

Oxide Growth

1. Introduction

Development of high-quality silicon dioxide (SiO_2) has helped to establish the dominance of silicon in the production of commercial integrated circuits. Among all the various oxidation methods (thermal oxidation, electrochemical anodization, and plasma enhanced chemical vaporization deposition), only thermal oxidation can provide the highest-quality oxides having the lowest interface trap densities. Silicon dioxide is an excellent insulator and dielectric material. Silicon dioxide is extensively used in semiconductors due to this property. One such example is a MOSFET.

1.1 MOSFET

MOSFET is a voltage controlled field effect transistor that has a “Metal Oxide” Gate electrode which is electrically insulated from the main semiconductor by a very thin layer of insulating material, usually SiO_2 . The aim of the MOSFET is to be able to control the voltage and current flow between the source and drain. It works as a switch. SiO_2 is used to avoid direct charge flow from the gate to the channel and vice-versa. SiO_2 layer is used as an electrical isolation between the gate and the channel through which major conduction will take place. SiO_2 is used as base insulating layer on which the other layers (Drain, Source, etc.) are grown. The gate potential causes charge build up at the bottom of the SiO_2 layer thereby aiding in turning ON of the device.

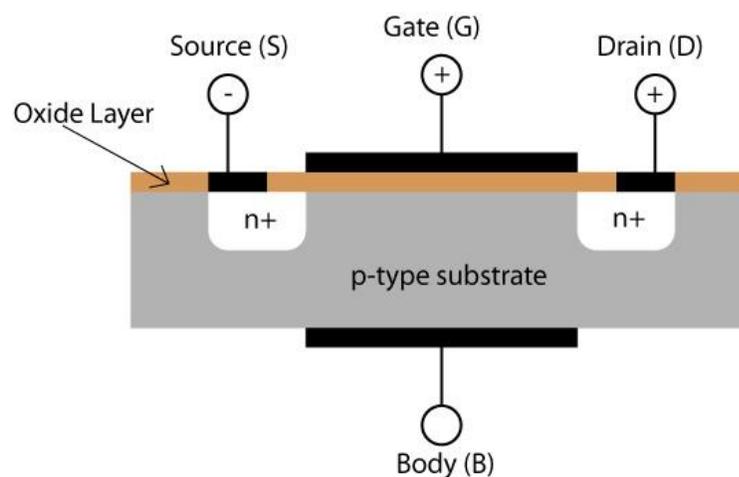


Figure 1. Basic Structure of a MOSFET[9]

2. Theory

2.1. Thermal oxidation process

There are two SiO₂ growth methods, dry and wet oxidation, depending on whether dry oxygen or water vapor is used:

- Dry oxidation: $\text{Si} + \text{O}_2 \rightarrow \text{SiO}_2$
- Wet oxidation: $\text{Si} + 2\text{H}_2\text{O} \rightarrow \text{SiO}_2 + 2\text{H}_2(g)$

The oxidizing ambient may also contain several percent of hydrochloric acid. The chlorine removes metal ions that may occur in the oxide. Dry oxidation is usually used to form thin oxides in a device structure because of its good Si-SiO₂ interface characteristics, whereas wet oxidation is used for thicker layers because of its higher growth rate. In this experiment, we will use dry oxidation to form the SiO₂ film.

SiO₂ incorporates silicon consumed from the substrate and oxygen supplied from the ambient. Thus, the oxide grows both down into the wafer and up out of it. Every unit thickness of silicon consumed yields 2.27-unit thickness of oxide [1].

