



OXYSIM

An Oxidation Simulator

User Manual

ICF Project

Under the guidance of

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Submitted By:

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In this manual, we will guide you through the various functionalities of OXYSIM and how to use them. This is a step-by-step tutorial for our Oxidation Simulator Tool OXYSIM.

1. **The Introduction Window:** This window displays the name of the tool, creators, and options to move on to the next window or exit.



Fig. 1: Introduction Window

Press Start to move on the menu window and press Quit to exit the tool.

2. **The Menu Window:** After you press Start on the Introduction window, the introduction window will disappear, and you will be guided to the Menu window on which you can see various options available. A brief description of the available options is given below:
 - **Single Stage Oxidation:** This option simulates Single Stage Oxidation with two models, namely, Deal Grove Model and Deal Grove Model with Massoud approximation. After the simulation, you will get the final oxide thickness. You can also plot the graph between the oxide thickness and time.
 - **Multi-Stage Oxidation:** This option simulates Multi-Stage Oxidation with two models, namely, Deal Grove Model and Deal Grove Model with Massoud

approximation. The tool supports five stages of oxidation. After the simulation, you will get the final oxide thickness after every stage. You can also plot the graph between the oxide thickness and time.

- Find Oxide Color: You can use this option to find the color of the oxide corresponding to a particular thickness of the oxide.
- Coefficients: This option displays the numerical values of the coefficients; we are using our tool for the calculations.
- Important Graphs: This option contains important graphs related to oxidation, such as Oxidation curves of silicon with $\langle 100 \rangle$, $\langle 111 \rangle$ orientations, and the linear and parabolic rate constant graphs. These graphs can come in handy to verify the results.
- Quit: To exit the Menu window, press this button.

The windowshot of the Menu window is shown below.

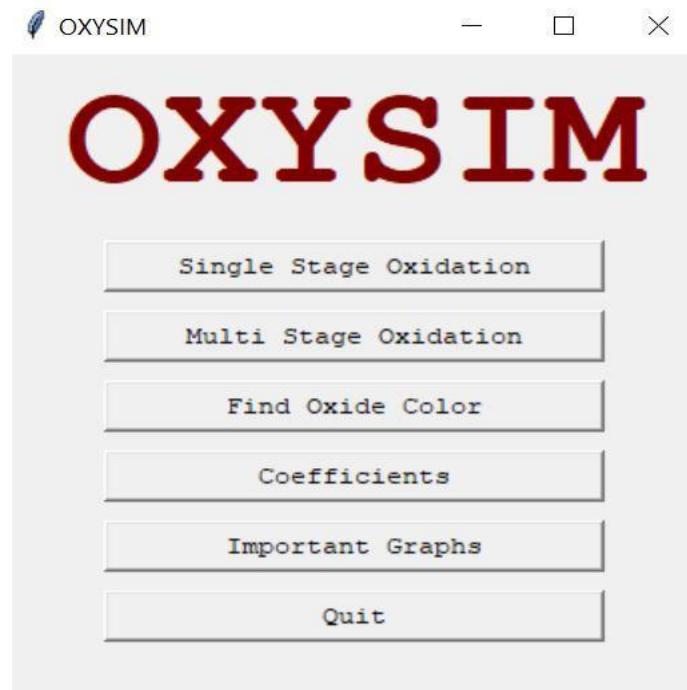


Fig. 2: Menu Window

3. **Single Stage Oxidation:** On pressing the Single Stage Oxidation Button on the Menu window, you will be guided to the following window.

