SOSim - A Software Simulator for Silicon Oxidation - Literature Review

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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. It is therefore 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, 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 a lot of 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].

Due to the above assumptions, the Deal-Grove model could correctly describe the oxidation growth with the thickness above 30nm. 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 for 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. 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. In addition, 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 outer surface of oxide, where it is adsorbed.

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

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

(2.2)
$$F_2 = -D\frac{\mathrm{d}C}{\mathrm{d}x} = D\frac{C_0 - C_i}{L}$$

(3) It reacts at the interface with silicon and form a new layer of SiO_2.

(2.3)
$$F_3 = kC_i$$

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

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

and

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

Introducing a time τ corresponding to the initial oxide thickness x_i,

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

The time required for a specific thickness can be calculated using

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

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

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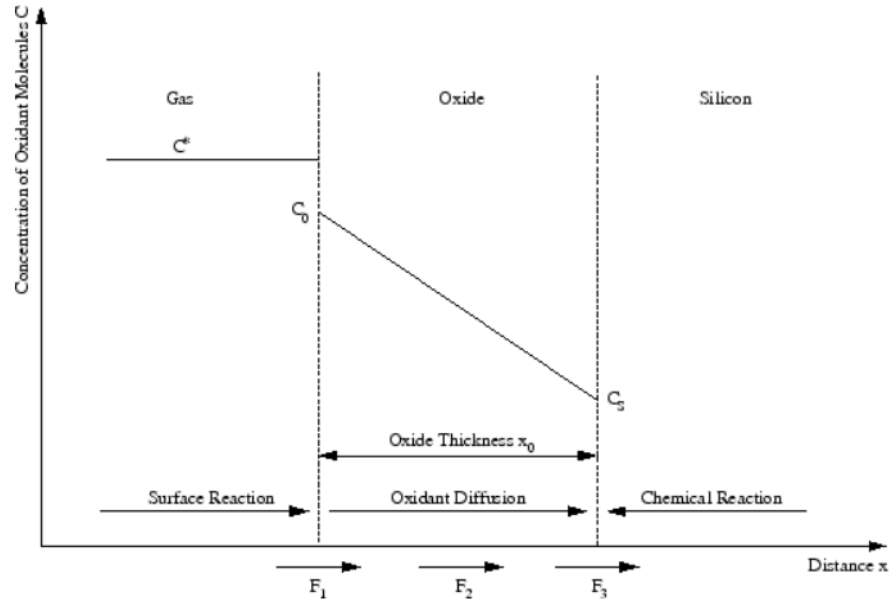

Figure 1. Model of Deal and Grove for the oxidation of silicon

3. The Massoud Model

The results of oxidation for the initial oxide growth in case of dry oxidation is 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 is treated as a non-steady process dependant on oxide thickness and temperature. The non-steady state is modelled by adding an additional rate-enhancement term to the oxidation equation. The enhancement term decays as the oxide thickness approaches 25nm, resuming the linear-parabolic relationship. The SiO_2 growth in Massoud Model is expressed as

$$(3.1) \qquad \frac{dxo}{dt} = \frac{B}{2xo + A} + C1 * exp(\frac{-xo}{L_1}) + C2 * exp(\frac{-xo}{L_2})$$
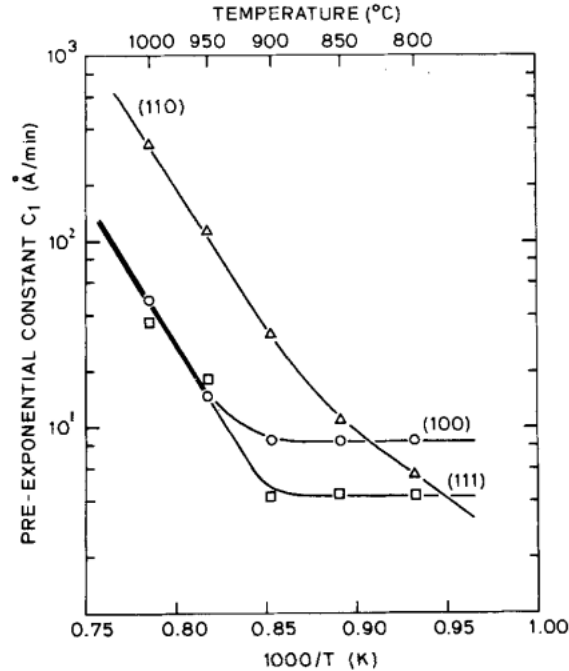

