

# SOSim: A Software Simulator for Silicon Oxidation Documentation

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**ABSTRACT.** The thermal oxidation of silicon is one of the most crucial processes in Integrated Circuit Fabrication. The silicon dioxide layer acts as a diffusion barrier, a good insulator, and a gate dielectric. The Deal-Grove model mathematically describes the growth of an oxide layer on a material's surface. In particular, it is used to predict and interpret thermal oxidation of silicon in semiconductor device fabrication. The model was first published in 1965 by Bruce Deal and Andrew Grove of Fairchild Semiconductor, building on Mohamed M. Atalla's work on silicon surface passivation by thermal oxidation at Bell Labs in the late 1950s. This served as a step in the development of CMOS devices and the fabrication of integrated circuits. The Massoud Model serves as an improvement over the Deal-Grove model by introducing more physical into the light for dry oxidation of silicon.

**Keywords:** Silicon Oxidation, Deal-Grove model, Massoud model, Simulator

## 1. INTRODUCTION

Thermal oxidation of silicon is one of the most integral parts of the fabrication process. The silicon oxide formed is a good insulator and a gate dielectric. Therefore, it is used extensively to create electrically insulating regions containing the conducting silicon regions and device areas [1]. With the development of the Very Large Scale Integration (VLSI) standards and the rapid miniaturization of circuits, a thinner oxide layer holds critical importance. Thermal oxidation of silicon is an excellent method to develop thin, uniform, the error-free oxide film on the surface of silicon [2]. Silicon oxide is one reason why silicon is still preferred in the semiconductor industry compared to other semiconductors like Germanium, Gallium Arsenide, etc [3].

In 1965, B. E. Deal and A. S. Grove formulated a straightforward method using Fick's law to find a relationship between the oxide thickness and oxidation/heating time [4]. Deal-Grove based their work on simplified assumptions like Fick's diffusion with a constant coefficient of diffusion. Due to the simplicity of their model, it attracted much attention in the fabrication industry. Many researchers started using the same assumptions as Deal-Grove had done in their work to come up with more innovative models [5].

The Deal-Grove model estimated the relationship between the oxide thickness and the oxidation time with a small margin of error; their assumptions were not always accurate. For example, the constant diffusion coefficient and linear dopant concentration profile did not satisfy the principle's continuity equation. Such assumptions led to minor inaccuracies in the theoretically calculated values and the experimentally calculated ones. Researchers concluded that the Deal-Grove model "provides a successful framework to explain the kinetics of the oxidation process for a wide range of oxide film thicknesses ... However, a characterization of the atomic processes occurring during oxidation is well beyond its scope" [6].

The Deal-Grove model could correctly describe the oxidation growth with a thickness above 30nm due to the above assumptions. The dynamics change rapidly for thicknesses lower than 30nm, and

there is a vast error in the theoretical estimates and the experimental values. When the Deal-Grove model was published in 1965, such thin oxides were not used. However, this limitation became noticeable with time as the device sizes started to shrink.

It has been observed experimentally that the oxidation rate is much faster than predicted by the Deal-Grove model at the initial stages of oxidation and thin oxide growths [7]. The Deal-Grove model was unable to consider this effect, and hence it had to be changed. The increased oxidation rate resulted from parallel oxidation methods, like oxygen vacancies, surface oxygen exchange, silicon interstitials within the oxide, etc [8].

In 1985, Massoud et al. [9]-[10] suggested some changes to the Deal-Grove model for dry oxidation, considering the increased oxidation rate for thickness less than 30nm. Their analytical model introduced some additional terms to the Deal-Grove model and proposed some changes to the equations' constants. In their work, they had assumed the various parallel oxidation mechanisms based on the experimental data.

## 2. BACKGROUND - THE MODELS

**2.1. The Deal-Grove Model.** Deal and Grove proposed a well-established model for thermal oxide growth in the mid-1960s, and it is still commonly applied because of its simplicity. One explanation for this simplicity is that two so-called Deal-Grove parameters, which have to be derived from experiments, contain the entire physics of the oxidation phase. Besides, the arrangement is considered to be one-dimensional. Thus, only oxide films grown on plane substrates can be added to the model.