2.2. Kinetics of growth: Deal-Grove model

The kinetics of thermal oxidation of silicon can be studied based on a simple model [1] illustrated in Figure 1. At the initial stage of oxidation, the oxidizing species (oxygen or water vapor) reacts with silicon atoms at the surface. This results in growth of a thin SiO₂ layer. Now, in order to oxidize Si, the oxidizing species has to diffuse through the SiO₂ layer to the Si-SiO₂ interface. The diffusive flux is

$$F_1 = D \frac{dC}{dx} \cong \frac{D(C_0 - C_s)}{x}, \quad (1)$$

where C_0 is the concentration of the oxidizing species in atmosphere adjacent to the SiO₂ surface, C_s is the concentration of the oxidizing species at the Si-SiO₂ interface, D is the diffusion coefficient of the oxidizing species, and x is the thickness of the oxide layer.

C_0 corresponds to the equilibrium bulk concentration of the oxidation species. At 1000°C and at a pressure of 1 atm, the concentration C_0 is 5.2×10^{16} molecules/cm³ for dry oxygen and 3×10^{19} molecules/cm³ for water vapor.

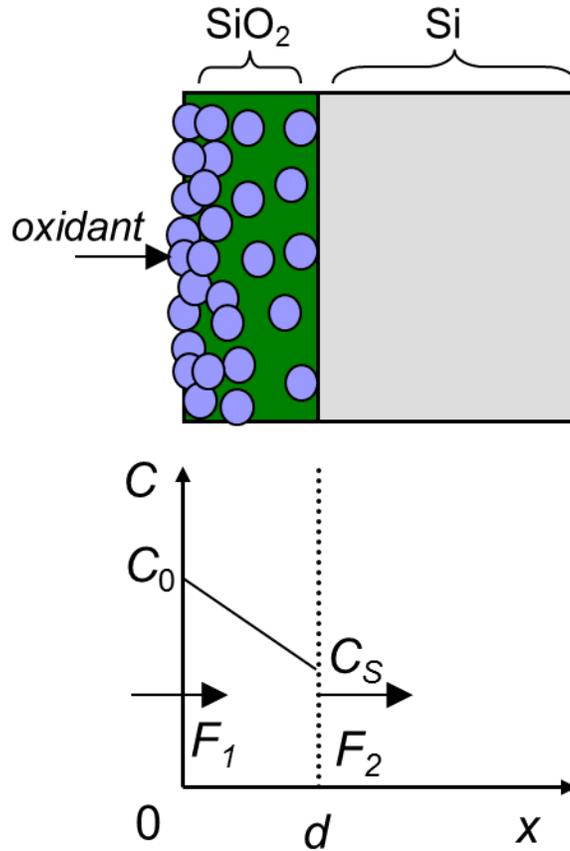


Figure 1. Deal-Grove model for the thermal oxidation of silicon [1].

The oxidizing species reacts with silicon at the Si-SiO₂ interface. Assuming that the reaction rate is proportional to the concentration C_s of the oxidizing species near the interface, the reactive flux is

$$F_2 = kC_s, \quad (2)$$

where k is the reaction rate. At a steady-state, $F_1 = F_2 = F$. Combining Eqs. (1) and (2) gives

$$F = \frac{DC_0}{x + D/k}. \quad (3)$$

The growth rate of the oxide layer is

$$\frac{dx}{dt} = \frac{F}{C_1} = \frac{DC_0/C_1}{x + D/k}, \quad (4)$$

where C_1 is the number of molecules of the oxidizing species required to produce a unit volume of the oxide. There are 2.2×10^{22} SiO₂ units per cm³ of silicon dioxide and production of each unit requires one oxygen molecule (O₂). Therefore, C_1 for oxidation in dry oxygen is 2.2×10^{22} cm⁻³. On the other hand, in wet oxidation, it is necessary to add two water molecules (H₂O) to

produce a single SiO₂ unit. Therefore, C₁ for oxidation in water vapor is 4.4×10²² cm⁻³.

Solving the differential equation (4) subject to the initial condition x(0) =0 yields

$$x^2 + \frac{2D}{k}x = \frac{2DC_0}{C_1}t. \quad (5)$$

This equation can be rewritten in a more compact form:

$$x^2 + Ax = Bt, \quad (6)$$

where

$$A = \frac{2D}{k} \text{ and } B = \frac{2DC_0}{C_1} \quad (7)$$

The values of A and B for dry oxidation at various temperatures are shown in Table 1.

