OXYSIM

An Oxidation Simulator

Documentation

ICF Project

Under the guidance of

Dr. S.S.Jamuar

Submitted By:

Mukul Garg	MT19147
Subodh Kumar Sharma	MT19161
Chandraveer Singh	MT19177
Puneet Kumar	MT19189

Objective:

The project aims to develop a tool named (OXYSIM), which is used to simulate the oxidation process. The tool takes the substrate and oxidation process information (substrate orientation, temperature, oxidation time, initial oxide thickness) as input and gives the oxide layer's thickness and color as the output. The tool implements the classic Deal-Grove linear parabolic model and the Massoud additional term to model the rapid initial oxidation regime. Users can select the models, the oxidation type (dry or wet oxidation), initial oxide thickness (in um), temperature, oxidation time, and crystal orientation (<100> or <111>) in their simulations.

Modelling Oxidation:

Deal-Grove Model:

This model gives the relation between the oxide thickness and the time for which oxidation is done. The rate of change of oxide thickness can be expressed in the given form:

$$\frac{dx}{dt} = \frac{B}{2x + A}$$

which gives oxide thickness as:

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

where

$$\tau = \frac{x_i^2}{B} + \frac{x_i}{B\ /\ A}$$

The values of B/A and B are calculated through the equations:

$$\frac{B}{A} = C_{B/A} \exp\left(-\frac{E}{KT}\right)$$

$$B = C_B \exp\left(-\frac{E}{KT}\right)$$

Parameters

x_0: Oxide thickness at time t

x_i: Initial oxide thickness (at t=0)

B/A: Linear rate constant

B: Parabolic rate constant

$C_{B/A}$: Coefficient of B/A

C_B: Coefficient of B

E: Activation energy

K: Boltzmann constant

T: Temperature

	Wet Oxidation(X_i=0nm)		Dry Oxidation(X_i=25nm)	
	C	E	C	E
<100>				
Linear (B/A)	9.7 * 10^7 um/hr	2.05eV	3.71 * 10^6 um/hr	2.00 eV
Parabolic (B)	386 um^2/hr	0.78eV	772 um^2/hr	1.23 eV
<111>				
Linear (B/A)	1.63 * 10^8 um/hr	2.05eV	6.23 * 10^6 um/hr	2.00 eV
Parabolic (B)	386 um^2/hr	0.78eV	772 um^2/hr	1.23 eV

Table 1: The values of coefficients and activation energy depending upon orientation and oxidation type [3]

The Deal-Grove model presents the general response of growth rate, which is linear in the initial stage and becomes parabolic with time. The Deal-Grove model does not model initial rapid oxidation thickness in the right way. Hence, the Massoud correction term should be used to show the initial oxidation growth rate i.e., an initial oxide thickness of about 25 nm should be used for reasonable answers [1], [3].

Massoud Model:

The Deal-Grove model needs to be updated for dry oxidation to address the thin oxide growth region. The complexity of the model increases by including the Massoud term. There is a trade-off between the accuracy and the complexity of the system [2].

The rate of change of oxide thickness can be expressed in the given form:

$$\frac{dx}{dt} = \frac{B}{2x + A} + C_1 e^{\frac{-x}{L_1}} + C_2 e^{\frac{-x}{L_2}}$$

The values of B/A and B are calculated through the equations:

$$B = C_B \exp\left(\frac{-E_B}{kT}\right)$$

$$\frac{B}{A} = C_{B/A} \exp\left(\frac{-E_{B/A}}{kT}\right)$$

Temperature	T<1000^{O}C		T>1000^{O}C	
Orientation	**<100>**	**<111>**	**<100>**	**<111>**
C_B(nm^2/min)	1.7 * 10^{11}	1.34 * 10^9	1.31 * 10^5	2.56 * 10^5
E_B(eV)	2.22	1.71	0.68	0.76
$C_{B/A}$(nm/min)	7.35 * 10^6	1.32 * 10^{71}	3.53 * 10^{12}	6.5 * 10^{11}
$E_{B/A}$(eV)	1.76	1.74	3.20	2.95