If one assumes that the oxidation process is dominated by the inward movement of the oxidant species, the transported species must go through the following stages:

- (1) It is transported from the bulk of the oxidizing gas to the oxide's outer surface, where it is adsorbed.

$$(2.1) \quad F_1 = h(C^* - C_0)$$

- (2) It is transported across the oxide film towards silicon.

$$(2.2) \quad F_2 = -D \frac{dC}{dx} = D \frac{C_0 - C_i}{L}$$

- (3) It reacts at the interface with silicon and forms a new layer of SiO<sub>2</sub>.

$$(2.3) \quad F_3 = kC_i$$

If we consider the fluxes to be in steady-states and we eliminate  $C_0$  and  $C_i$ , then:

$$(2.4) \quad F = F_1 = F_2 = F_3 = \frac{C^*}{\frac{1}{k} + \frac{1}{h} + \frac{L}{D}}$$

and

$$(2.5) \quad R = \frac{dL}{dt} = \frac{F}{N} = \frac{\frac{C^*}{N}}{\frac{1}{k} + \frac{1}{h} + \frac{L}{D}} = \frac{B}{A + 2L}$$

Introducing a time  $\tau$  corresponding to the initial oxide thickness  $x_i$ ,

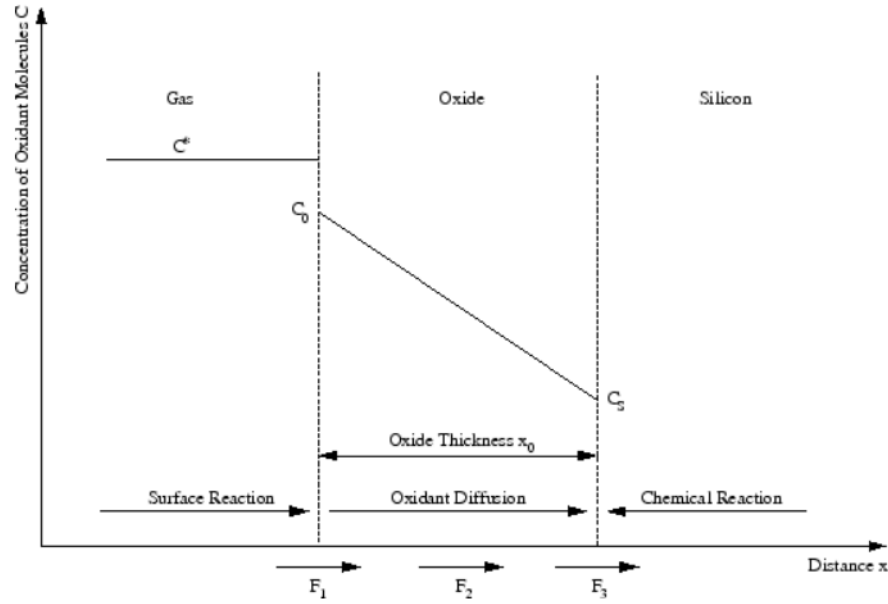
$$(2.6) \quad \tau = \frac{x_i^2 + Ax_i}{B}$$

The time required for a specific thickness can be calculated using

$$(2.7) \quad t = \frac{x_0^2 - x_i^2}{B} + \frac{x_0 - x_i}{B/A}$$

On the other hand, to find the thickness using time, we can solve the above equation and get,

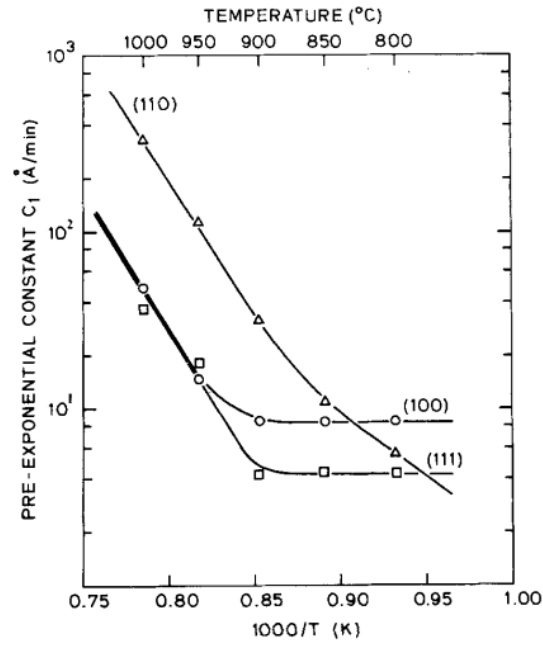
$$(2.8) \quad x_0 = \frac{A}{2} \left( \sqrt{1 + \frac{4B}{A^2}(t + \tau)} - 1 \right)$$