Fig. 3: Single Stage Oxidation Main Window

The various inputs in this window are described below:

1. Oxidation Model: Using this dropdown, you can select the model you want to choose for the calculations. OXYSIM supports two models, namely the Deal Grove Model and Deal Grove model with Massoud approximation. Default is the Deal Grove Model.
2. Crystal Orientation: Using this dropdown, you can select the crystal orientation as $\langle 100 \rangle$ or $\langle 111 \rangle$. Default is $\langle 111 \rangle$ orientation.
3. Oxidation Type: Using this dropdown, you can select the Oxidation type as Wet or Dry. The default is Wet.
4. Temperature: This is the entry field for Temperature in the units of degree Celcius. If you don't enter anything, the tool takes the default value as 1100 degrees Celsius.
5. Duration of oxidation: This is the entry field for the time of oxidation in hours. If you don't enter anything, the tool takes the default value as 1 hour.
6. If you have an initial thickness, then select Y in the dropdown and enter the initial thickness in the textbox. If Y is not selected, the tool will not take the initial thickness value for calculation.

Click on Submit, and you will get the final oxide thickness with an option to plot the graph.

Single Stage Oxidation

Oxidation Model: Deal Grove + Massoud Model

Crystal Orientation: 100

Oxidation Type: Dry

Temperature(degree Celcius): 1200

Duration of Oxidation(in hours): 2

Do you have initial oxide thickness(Y/N): Y

Enter the initial oxide thickness(in um): 0.2

Submit

The calculated oxide thickness (in um): 0.335

Do you want to plot the graph?: Yes No

Fig. 4: Single Stage Oxidation Window for (Deal Grove + Massoud) Models

Press Yes to plot the graph and press No to exit the Single Stage Oxidation Window.

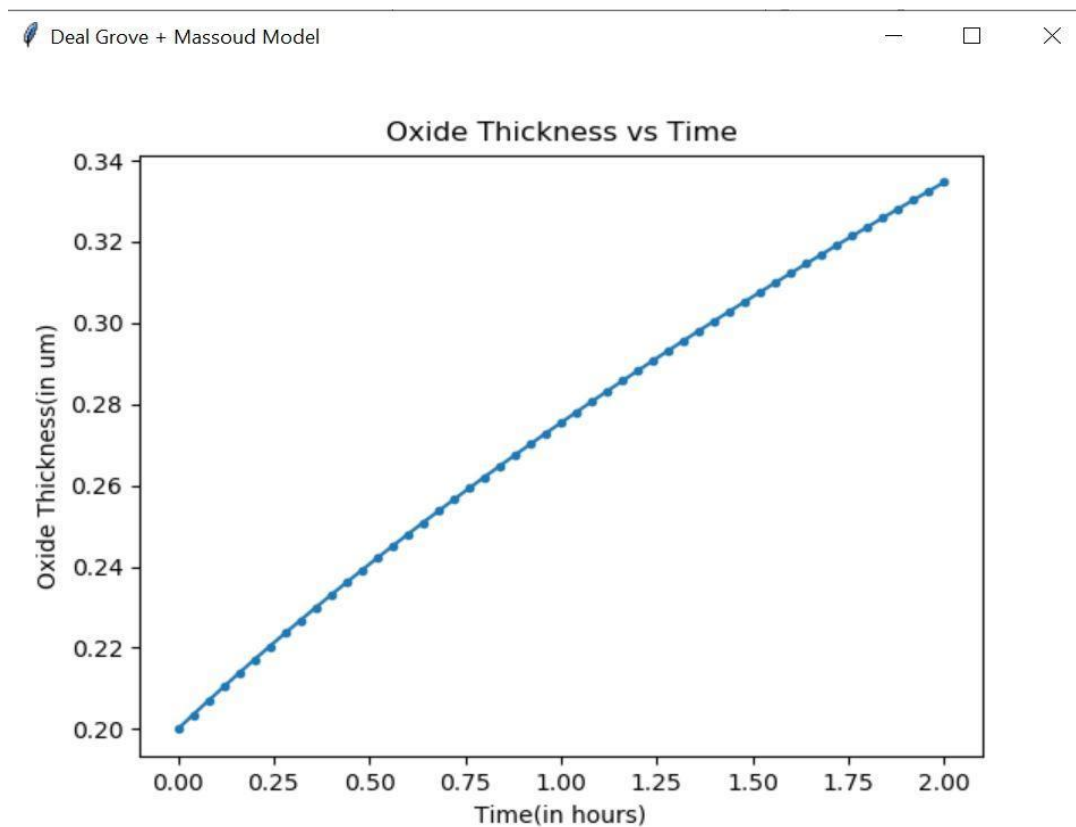


Fig. 5: Graph for Single Stage Oxidation (Deal Grove + Massoud Model)

