

# **Biomedical Ultrasound Fundamentals of Imaging and Micromachined Transducers**

**TA : Srinivas Bhaskara, Course Instructor : Dr. Hardik J. Pandya**

**Department of Electronic Systems Engineering**

**Indian Institute of Science, Bangalore**

## **Lecture - 17**

Greetings, and welcome back to the course on Biomedical Ultrasound: Fundamentals of Imaging and Micromachine Transducers. I am Srinivas Bhaskara, the teaching assistant for this course. Today, we will discuss thermal oxidation, with a focus on the Deal-Grove model and its mathematical aspects, as well as empirical observations.

Let's begin by distinguishing between dry oxidation and wet oxidation. The terms "dry" and "wet" are quite straightforward. In dry oxidation, only oxygen is used to oxidize the silicon, while in wet oxidation, water vapor is used for the oxidation process. It's important to be clear on this terminology.

Now, let's talk about oxide formation. Oxides can either be grown or deposited. What's the difference? In grown oxide, the silicon wafer already exists as the precursor. When oxygen or water vapor is introduced, it reacts with the silicon, forming silicon dioxide along with byproducts like residual gases. In this case, the silicon wafer is already present, and the oxide grows on top of it, much like how fruit grows on a tree.

In contrast, in deposited oxide, both silicon and oxygen are introduced as precursors. These react on the surface to form silicon dioxide. However, for today's discussion, we are focusing solely on grown oxide and not on deposited oxide, which involves different processes and concepts.

So, with that in mind, let's return to the topic of dry and wet oxidation, focusing specifically on the growth of oxides.

When silicon reacts with oxygen, it undergoes dry oxidation, forming silicon dioxide ( $\text{SiO}_2$ ). In the case of silicon reacting with water molecules, wet oxidation occurs, producing silicon dioxide and releasing hydrogen ( $\text{H}_2$ ) as a byproduct. The two types of oxidations - wet and dry, differ not only in process but also in speed. Wet oxidation is approximately 10 times faster than dry oxidation, although both operate within the same temperature range of 900 to 1200°C. We will explore the mathematical proof of this later, but for now, consider it as a factual statement.

This high temperature is necessary for the oxidation process, but have you noticed that silicon left in the atmosphere at room temperature also forms a very thin layer of oxide? In our labs, silicon

wafers exposed to the air naturally develop a native oxide layer after a few months. This layer, usually just a few nanometers thick, is a result of silicon reacting with the oxygen and water vapor present in the environment. Although unintentional, this native oxide forms due to the presence of oxygen and humidity in the air. However, the quality of this naturally formed silicon dioxide is not ideal.

Now, why do we need such high temperatures for oxidation? This is where the concept of diffusion comes into play. For those familiar with diffusion, the diffusion constant follows the formula  $e^{-\frac{E_g}{kT}}$ , where  $E_g$  is the activation energy and  $T$  is the temperature. As temperature increases, the term  $kT$  increases, reducing the exponential value and thus increasing diffusion. Higher diffusion rates, in turn, result in thicker oxide layers, and this relationship between diffusion and temperature is the key concept that we will explore in more detail throughout this lecture.

Dry oxidation is an excellent insulator, often used in MOS transistors. Imagine a typical MOS transistor structure, where you have a source, a drain, and a gate in between. The gate, which applies voltage, is separated from the channel by a very thin oxide layer, known as the gate oxide. This gate oxide must possess high-quality insulating properties.

Now, if you compare dry oxidation and wet oxidation, which one do you think produces a better oxide material? The answer is dry oxidation. In dry oxidation, only silicon dioxide ( $\text{SiO}_2$ ) forms, making it purer and more effective as an insulator. However, in wet oxidation, hydrogen ( $\text{H}_2$ ) is also a byproduct. The hydrogen gas, being in a gaseous form, must escape the reaction, creating microscopic holes in the oxide film. These holes compromise the material's insulating properties compared to the high-quality oxide formed during dry oxidation.

The drawback of dry oxidation is that it's much slower than wet oxidation. The diffusion constants of oxygen and water vapor help explain this difference—oxygen diffuses more slowly, resulting in a slower oxide growth. We'll examine the relevant equations and the diffusion constants more closely, but for now, understand that dry oxidation, despite being slower, is typically used in applications requiring high-quality gate oxides, such as gate insulation in MOS transistors.

Wet oxidation is frequently used in various applications such as thin film oxide layers and masking oxides, despite the presence of hydrogen gas diffusion, which can create electron pathways that degrade the insulating properties. As previously discussed, native oxide forms at room temperature on silicon surfaces, but this oxide layer is very thin and of poor quality compared to high-temperature dry oxidation. The key factor here is that high temperatures promote better crystallinity in the oxide layer.

