

Direction Dependent Three-Dimensional Silicon Carbide Oxidation Growth Rate Calculations

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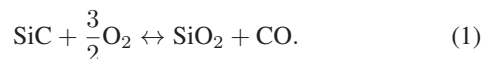
Abstract—We propose a direction dependent interpolation method for silicon carbide oxidation growth rates and we compute these rates for three-dimensional simulations according to known growth rate values. Additionally, we analyze the temperature dependence of silicon carbide oxidation for different crystal directions. 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.

I. INTRODUCTION

Silicon carbide (SiC) is a wide bandgap semiconductor and has superior physical properties for power device applications, such as approximately three times wider band gap, ten times larger electrical break-down field, and three times higher thermal conductivity, compared to silicon (Si) [1], [2]. Taking advantages of these properties, the on-state resistance for unipolar devices such as metal-oxide-semiconductor field-effect-transistors (MOSFETs) can be reduced by a factor of a few hundreds when replacing Si with SiC [3], [4].

3C-SiC, 4H-SiC, 6H-SiC, and 15R-SiC are the most common polytypes presently being developed for device applications. These polytypes are characterized by the stacking sequence of the bi-atom layers of the SiC structure. Changing of the stacking sequence has a profound effect on the electrical properties. In this work we focus only 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 [5].

Thermally grown silicon oxide (SiO₂) plays a unique role in device fabrication. Among the wide bandgap semiconductors, SiC is the only compound semiconductor which can be thermally oxidized in the form of SiO₂, similar to the Si substrate. The oxidation reaction of SiC is defined by [5]:



However, thermal oxidation of SiC is considerably more complicated compared to the oxidation of Si [2] and is about one order of magnitude slower under the same conditions [6], [7]. The oxidation of SiC additionally includes the out-diffusion of product gasses (e.g. CO) through the oxide film. Another unique phenomenon has been observed: The oxidation of SiC is a face-terminated oxidation, i.e., the top and the bottom face

have different oxidation rates [8]–[10]. Fig. 1 shows popular faces of 4H-SiC.

In Section II we discuss thermal oxidation models of Si and SiC, in Section III we introduce the temperature dependence of oxidation growth rates with Arrhenius plots, and in Section IV we discuss geometrical aspects of SiC, proposed interpolation methods, and results.

II. THERMAL OXIDATION MODELS

There are several one-dimensional Si and SiC oxidation models available [1], [2], [5], [11]–[17], of which the most popular one is the Deal-Grove model [5], [11], [14] and the more accurate Massoud empirical relation [1], [12]. The Deal-Grove model assumes that the oxidation occurs by diffusion of the oxidant to the SiO₂/Si interface, where it reacts with Si. This process is expressed by the following parabolic ordinary differential equation for the oxide thickness X over time [11],

$$\frac{dX}{dt} = \frac{B}{A + 2X}, \quad (2)$$

where B/A and B denote the linear and parabolic rate constants of oxidation, respectively. The oxidation process cannot be characterized by the Deal-Grove model for the thin oxide region, hence Massoud *et al.* have proposed an empirical relation to describe the growth rate enhancement. This model includes an additional exponential term [12],

$$\frac{dX}{dt} = \frac{B}{A + 2X} + C \exp\left(-\frac{X}{L}\right), \quad (3)$$

where C and L are the exponential prefactor and the characteristic length, respectively. All of the above parameters (B/A , B , C and L) are highly dependent on the crystal orientation of SiC [1], [5], i.e., the parameter values are different for the surface oxidation on different faces of the crystal.

The Deal-Grove and Massoud *et al.* models were originally proposed for Si oxidation, but can be applied in a modified form to SiC oxidation [2]. However, due to the one-dimensional nature those models cannot correctly predict oxidation growth for three-dimensional SiC structures. Our approach extends these models by incorporating the crystal direction dependence into the oxidation growth rates.