Single Stage Oxidation

Oxidation Model: Deal Grove Model

Crystal Orientation: 100

Oxidation Type: Wet

Temperature(degree Celcius): 1200

Duration of Oxidation(in hours): 2

Do you have initial oxide thickness(Y/N): Y

Enter the initial oxide thickness(in um): 0.2

Submit

The calculated oxide thickness (in um): 1.265

Do you want to plot the graph?: Yes No

Fig.6: Single Stage Oxidation Window for Deal Grove Model

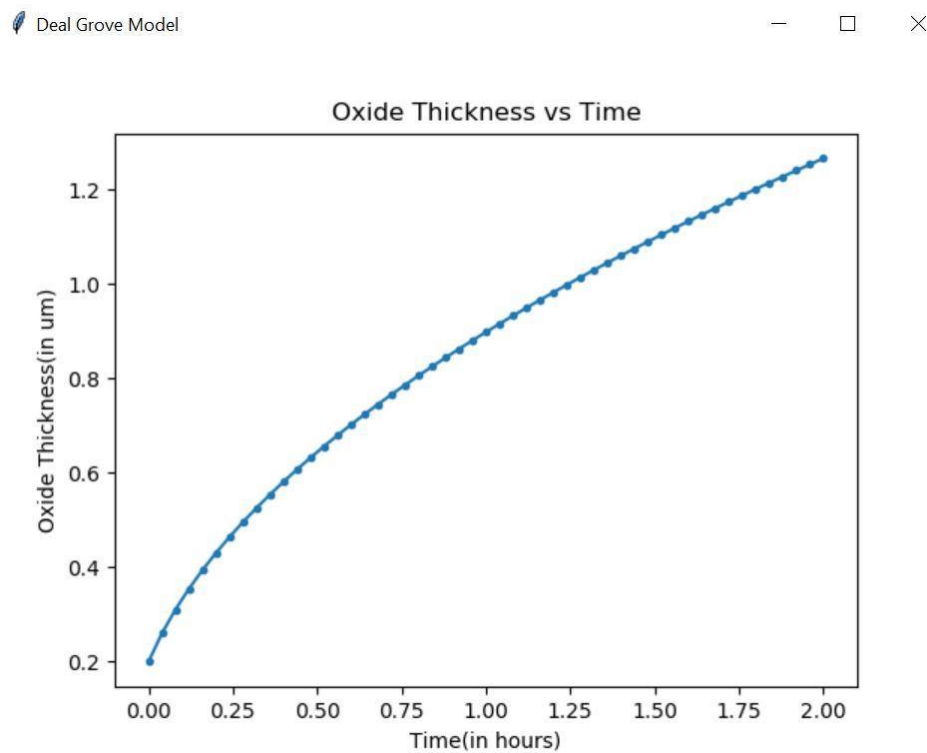
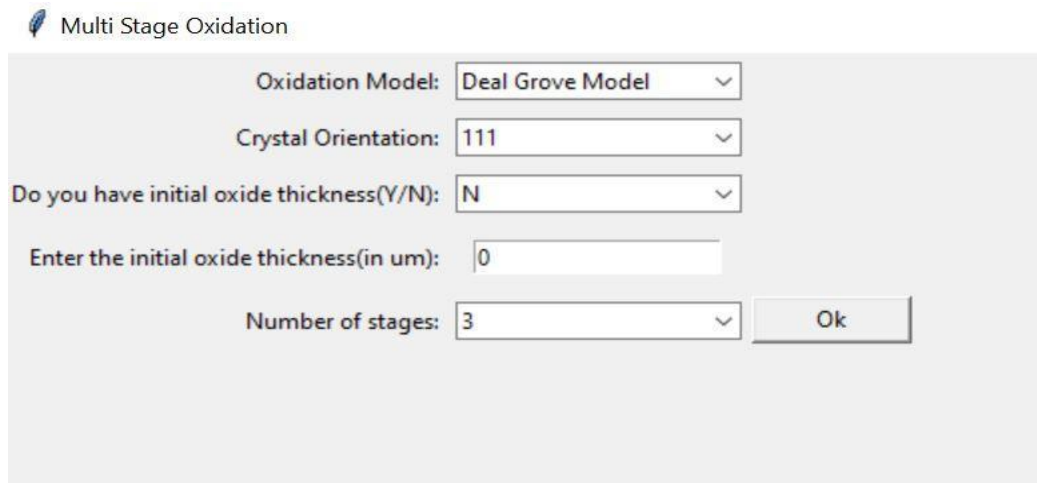