Table 1. Oxidation coefficients for (100) silicon surface.

Temperature (°C)	A (μm)	B(μm ² /hr)
800	0.370	0.0011
920	0.235	0.0049
1000	0.165	0.0117
1100	0.090	0.027
1200	0.040	0.045

Time-dependence of the SiO₂ thickness predicted by Eq. (6) is shown in Figure 2. At the early stages of oxidation, the oxide thickness is relatively small so that the timescale of diffusion of oxidizing species through the oxide layer is much smaller than the timescale of the oxidation reaction, i.e. oxidation is *reaction-limited*. As the oxide layer becomes thicker, the timescale of diffusion through this layer exceeds the reaction timescale at the Si-SiO₂ interface, thus the reaction becomes *diffusion-limited*.

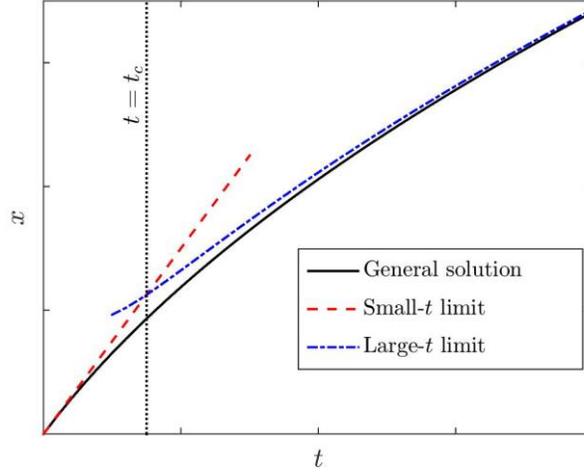


Figure 2. Time dependence of the SiO₂ thickness predicted by Eq. (6). The small- and large-time limits are given by Eqs. (10) and (11), respectively.

Both the reaction- and diffusion-limited stages of oxidation are predicted by the Deal-Grove model. To see this, write the solution of Eq. (6) as follows:

$$x(t) = \frac{A}{2} \left[\sqrt{1 + \frac{t}{t_c}} - 1 \right]. \quad (8)$$

where

$$t_c = \frac{A^2}{4B}. \quad (9)$$

is the time corresponding to transition between the two regimes.

The reaction- and diffusion-limited regimes correspond to $t \ll t_c$ and $t \gg t_c$, respectively. In these cases, Eq. (8) reduces to

$$x \approx \frac{At}{4t_c} = \frac{B}{A} t = \frac{C_0}{C_1} kt \quad \text{for } t \ll t_c \text{ and} \quad (10)$$

$$x \approx \frac{A}{2} \left[\left(\frac{t}{t_c} \right)^{\frac{1}{2}} - 1 + \frac{1}{2} \left(\frac{t_c}{t} \right)^{\frac{1}{2}} \right] \approx \frac{A}{2} \left(\frac{t}{t_c} \right)^{\frac{1}{2}} = \sqrt{Bt} \text{ for } t \gg t_c \quad (11)$$

I.e., during the reaction-controlled oxide growth, the oxide thickness grows linearly with time, whereas in the diffusion-controlled regime, the thickness grows as the square root of time. In Figure 2, these regimes are shown by the red and blue lines, respectively.

2.3. Oxidation Reactor

The basic thermal oxidation reactor is shown in Figure 3. The reactor consists of a resistance-heated furnace, a cylindrical fused-quartz tube containing the silicon wafers held vertically in a slotted quartz boat, and a source of either pure dry oxygen or pure water vapor.

