dependent interpolation method for silicon carbide (SiC) oxidation growth rates.
- The rates for the three-dimensional simulations are computed according to the four known growth rate values.
- Our approach is an essential step towards highly accurate three-dimensional oxide growth simulations and helps to better understand the silicon carbide anisotropic nature and oxidation mechanism.





Thermal Oxidation Models

Deal-Grove [1]

$$\frac{dX}{dt} = \frac{B}{A + 2X}$$

- $B/A \rightarrow$ linear rate constant
- B $\rightarrow$ parabolic rate constant

Massoud empirical relation [2]

$$\frac{dX}{dt} = \frac{B}{A + 2X} + C \exp\left(-\frac{X}{L}\right)$$

- $C \rightarrow$ exponential prefactor
- $L \rightarrow$ characteristic length

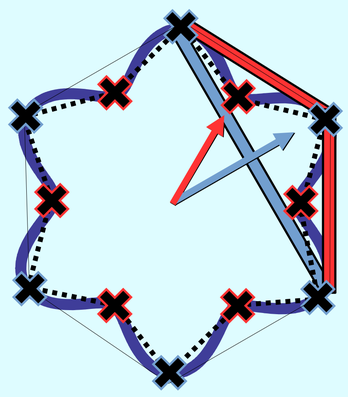
- All parameters depend highly on the crystal orientation of SiC.
- Due to the one-dimensional nature those models cannot correctly predict oxidation growth for three-dimensional SiC structures.
- We extend these models by incorporating the crystal direction dependence into the oxidation growth rates.

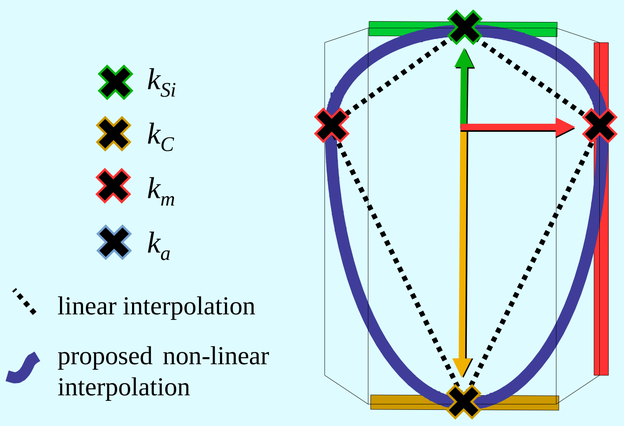
Interpolation Method

- The non-linear interpolation is written as a parametric function.
- A symmetric star shape in the x-y plane and a tangent-continuous union of two half-ellipses in z direction are used:

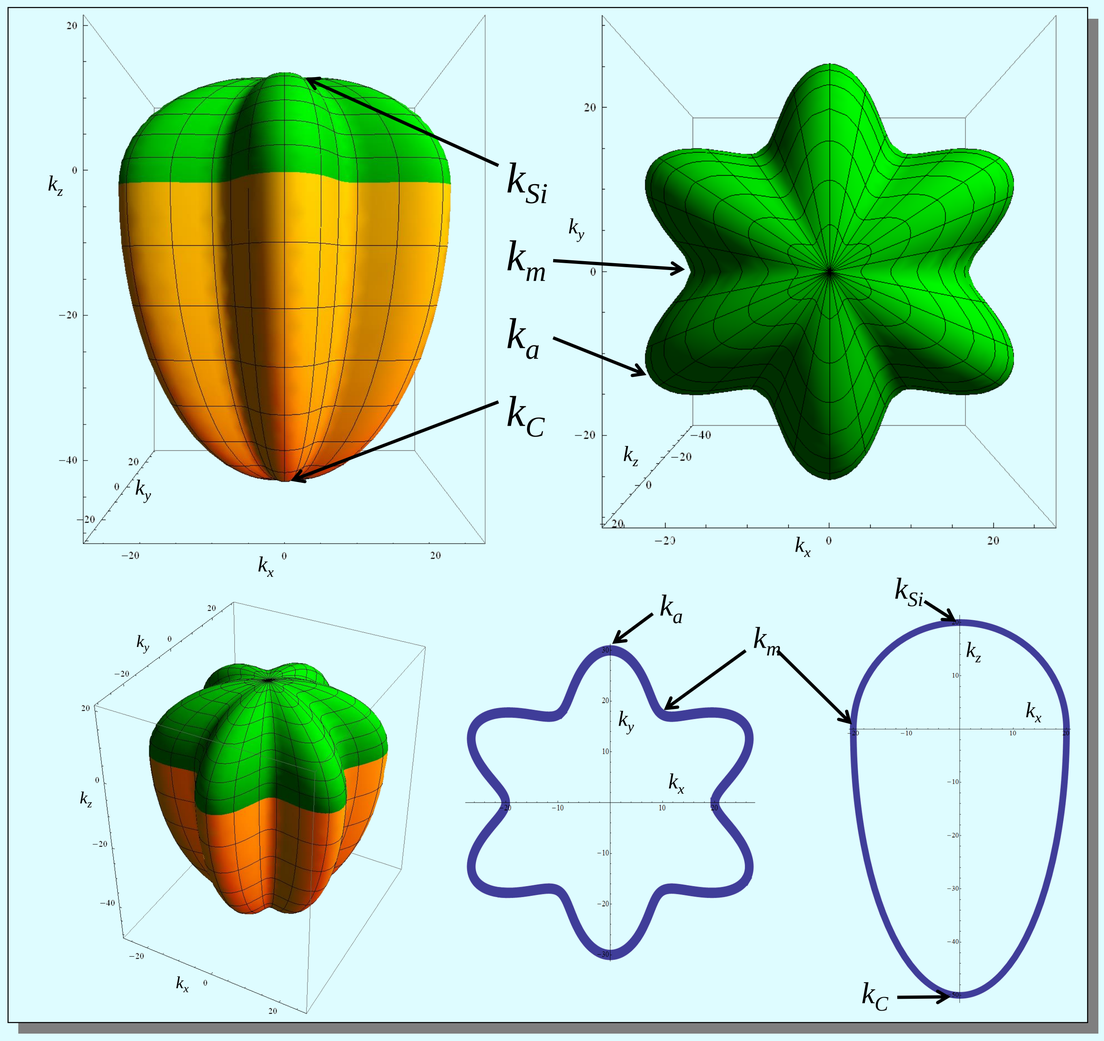
$$x = \left(k_y + \left(k_x - k_y\right)\cos^2\left(3t\right)\right)\cos\left(t\right)\cos\left(u\right)$$
$$y = \left(k_y + \left(k_x - k_y\right)\cos^2\left(3t\right)\right)\sin\left(t\right)\cos\left(u\right)$$
$$z = k_z^+ \sin\left(u\right) \text{ for } u \geq 0$$
$$z = k_z^- \sin\left(u\right) \text{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

- $t \in [0, 2\pi]$ and $u \in [-\pi/2, \pi/2] \rightarrow$ arbitrary parametric variables
- $k_{x,y,z} \rightarrow$ known oxidation growth rates in x, y, and z direction

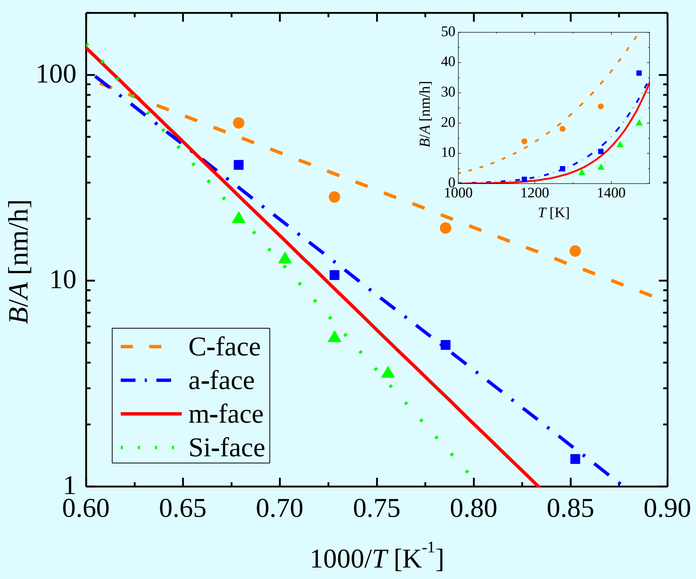




Results – The Growth Rate Surface



Growth Rates – Arrhenius Plot



- The relation between the temperature and the rate constant of the chemical reaction is defined by an Arrhenius equation:

$$k = Z \exp\left(-\frac{E_a}{RT}\right)$$

- We have obtained the growth rates and activation energies of the Si-, a-, and C-face from experimentally measured data [3].
- We have approximated the growth rate and activation energy for the m-face, based on published oxide thicknesses [4].

Conclusions

- The proposed interpolation method matches with the three-dimensional behavior of SiC oxidation.
- The method converts an arbitrary crystal direction into a growth rate value according to four known growth rate values.
- The necessary growth rates are provided with Arrhenius plots.

Acknowledgement

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

[1] B. E. Deal and A. Grove, Journal of Applied Physics **36** (1965).
[2] H. Z. Massoud et al., Journal of the Electrochemical Society **132** (1985).
[3] D. Goto et al., Journal of Applied Physics **117** (2015).
[4] J. Ahn et al., Nanoscale Research Letters **6** (2011).