Fig. 7: Output Graph for Single Stage Oxidation (Deal Grove Model)

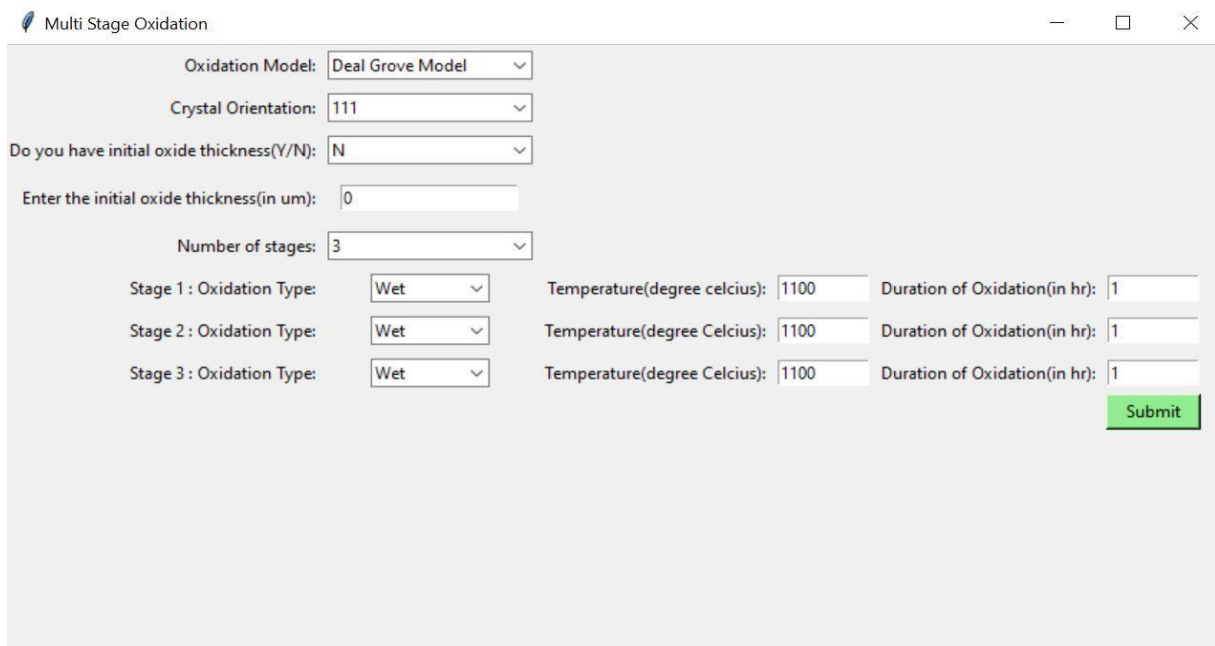
4. **Multi-Stage Oxidation:** On pressing the Multi-Stage Oxidation Button on the Menu window, you will be guided to the following window.