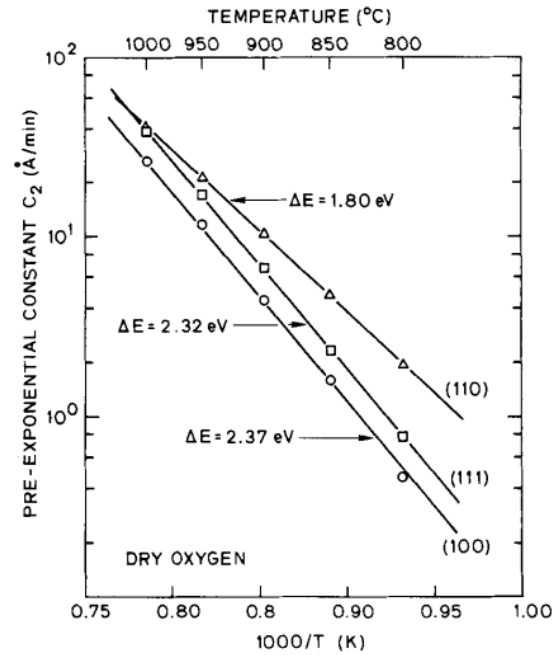
**Figure 1.** Model of Deal and Grove for the oxidation of silicon

**2.2. The Massoud Model.** The oxidation results for the initial oxide growth in the case of dry oxidation are faster than predicted by the Deal-Grove Model. The Deal-Grove Model assumes a linear growth for the first 30 nm of oxide growth. However, it is faster and non-linear. To model the thin film oxidation, the Massoud Model was developed with some changes in parabolic constants of Deal-Grove's model. The initial stages of oxidation are treated as a non-steady process depending on oxide thickness and temperature. The non-steady-state is modeled by adding the rate-enhancement term to the oxidation equation. The enhancement term decays as the oxide thickness approaches 25nm, resuming the linear-parabolic relationship. The  $\text{SiO}_2$  growth in Massoud Model is expressed as

$$(2.9) \quad \frac{dx_o}{dt} = \frac{B}{2x_o + A} + C1 * \exp\left(\frac{-x_o}{L_1}\right) + C2 * \exp\left(\frac{-x_o}{L_2}\right)$$



**Figure 2.** Temperature dependence of Pre-Exponential constant  $C_1$  for lightly doped (100), (111) and (110) silicon oxidized in the temperature range 800-1000°C [10]



**Figure 3.** Temperature dependence of Pre-Exponential constant  $C_2$  for lightly doped (100), (111) and (110) silicon oxidized in the temperature range 800-1000°C [10]

The first term in the equation is a linear-parabolic relationship, as given by Deal-Grove's model. However, the value of linear and parabolic constants are different. The second and third terms are rate enhancement terms.  $C_1$  and  $C_2$  are pre-exponential constants dependant on the activation energy and temperature. The characteristic length  $L_1$  and  $L_2$  is of the order of 1nm and 7nm, respectively. The second term vanishes after oxide thickness greater than 5nm. The second term vanishes after 25nm.

Another formulation of the above equation is derived as :

$$(2.10) \quad \frac{dxo}{dt} = \frac{B + K_1 \exp(\frac{-t}{\tau_1}) + K_2 \exp(\frac{-t}{\tau_2})}{2xo + A}$$

Here, the two terms representing the rate enhancement in the thin regime are decaying exponentially with time.

Unlike Deal-Grove's model, the linear, parabolic, and pre-exponential constants in Massoud's model are dependant on the temperature. With the device length scaling, thin oxides need to be modeled. Massoud's model could accurately predict the thermal oxidation results for thin-film oxides, an advantage over the Deal-Grove model.