Table 2: The values of coefficients and activation energy depending upon orientation, oxidation type and temperature [2]

Arrhenius expression:

$$k_1 = k_1^O \exp\left(\frac{-E_{k_1}}{kT}\right)$$

$$k_2 = k_2^O \exp\left(\frac{-E_{k_2}}{kT}\right)$$

$$\tau_1 = \tau_1^o \exp\left(\frac{-E_{\tau_1}}{kT}\right)$$

$$\tau_2 = \tau_2^o \exp\left(\frac{-E_{\tau_2}}{kT}\right)$$

Crystal Orientation	<100>	<111>
k_1^O(nm^2/min)	2.49 * 10^{11}	2.70 * 10^9
E_{k_1}	2.18	1.74
k_2^O(nm^2/min)	3.72 * 10^{11}	1.33 * 10^9
E_{k_1}	2.28	1.76
τ_1^o(min)	4.14 * 10^{-6}	1.72 * 10^{-6}
E_{τ_1}	1.38	1.45
τ_2^o(min)	2.71 * 10^{-7}	1.56 * 10^{-7}
E_{τ_2}	1.88	1.90

Table 3: Arrhenius expression coefficients [2]

The final oxide thickness is given by:

$$x_o = \text{sqrt}\left\{ \left(\frac{A}{2}\right)^2 + Bt + M_1\left[1 - \exp\left(-\frac{t}{\tau_1}\right)\right] + M_2\left[1 - \exp\left(-\frac{t}{\tau_2}\right)\right] + M_o \right\} - \left(\frac{A}{2}\right)$$

Parameters:

$M_o = x_i^2 + Ax_i$

$M_1 = k_1 \tau_1$

$M_2 = k_2 \tau_2$

x_i = Initial oxide thickness

k_1^O, k_2^O = Pre-exponential coefficients

τ_1^o, τ_2^o = Time constant coefficients

E_{k_1}, E_{k_2}, E_{τ_1}, E_{τ_2} = Activation energies

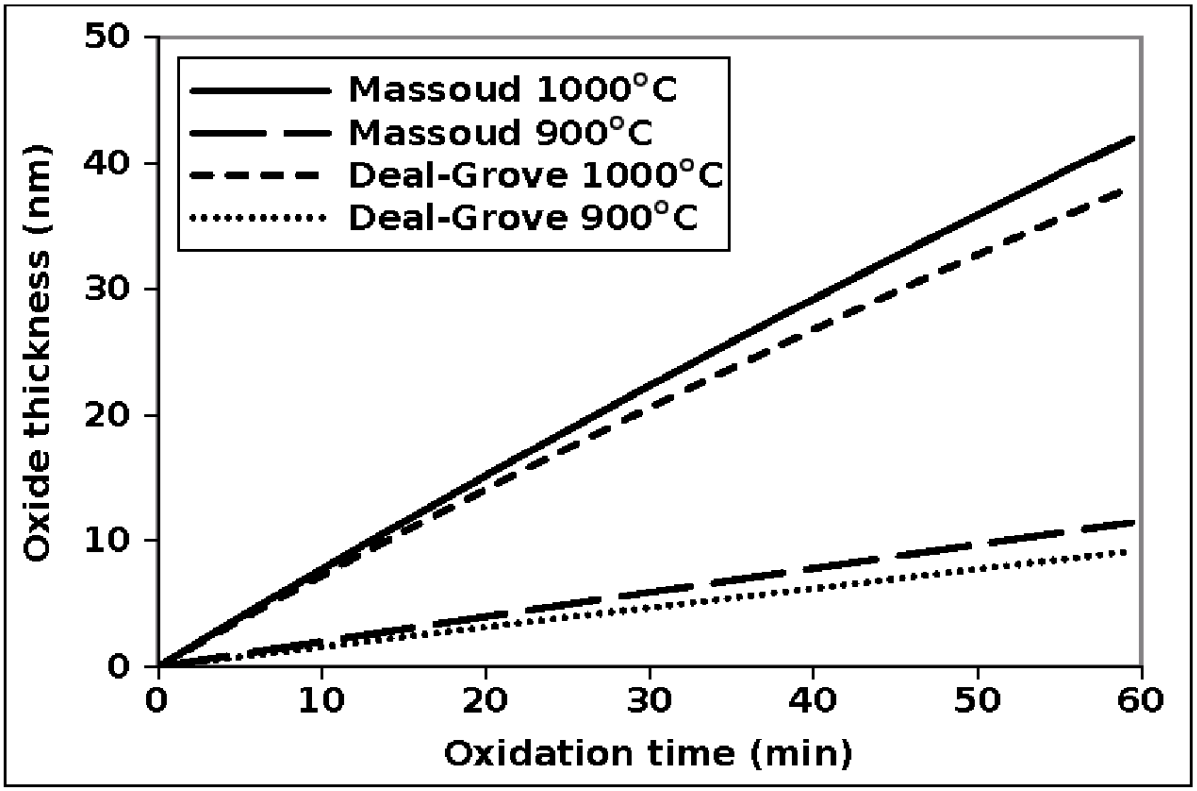

Fig. 2: Comparison between the Deal Grove and Massoud models for the oxide thickness during the first hour of oxidation in a dry ambient [2]

Color Chart:

This table gives the color of oxide depending upon the oxide thickness [3]. We have used this table in our code by taking the range using mid-point of thickness so that color can be Obtained for any oxide thickness between 0.05um and 1.54um.

Film Thickness (μm)	Color and Comments	Film Thickness (μm)	Color and Comments
0.05	Tan	0.63	Violet red
0.07	Brown	0.68	"Bluish" (not blue but borderline between violet and blue green; appears more like a mixture between violet red and blue green and looks grayish)
0.10	Dark violet to red violet		
0.12	Royal blue		
0.15	Light blue to metallic blue		
0.17	Metallic to very light yellow green	0.72	Blue green to green (quite broad)
		0.77	"Yellowish"
0.20	Light gold or yellow; slightly metallic	0.80	Orange (rather broad for orange)
		0.82	Salmon
0.22	Gold with slight yellow orange	0.85	Dull, light red violet
		0.86	Violet
0.25	Orange to melon	0.87	Blue violet
0.27	Red violet	0.89	Blue
0.30	Blue to violet blue	0.92	Blue green
0.31	Blue	0.95	Dull yellow green
0.32	Blue to blue green	0.97	Yellow to "yellowish"
0.34	Light green	0.99	Orange
0.35	Green to yellow green	1.00	Carnation pink
0.36	Yellow green	1.02	Violet red
0.37	Green yellow	1.05	Red violet
0.39	Yellow	1.06	Violet
0.41	Light orange	1.07	Blue violet
0.42	Carnation pink	1.10	Green
0.44	Violet red	1.11	Yellow green
0.46	Red violet	1.12	Green
0.47	Violet	1.18	Violet
0.48	Blue violet	1.19	Red violet
0.49	Blue	1.21	Violet red
0.50	Blue green	1.24	Carnation pink to salmon
0.52	Green (broad)	1.25	Orange
0.54	Yellow green	1.28	"Yellowish"
0.56	Green yellow	1.32	Sky blue to green blue
0.57	Yellow to "yellowish" (not yellow but is in the position where yellow is to be expected; at times appears to be light creamy gray or metallic)	1.40	Orange
		1.45	Violet
		1.46	Blue violet
		1.50	Blue
0.58	Light orange or yellow to pink	1.54	Dull yellow green
0.60	Carnation pink		

Fig. 2: Color Chart [3]

OXYSIM Tool Link:

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

Click here: Google Drive Link

References:

[1] "2.3.1 Deal-Grove Model." https://www.iue.tuwien.ac.at/phd/filipovic/node31.html#sect:dealgrove (accessed Nov. 13, 2020).

[2] "2.3.3 Massoud Model." https://www.iue.tuwien.ac.at/phd/filipovic/node33.html#equ:massoud12 (accessed Nov. 13, 2020).

[3] R. C. Jaeger, G. W. Neudeck, and R. F. Pierret, "Introduction to Microelectronic Fabrication, 2002." Prentice Hall.