The loading end of the furnace tube protrudes into a vertical flow hood where a filtered flow of air is maintained. Flow is directed as shown by the arrow in Figure 3. The hood reduces dust and particular matter in the air surrounding the wafers and minimizes contamination during wafer loading. The oxidation temperature is generally in the range of 900°C to 1200°C, and the typical gas flow rate is about 1 L/min. The oxidation system uses microprocessors to regulate the gas flow sequence, to control the automatic insertion and removal of silicon wafers, to ramp the temperature up (i.e., to increase the furnace temperature linearly) from a low temperature to the oxidation temperature so that the wafers will not warp due to sudden temperature change, to maintain the oxidation temperature to within $\pm 1^\circ\text{C}$, and to ramp the temperature down when oxidation is completed.

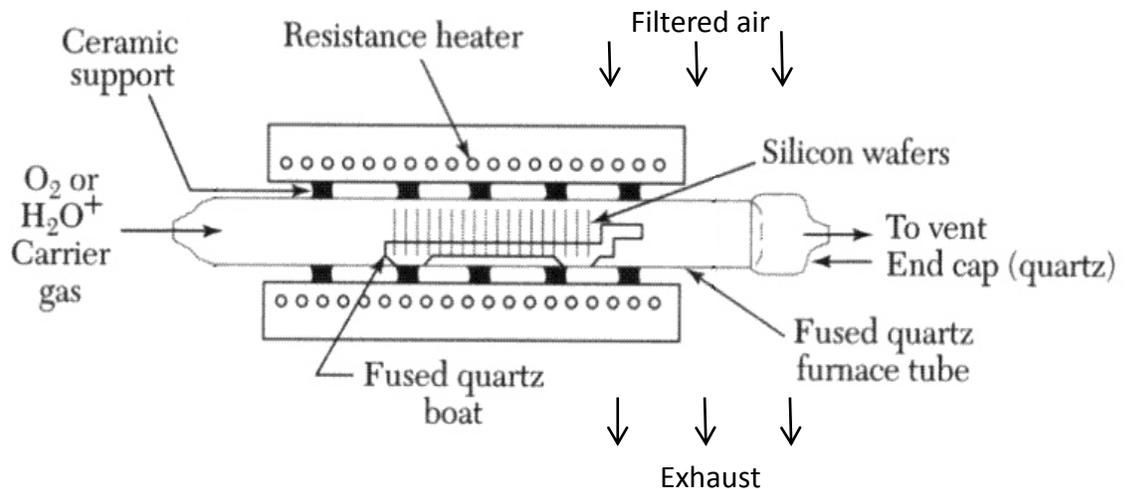


Figure 3. Schematic cross section of a resistance-heated oxidation furnace [2].

2.4. Oxide quality

The simplest method for determining the thickness of an oxide is to compare the color of the wafer with a reference color chart. When an oxide-coated wafer is illuminated with white light perpendicular to the surface, the light penetrates the oxide and is reflected by the underlying silicon wafer. Constructive interference leads to enhancement of a certain wavelength of reflected light, and the color of the wafer corresponds to that wavelength. For example, a wafer with a 500 nm silicon dioxide layer will appear blue green.

Clearly, color chart comparisons are subjective and are therefore not the most accurate mechanism for determining oxide thickness. A more accurate measurement can be obtained using techniques such as ellipsometry.

Ellipsometry is a very powerful and accurate optical method to measure the thickness of thin films [3], [4], [5]. The technique uses plane polarized monochromatic light to illuminate the oxidized silicon surface at an angle. The film thickness is determined from interference between the light reflected by the SiO₂ surface and the light traveling through the SiO₂ layer and reflected by the silicon substrate. This light interference is determined by the film thickness and the refractive index of SiO₂. This technique requires that the thickness is known to be within approximately 250 nm since the measured quantities are periodic functions of this thickness. Thicknesses down to the very thin (<5nm) regime may be measured. However, inaccuracies in this regime may be present. The technique assumes that the refractive index does not vary with thickness. More complicated methods, such as spectral or multiple wavelength ellipsometry [6], [7] or multiple angle ellipsometry are now being used to improve the accuracy of these measurements to <1nm [7], [8].

3. References

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