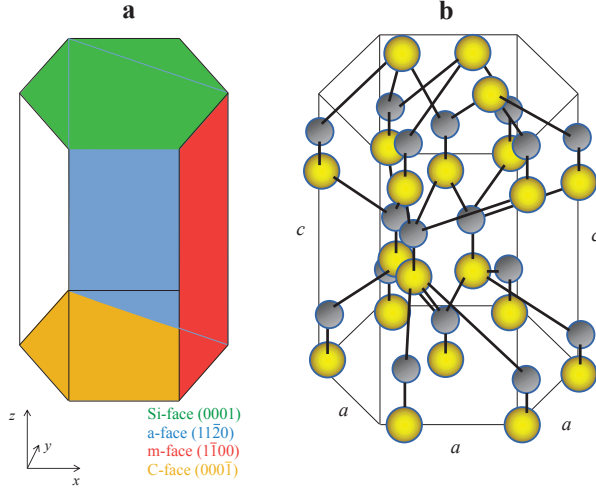


Fig. 1. A schematic illustration of **a**) common faces of a hexagonal structure and **b**) atomic view of a 4H-SiC polytype with sequence ABAC. Green, blue, red, and orange shapes show the Si-, a-, m-, and C-face, respectively. Yellow spheres show the Si atoms, gray spheres C atoms, a is crystal dimension, and c is the crystal height. The ratio between c and a for 4H-SiC is approximately three and for 6H-SiC approximately five.

III. GROWTH RATES OF OXIDATION

The rate of any chemical reaction depends on various physical quantities, e.g., temperature and pressure. As the temperature increases, the molecules move faster and collide more frequently with each other. The proportion of collisions influences the kinetic energy of the molecules and the activation energy of the chemical reaction. The relation between the temperature T and the rate constant of the chemical reaction k is defined by the Arrhenius equation [18]

$$k = Z \exp\left(-\frac{E_a}{RT}\right), \quad (4)$$

where Z is the pre-exponential factor, E_a is the activation energy of the chemical reaction, and R is the ideal gas constant. The Arrhenius equation can be used to determine the activation energy [1] when applying the natural logarithm on both sides of the equation.

$$\ln(k) = -\frac{E_a}{R} \frac{1}{T} + \ln(Z) \quad (5)$$

The equation has the form of a linear function $y = mx + n$, with the slope $m = -E_a/R$ and the intercept $n = \ln(Z)$.

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 of oxidation. Fig. 2 and Fig. 3 show Arrhenius plots of the linear growth rates B/A and initial growth rates $B/A + C$ for the four SiC faces, respectively. The data points are measured values, the dashed lines are fits using Massoud's empirical relation (Eq. 3), and the solid lines are approximated values. We have obtained the growth rates and activation energies of the Si-, a-, and C-face from experimentally measured data [1]. Additionally, we have approximated the growth rate and activation energy for the m-face, based on published oxide thicknesses [19], as there are

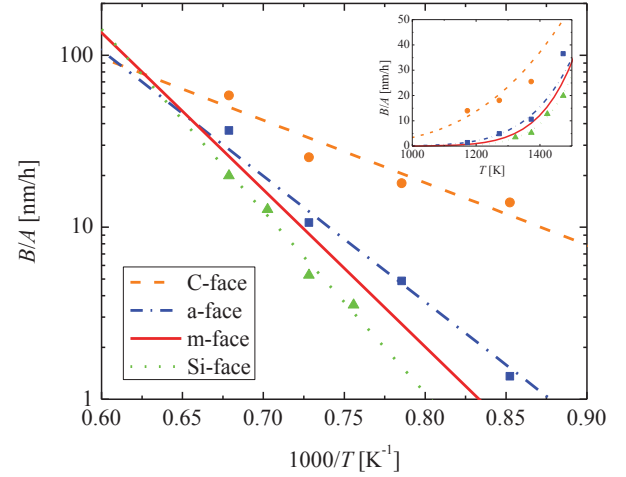


Fig. 2. Arrhenius plots of 4H-SiC oxidation, linear growth rates B/A versus oxidation temperature for the Si- (green), m- (red), a- (blue), and C-face (orange). Experimental data for the Si-, a-, and C-face (symbols) were obtained from [1] and the data for the m-face (solid lines) were approximated from [19].