Temperature Range	T < 1000 °C			T > 1000C	
Crystal Orientation	100	111	110	100	111
$C_B$ [nm <sup>2</sup> /min]	$1.70 \times 10^{11}$	$1.34 \times 10^9$	$3.73 \times 10^8$	$1.31 \times 10^5$	$2.56 \times 10^5$
$E_B$ [eV]	2.22	1.71	1.63	0.68	0.76
$C_{B/A}$ [nm/min]	$7.35 \times 10^6$	$1.32 \times 10^7$	$4.73 \times 10^8$	$3.53 \times 10^{12}$	$6.50 \times 10^{11}$
$E_{B/A}$ [eV]	1.76	1.74	2.10	3.20	2.95

**Table 1.** Pre-exponential constants and activation energies for B and B/A

The parabolic and linear rate constants are expressed in-terms of Arrhenius-expression as:

$$(2.11) \quad B = C_B * \exp(\frac{-E_B}{kT})$$

$$(2.12) \quad B/A = C_{B/A} * \exp(\frac{-E_B}{kT})$$

The relationship describing the oxide-growth in dry oxygen is derived from solving the above differential equation.

$$(2.13) \quad xo = \sqrt{(\frac{A}{2})^2 + Bt + M_1[1 - \exp(-\frac{t}{\tau_1})] + M_2[1 - \exp(-\frac{t}{\tau_2})] + M_0} - \frac{A}{2}$$

where the constants are described as

$$(2.14) \quad M_0 = (x_i^2 + Ax_i^2)$$

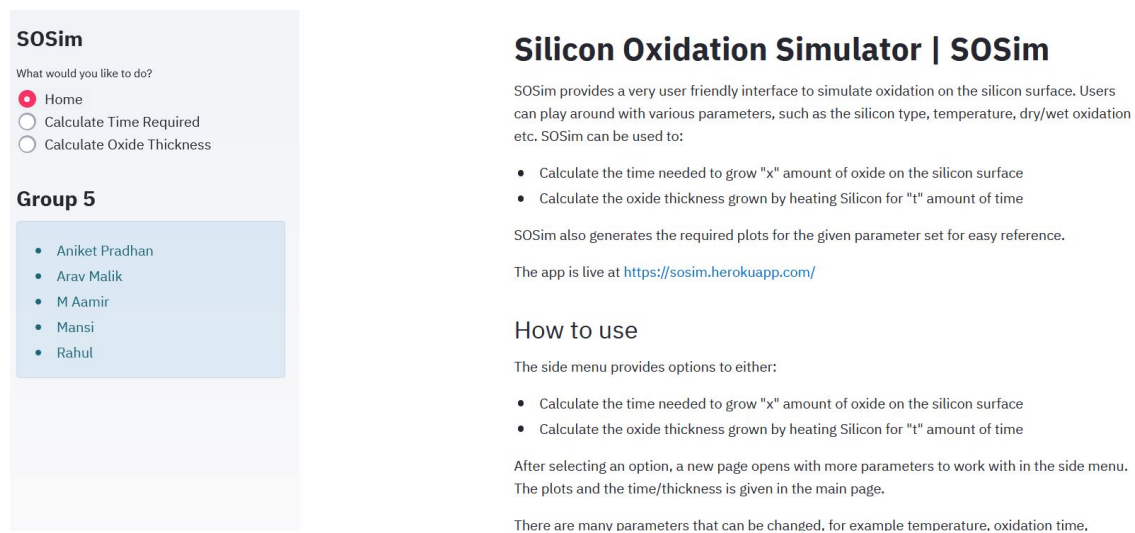
Here,  $x_i$  represents the initial oxide thickness

$$(2.15) \quad M_1 = K_1\tau_1$$

$$(2.16) \quad M_2 = K_2\tau_2$$

### 3. ABOUT THE APP

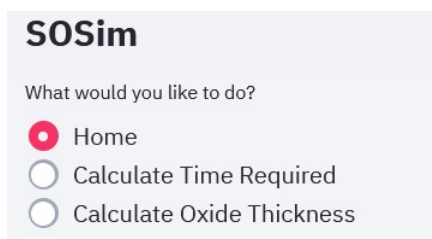
SOSim provides a very user-friendly interface to simulate oxidation on the silicon surface. Users can play around with various parameters, such as the silicon type, temperature, dry/wet oxidation, etc.