The image shows a software window titled "Multi Stage Oxidation". It contains several input fields and a button. The fields are: "Oxidation Model:" with a dropdown menu showing "Deal Grove Model"; "Crystal Orientation:" with a dropdown menu showing "111"; "Do you have initial oxide thickness(Y/N):" with a dropdown menu showing "N"; "Enter the initial oxide thickness(in um):" with a text input field containing "0"; and "Number of stages:" with a dropdown menu showing "3". To the right of these fields is an "Ok" button.

Fig. 8: Multi Stage Oxidation Main Window

On giving inputs for Oxidation Model, Crystal Orientation, Initial Thickness, and Number of stages click on, Ok. Once you click Ok, depending on the number of stages, Oxidation Type, Duration, and Temperature of oxidation will be asked for various stages. After submitting, you will get the oxide thickness after every stage. Similar to the Single Stage Oxidation, you can also plot a graph for the Oxidation Thickness vs. Time.



The image shows a software window titled "Multi Stage Oxidation" with standard window controls (minimize, maximize, close) in the top right corner. It contains the same initial input fields as Figure 8: "Oxidation Model:" (Deal Grove Model), "Crystal Orientation:" (111), "Do you have initial oxide thickness(Y/N):" (N), "Enter the initial oxide thickness(in um):" (0), and "Number of stages:" (3). Below these, there are three rows of inputs for each stage. For each stage, there is a dropdown for "Oxidation Type:" (all set to "Wet"), a text input for "Temperature(degree celcius):" (all set to "1100"), and a text input for "Duration of Oxidation(in hr):" (all set to "1"). A green "Submit" button is located at the bottom right of the window.

Fig. 9: Multi Stage Oxidation Window for Deal Grove model

Multi Stage Oxidation

Oxidation Model: Deal Grove Model

Crystal Orientation: 100

Do you have initial oxide thickness(Y/N): Y

Enter the initial oxide thickness(in um): 0.12

Number of stages: 3

Stage 1 : Oxidation Type: Wet Temperature(degree celcius): 1100 Duration of Oxidation(in hr): 1

Stage 2 : Oxidation Type: Dry Temperature(degree Celcius): 1200 Duration of Oxidation(in hr): 5

Stage 3 : Oxidation Type: Wet Temperature(degree Celcius): 1150 Duration of Oxidation(in hr): 1

Submit

Oxide Thickness after Stage 1: 0.666 Oxide Thickness after Stage 3: 1.39 Oxide Thickness after Stage 5:

Oxide Thickness after Stage 2: 0.818 Oxide Thickness after Stage 4:

Do you want to plot the graph?: Yes No

Fig. 10: Multi Stage Oxidation Output Window For Deal Grove Model

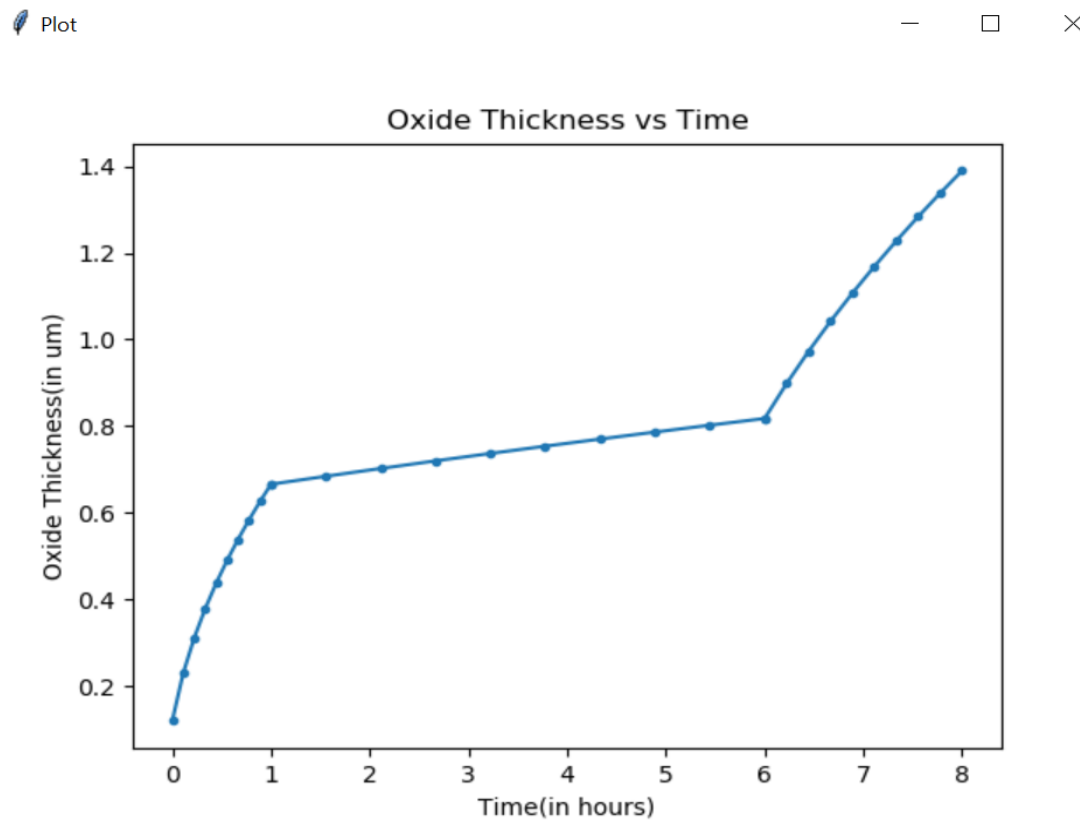


Fig. 11: Output Graph For Multi Stage Oxidation (Deal Grove Model)

5. **Find Oxide Color:** Using this option, you can find the oxide's color corresponding to the thickness of the oxide. Just enter the oxide thickness in micrometers, and you will get the color of the oxide.

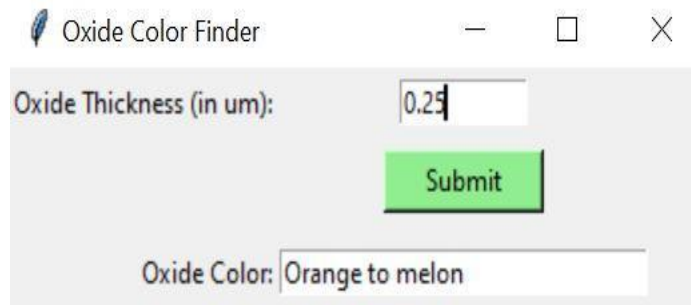


Fig. 12: Oxide Color Finder Window

6. **Coefficients:** This option contains the information of various coefficients we have used for the oxide thickness calculation, such as Linear and Parabolic growth rate constants and activation energies. On clicking this window, you will be guided to the following window in which you can select the process for which you want to see the coefficients. Once you click on a particular process, the coefficients will be displayed.



Fig. 13: Window for various Coefficients

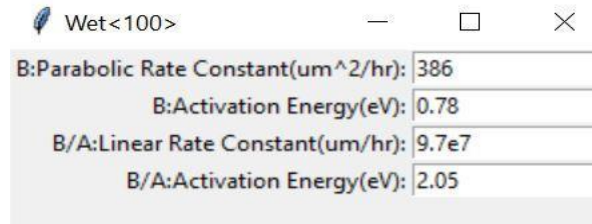


Fig. 14: Output Window for Wet<100> Coefficients

7. Important Graphs: Using this option, you can see the various graphs important for the oxidation process, as given in the following window.