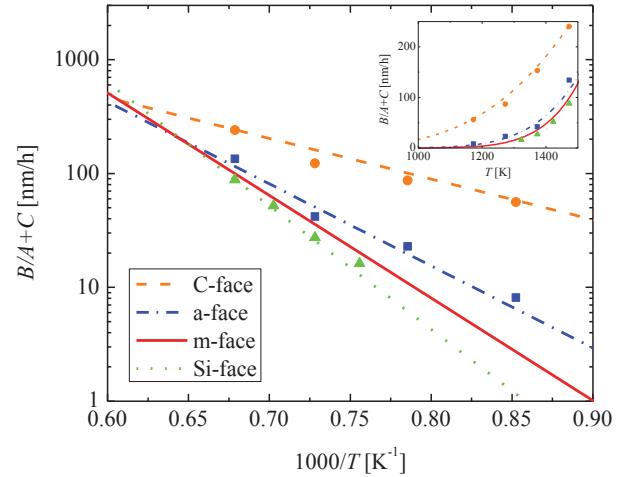


Fig. 3. Arrhenius plots of 4H-SiC oxidation, initial growth rates $B/A + C$ versus oxidation temperature for the Si- (green), m- (red), a- (blue), and C-face (orange). Experimental data for the Si-, a-, and C-face (symbols) were obtained from [1] and the data for the m-face (solid lines) were approximated from [19].

no experimental data available. These plots allow to directly obtain fixed growth rate values for different oxidation temperatures in order to perform growth rate surface calculations.

The linear growth rates are used when the oxide thickness X is far below the characteristic thickness A , in which the rate-limiting step is the interface oxidation reaction. The initial growth rates are used for the thin oxide region when X is approximated by zero. We do not show the Arrhenius plot of the parabolic rate constant B , as its value and activation energy do not depend on the crystal orientation [1].

IV. GEOMETRY OF SiC

Geometrical aspects of SiC must be described mathematically in order to calculate growth rate variations for different crystal directions. We propose a direction dependent interpolation method to convert an arbitrary crystal direction into a growth rate for oxidation, according to a set of known growth rate values [1]. For fixed points of oxidation growth rates we use the (0001), (10 $\bar{1}$ 0), (11 $\bar{2}$ 0), and (000 $\bar{1}$) directions, which have been examined experimentally [1], [5], [19] and correspond to the Si-, m-, a-, and C-face, respectively (see Fig. 1). Note, the hexagonal structure includes six m- and six a-faces, while it has only one Si- and one C-face.

The proposed interpolation is written as a parametric function, which consists of a symmetric star shape in the x-y plane and a tangent-continuous union of two half-ellipses in z direction. Fig. 4 shows the fixed points of the growth rates and the interpolation curves between them in the x-y and x-z planes. A linear star-shaped interpolation with sharp edges would fit the geometry of SiC well enough, but rather more accurate and realistic is a non-linear interpolation.

The parametric function of the three-dimensional interpolation method is

$$\begin{aligned} x &= \left(k_y + (k_x - k_y) \cos^2(3t) \right) \cos(t) \cos(u), \\ y &= \left(k_y + (k_x - k_y) \cos^2(3t) \right) \sin(t) \cos(u), \\ z &= k_z^+ \sin(u) \text{ for } u \geq 0, \\ z &= k_z^- \sin(u) \text{ for } u < 0, \end{aligned} \quad (6)$$

where $t \in [0, 2\pi]$ and $u \in [-\pi/2, \pi/2]$ are arbitrary parametric variables and $k_{x,y,z}$ are known oxidation 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 is different. The growth rates k_x , k_y , k_z^+ and k_z^- correspond to k_m , k_a , k_{Si} and k_C , which are the growth rates in the directions of the m-, a-, Si- and C-face, respectively. The growth rate surface is given by a non-linear interpolation between these 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 faces.

The hexagonal structure of SiC gives geometrical symmetry in the x-y plane so that the crystal directions towards a- and m-faces repeat six times with an enclosed angle of $\pi/6$. Hence, the proposed interpolation method match with the three-dimensional behavior of SiC oxidation. The SiC oxidation growth rate surface is shown in Fig. 5, Fig. 6, and Fig. 7, respectively.

The distance from the origin $0 = (0, 0, 0)$ to any point on the growth rate surface gives the growth rate in direction to this point. The set of growth rate values together with the SiC oxidation models can be used for three-dimensional oxidation growth simulations.