**Figure 4.** The complete UI of the app on a desktop/laptop

SOSim can be used to:

- Calculate the time needed to grow "x" amount of oxide on the silicon surface
- Calculate the oxide thickness grown by heating Silicon for "t" amount of time



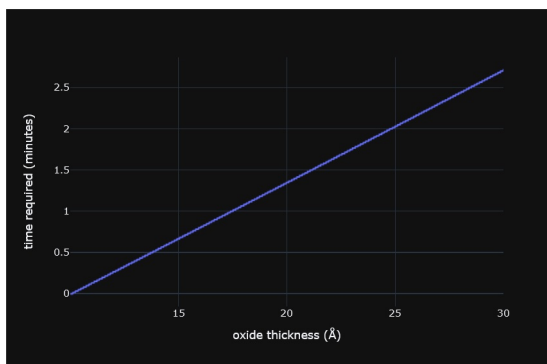
**Figure 5.** Main options for the desired result (to be selected in the left pane)

After selecting an option, a new page opens with more parameters to work within the side menu. The plots and the time/thickness are given on the main page.

00:01:21 (HH/MM/SS) of heating is required

For oxidising 20.0 Å of silicon at 1000 °C

Algorithm used: Deal-Grove

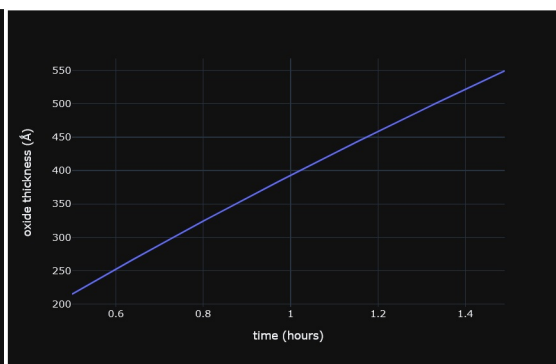


(A) Resultant plot with figures for time

392.76 Å thick oxide is formed

After heating silicon at 1000.00 °C for 1.0 hours

Algorithm used: Deal-Grove



(B) Resultant plot with figures for thickness

**Figure 6.** How the main pane looks after the parameters

Many parameters can be changed, for example, temperature, oxidation time, crystal orientation, ambient (dry/wet), and the oxidation model (Deal-Grove/Massoud). All parameters are available on the side panel.

SOSim also generates the required plots for the given parameter set for easy reference.

The plots are interactive and can be varied appropriately. They can be zoomed in, downloaded in high quality, annotated, etc.



### Calculate Time Required

Algorithm

☒ Deal-Grove  
☐ Massoud

Ambient

☒ Dry  
☐ Wet

Partial Pressure: 1 atm

Crystal Orientation

<100>

Initial Oxide Thickness (Å)

10

Temperature (°C)

700 1000 1200

Final Oxide Thickness (Å)

20

(A) Options available for time required

### Calculate Oxide Thickness

Algorithm

☒ Deal-Grove  
☐ Massoud

Ambient

☒ Dry  
☐ Wet

Partial Pressure: 1 atm

Crystal Orientation

<100>

Initial Oxide Thickness (Å)

10

Temperature (°C)

700 1000 1200

Time (hours)

1

Time (minutes)

0

(B) Options available for thickness

**Figure 7.** How the left pane looks to select parameters

### Theme

Theme

plotly\_dark

**Figure 8.** Option to select a theme for the plot from different available options

The app is live at [Silicon Oxidation Simulator | SOSim](#)

#### 4. HOW TO RUN FROM SOURCE

It is straightforward to run SOSim for the user's requirement. The requirements are specified in the `requirements.txt` file, which can be installed via `pip`. We use Python to run SOSim.