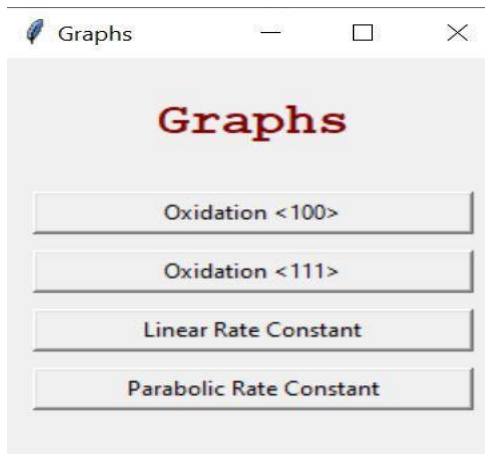


Fig. 15: Graph Window

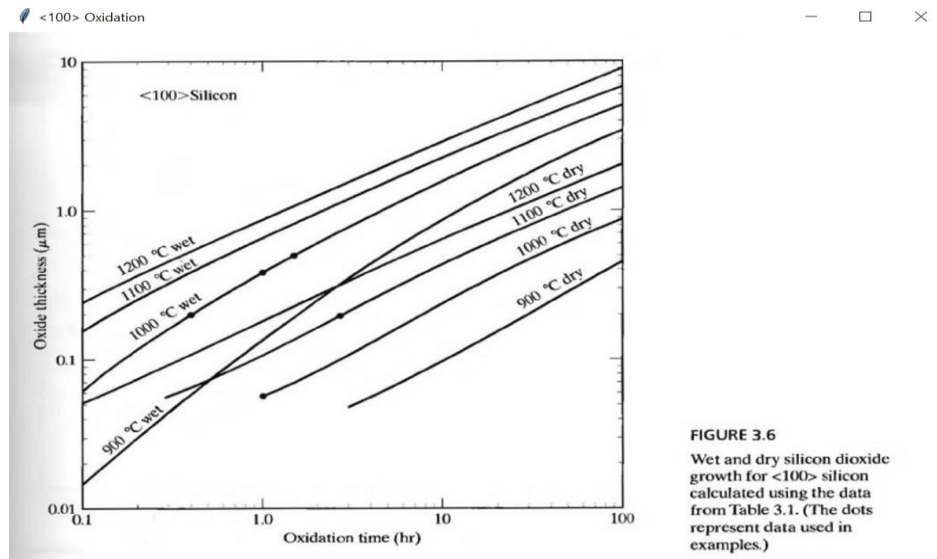


Fig. 16: Graph (Oxidation Thickness vs Time) for <100> orientation

FIGURE 3.5

Dependence of the linear rate constant B/A on temperature for the thermal oxidation of silicon in pyrogenic H_2O (640 torr) or dry O_2 . Reprinted by permission of the publisher, The Electrochemical Society, Inc., from Ref. [10].

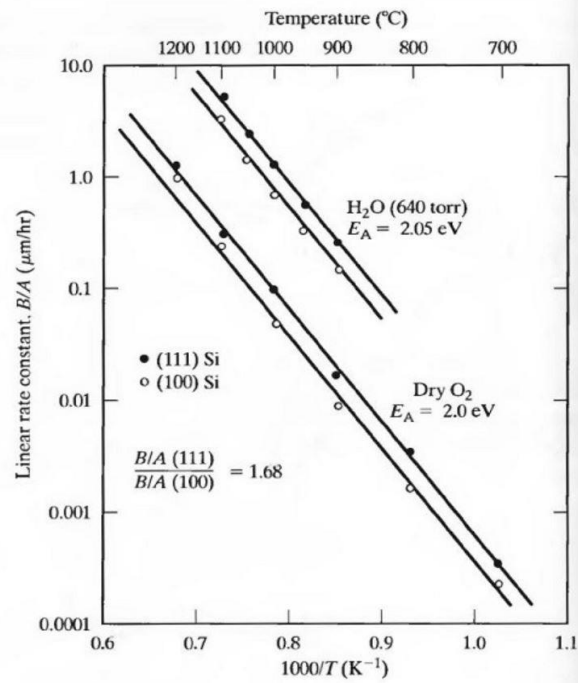


Fig. 17: Graph (Linear rate Constant vs Temperature)

OXYSIM Tool Link:

You can download the tool (**OXYSIM**) from the link given below (Ctrl+Click)

Click here: [Google Drive Link](#)