Figure 2. Temperature dependence of Pre-Exponential constant C1 for lightly doped (100),(111) and (110) silicon oxidized in the temperature range 800-1000C [10]
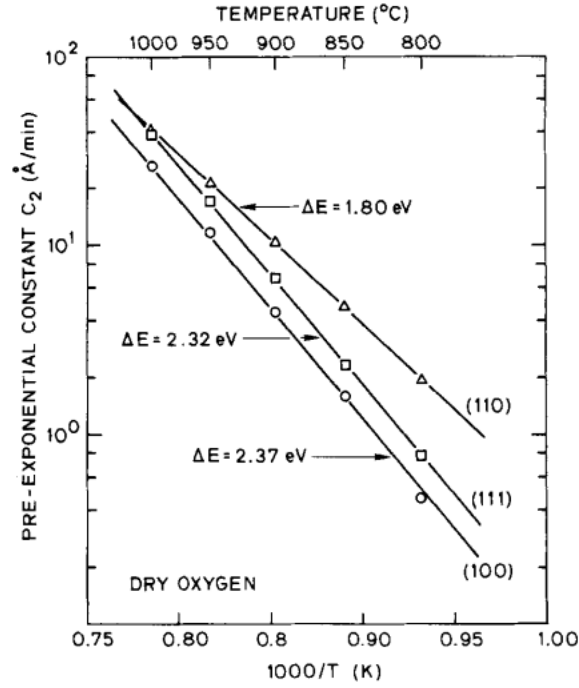
Figure 3. Temperature dependance of Pre-Exponential constant C2 for lightly doped (100),(111) and (110) silicon oxidized in the temperature range 800-1000C [10]

The first term in the equation is a linear-parabolic relationship as given by the Deal-Grove's model. However, the value of linear and parabolic constants are different. The second and third term are rate enhancement terms. C1 and C2 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 :

$$(3.2) \qquad \frac{dxo}{dt} = \frac{B + K_1 exp(\frac{-t}{\tau_1}) + K_2 exp(\frac{-t}{\tau_2})}{2xo + A}$$

Here, the two terms which represent 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 modelled. 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^2/min]	1.70 x 10^{11}	1.34 x 10^9	3.73 x 10^8	1.31 x 10^5	2.56 x 10^5
E_B	[eV]	2.22	1.71	1.63	0.68	0.76
$C_{B/A}$	[nm/min]	7.35 x 10^6	1.32 x 10^7	4.73 x 10^8	3.53 x 10^{12}	6.50 x 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:

$$(3.3) \qquad B = C_B * exp(\frac{-E_B}{kT}) https://www.iue.tuwien.ac.at/phd/hollauer/img217.png$$

$$(3.4) \qquad B/A = C_{B/A} * exp(\frac{-E_B}{kT})$$

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

$$(3.5) \qquad xo = \sqrt{(\frac{A}{2})^2 + Bt + M_1[1 - exp(-\frac{t}{\tau_1})] + M2[1 - exp(-\frac{t}{\tau_2})] + M_0} - \frac{A}{2}$$

where the constants are described as

$$(3.6) \qquad M_0 = (x_i^2 + Ax_i^2)$$

here, x_i represents the initial oxide thickness

$$(3.7) \qquad M_1 = K_1\tau_1$$

$$(3.8) \qquad M_2 = K_2\tau_2$$

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