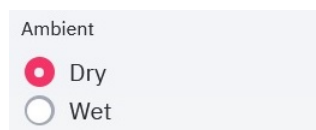
- (optional) First, create a virtual environment using `virtualenv` or `pipenv`
- Install the requirements using `pip`  
`pip install -r requirements.txt`
- Run the app using `streamlit`  
`streamlit run app.py`
- A webpage should open automatically, otherwise the user can open `localhost:8501` on their web browser which will then show the SOSim Screen/UI.
- The user can select which operation would they like to do, and it will render the solutions and provide them with the plots in almost no time.

#### 5. PROCEDURE

The user can first select what they want to calculate: the time using the thickness or vice versa. Then, they can select the desired oxidation process parameters in the left pane, including the model, initial oxide thickness, ambient, crystal orientation, etc. and the oxidation time and thickness are displayed on the main pane, along with a plot of the oxide thickness vs. time for the process duration below them.

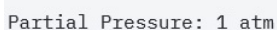
Additional details on the various process parameters are described in the following subsections.

**5.1. Ambient.** The user can choose the ambient, either Wet or Dry, which depends on whether the gaseous oxidizing species in the furnace is water vapor or oxygen, respectively. Compared to the dry oxidation, the wet oxidation is much quicker due to the much higher solubility of  $H_2O$  (compared with  $O_2$ ) in  $SiO_2$  which yields a much larger concentration of oxidant within the oxide. The Massoud model is limited to dry oxidation only. However, the Deal-Grove model can be used for both dry and wet oxidation.



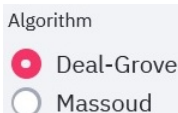
**Figure 9.** Ambient option in the left pane

**5.2. Partial Pressure.** The user can enter the partial pressure of the oxidizing species in atm (standard atmosphere). The higher the partial pressures of the oxidizing species, the higher will be the oxidation rates. For wet oxidation using pyrogenic steam, corresponding to the industry standard, the default partial pressure is 0.92 atm. For bubbler systems or flash vaporization, this value does not need to be accurate. For dry oxidation, the default partial pressure is 1.00 atm (100% oxygen ambient). This value can also be adjusted for local differences in the atmospheric pressure due to altitude to be accounted for. In our SOSim App, the app fixes the oxygen partial pressure at 1.00 atm when the Massoud model is chosen.



**Figure 10.** Partial Pressure option in the left pane

**5.3. Model.** The user can choose the algorithm to be used from either the Deal–Grove model or the Massoud one. The phenomenological Deal–Grove algorithm works well for dry and wet oxidation of the thicker oxide films, but the performance drops significantly in the case of dry oxidation of thin oxides (which is less than 500 Å), where the experimental oxidation rate is faster than predicted by this algorithm. For such thin and dry oxides, the Massoud model has far more improved accuracy (particularly in the 800–1000 °C temperature range).



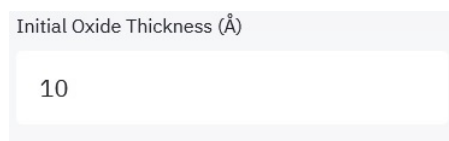
**Figure 11.** Model option in the left pane

**5.4. Crystal Orientation.** The user can choose between either the  $\langle 100 \rangle$ , the  $\langle 111 \rangle$ , or the  $\langle 110 \rangle$  which depends on the *Si* surface's crystal orientation being oxidized. The oxidation is fastest for the *Si* with the crystal orientation  $\langle 111 \rangle$  and the slowest for the *Si* with the crystal orientation  $\langle 100 \rangle$ . The Deal-Grove model hypothesized that this difference could be accounted to the variations in the atomic surface densities, i.e., the available oxidation sites for these crystal orientations.



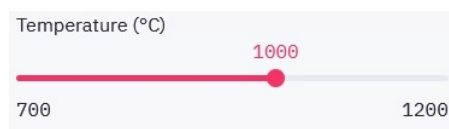
**Figure 12.** Crystal Orientation option in the left pane

**5.5. Initial Oxide Thickness.** The user can enter the desired initial oxide thickness present on the wafers in Å before the oxidation process. The oxidation process is non-linear, generally where the oxidation rate decreases with time as the process undergoes a transition from being rate limited due to the surface-reaction to being limited by the oxidant's diffusion through the  $\text{SiO}_2$ . The sequential oxidation steps should be handled using the thickness of the final oxide after one step as the initial oxide for the next step, as such (e.g., to model a dry–wet–dry sequence).