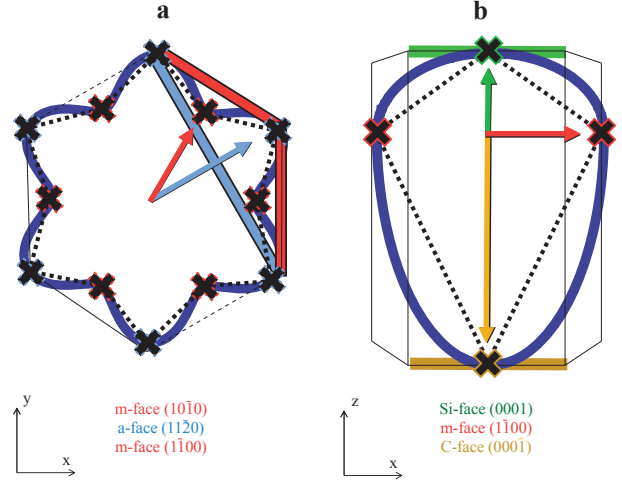


Fig. 4. Schematic representation of the two-dimensional interpolation in the **a)** x-y and **b)** x-z plane. A linear (black dotted) and a non-linear (dark blue line) interpolation is used according to known growth rate values (black crosses) of Si- (green), m- (red), a- (blue), and C-face (orange square). Colored arrows represent crystal directions towards the corresponding faces.

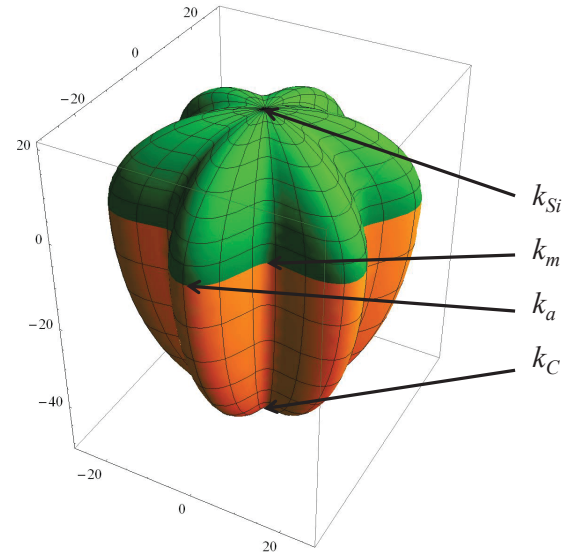


Fig. 5. Three-dimensional parametric plot of 4H-SiC oxidation growth rates. An arbitrary direction growth rate is calculated according to the four known growth rates (k_{Si} , k_m , k_a , and k_C) shown with black arrows. The surface color shows calculations for positive (green) and negative (orange) z direction.

V. 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 the provided Arrhenius plots.

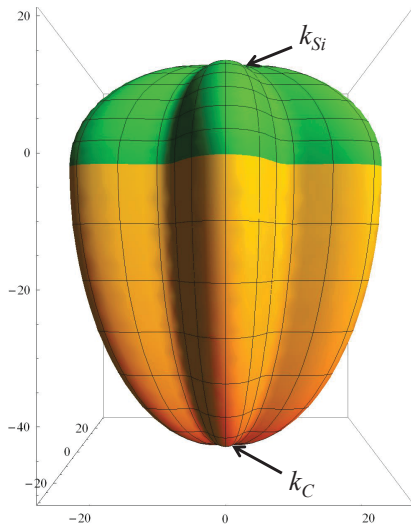


Fig. 6. Front view of the three-dimensional parametric plot of 4H-SiC oxidation growth rates. The two fixed points k_{Si} and k_C are shown with black arrows and correspond to Si- and C-face, respectively. The surface color shows calculations for positive (green) and negative (orange) z direction.

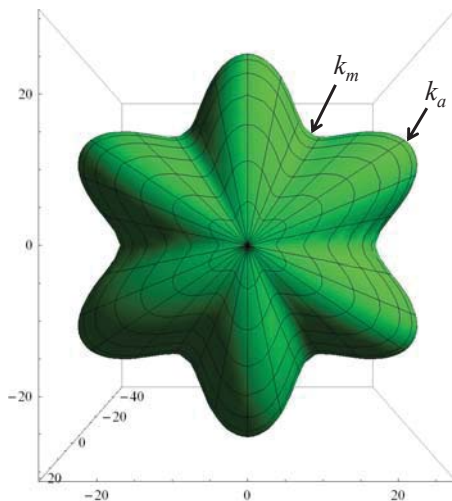


Fig. 7. Top view of the three-dimensional parametric plot of 4H-SiC oxidation growth rates. Black arrows show one of the six fixed points k_m and k_a , which correspond to an m- and a-face, respectively.

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