A screenshot of a software interface showing a text input field for 'Initial Oxide Thickness (Å)'. The field contains the number '10'.

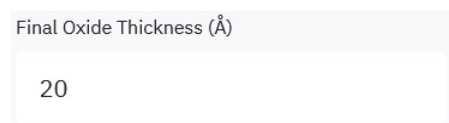
**Figure 13.** Initial Oxide Thickness option in the left pane

**5.6. Temperature.** The user can enter the desired temperature in °C at which the oxidation reaction should take place, which is limited to the 700–1200 °C range. Due to the Arrhenius-like, i.e., exponential behavior of the diffusivities of the oxidant and their surface reaction rates, the oxidation process is highly dependent on the temperature. The Massoud algorithm provides the most accurate results in the 800–1000 °C range of the temperature for which it was developed. Though the app will still return a result, any temperature which is outside this range should be used with caution.

A screenshot of a software interface showing a temperature slider. The slider is labeled 'Temperature (°C)' and has a range from 700 to 1200. A red dot is positioned at 1000, which is also labeled in red text above the slider.

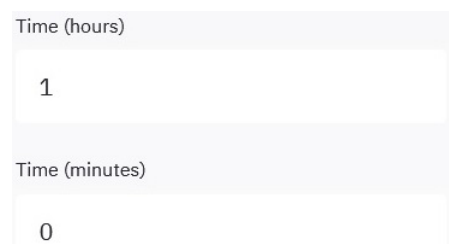
**Figure 14.** Temperature option in the left pane

**5.7. Final Oxide Thickness.** The user can select this option and enter the desired thickness of the final oxide in Å while also including the initial oxide thickness to calculate the oxidation time.

A screenshot of a software interface showing a text input field for 'Final Oxide Thickness (Å)'. The field contains the number '20'.

**Figure 15.** Final Oxide Thickness option in the left pane

**5.8. Oxidation Time.** The user can select this option and enter the desired total oxidation time in HH:MM:SS format to solve the thickness of the final oxide, including the initial oxide thickness.

A screenshot of a software interface showing two stacked text input fields for 'Oxidation Time'. The top field is labeled 'Time (hours)' and contains the number '1'. The bottom field is labeled 'Time (minutes)' and contains the number '0'.

**Figure 16.** Oxidation Time option in the left pane

## 6. RESULTS

The following results are provided when the form is submitted:

6.1. **Oxidation Time.** Total oxidation time, in HH:MM:SS format and in minutes.

00:01:21 (HH/MM/SS) of heating is required

**Figure 17.** Oxidation Time as result in the main pane

6.2. **Oxide Thickness.** Total oxide thickness, including any initial oxide, in Å.

392.76 Å thick oxide is formed

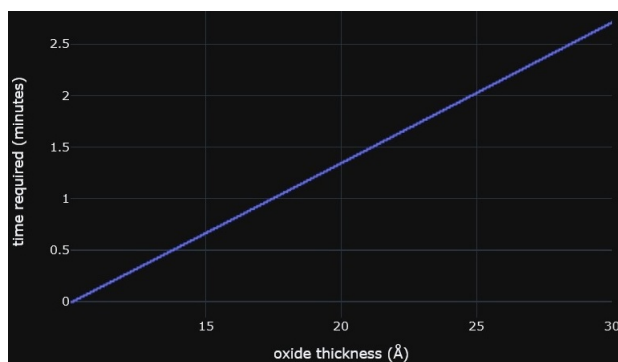
**Figure 18.** Oxide Thickness as result in the main pane

6.3. **Si Thickness Consumed.** The total thickness of *Si* in Å consumed during the oxidation process, including any initial oxide thickness, which is assumed to be grown via thermal oxidation.

For oxidising 20.0 Å of silicon at 1000 °C

**Figure 19.** *Si* Thickness Consumed as result in the main pane

6.4. **Thickness vs. Time Plot.** A plot of the oxide thickness in Å as a function of the oxidation time taken in minutes. Hover the mouse-over the plot to observe over the individual datapoints and also discover other functionalities of the plot.



**Figure 20.** Thickness vs. Time Plot as result in the main pane

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