Now, let's consider an example. Suppose you have a 500-micron-thick silicon wafer, and your goal is to grow a 100-micron-thick silicon dioxide ( $\text{SiO}_2$ ) layer on it. One might assume that after oxidation, the total thickness would simply be 600 microns (500 microns of silicon + 100 microns

of SiO<sub>2</sub>). However, it doesn't work like that. During the oxidation process, part of the silicon is consumed, and part of the SiO<sub>2</sub> grows on top of the existing silicon.

Specifically, if the final SiO<sub>2</sub> thickness is X, then 0.46X of the silicon is consumed, and 0.54X of SiO<sub>2</sub> is grown on top. So, for a desired 100-micron-thick SiO<sub>2</sub> layer, 46 microns of the silicon will be consumed, and 54 microns of SiO<sub>2</sub> will be added on top of the wafer. The total thickness after oxidation would then be 554 microns, not 600 microns.

This ratio (0.46:0.54) is derived from the relationship between the densities of silicon and silicon dioxide, and understanding this is crucial, especially for exams and assignments. It's important to note how much silicon is consumed during oxidation and how the final thickness is calculated based on this ratio.

Let's discuss how the oxidation process occurs. First, you have a furnace, typically made of quartz, which is capable of withstanding very high temperatures. Inside the furnace, there is a boat where silicon wafers are stacked for the oxidation process. Depending on the furnace's length, you can oxidize multiple wafers simultaneously. The chamber housing the wafers is also made of quartz to handle the intense heat.

For dry oxidation, you need a source of oxygen. However, it's not ideal to rapidly increase the temperature to the desired level (around 900 to 1200°C). Instead, you gradually increase the temperature to prevent premature oxidation. During the heating process, nitrogen can be introduced into the chamber to prevent unwanted oxidation at lower temperatures. Once the temperature reaches the target range, oxygen is gradually introduced to begin the oxidation process.

For wet oxidation, the process is slightly different. You still need oxygen, but in addition, hydrogen is used to create water vapor (H<sub>2</sub>O). This is achieved using a bubbler, where oxygen passes through water, creating water vapor. The water vapor is then introduced into the furnace chamber, where it reacts with the silicon, forming silicon dioxide (SiO<sub>2</sub>). The same temperature range, 900 to 1200°C, is maintained, but in this case, the reaction is faster due to the presence of water vapor.

As the temperature increases, diffusion - the movement of oxygen or water molecules into the silicon also increases, speeding up the oxidation process. We'll explore the principles of diffusion and how they influence oxidation more deeply in the upcoming sections. The atmosphere inside the furnace is very high and piranha cleaning is implemented.

In the pre-cleaning step, the components typically used are H<sub>2</sub>O<sub>2</sub> and H<sub>2</sub>SO<sub>4</sub> in various ratios, such as 1:2, 2:4, or other combinations. This cleaning process, known as piranha cleaning, is essential to remove contaminants from the silicon wafer. However, since oxidizing agents are involved, a thin layer of silicon dioxide (SiO<sub>2</sub>) will inevitably form on the wafer surface during the process. This silicon dioxide layer is usually just a few nanometers thick, but its quality is not very high.

To avoid the growth of unwanted silicon dioxide after piranha cleaning, a common practice is to perform an HF (hydrofluoric acid) dip. This involves immersing the wafer in a very dilute HF solution (in a 1:50 ratio of concentrated HF to water) for about 30 seconds. This step effectively removes the native oxide layer, making it suitable for further processing if no oxide growth is desired.

After pre-cleaning, various oxides like gate oxides, tunneling oxides, and pad oxides are used in different stages of the fabrication process to insulate devices from each other. Additionally, field oxides are used for similar insulating purposes, while masking oxides are applied during processes like diffusion or ion implantation. For example, if you want to process only a specific area of the wafer, masking oxides are used to protect other regions from exposure.

You can use masking to shield specific areas during processes like ion implantation, allowing you to work only on targeted regions while protecting the rest of the surface. This technique is essential in controlling where modifications occur on the wafer.

Now, consider using deposited oxides or metal oxides as insulators between metals. For example, imagine you have a silicon wafer with a layer of metal, such as aluminum, on top. If you want to grow silicon dioxide on top of this, exposing the aluminum to high temperatures (like 800°C or 1200°C) would cause the aluminum to diffuse into the silicon, damaging its properties.

To avoid this, you can use a process called sputtering, which typically occurs at room temperature. Sputtering allows you to coat the surface with a layer of silicon dioxide without the risk of high-temperature damage. This technique is crucial when dealing with metal contamination, as exposing the wafer to high temperatures can compromise its quality.

Now, when it comes to understanding the actual oxidation process and how it can be modeled, we use a well-established mathematical framework known as the Deal-Grove model. This model helps predict how oxidation occurs under different conditions, including thickness and temperature. While there are certain limitations and scenarios where the model may not hold, it is widely accepted and used across the industry to understand silicon dioxide growth.

The Deal-Grove model attempts to simulate the real-time behavior of oxidation as it occurs on a silicon wafer. Initially, there is no silicon dioxide ( $\text{SiO}_2$ ) on the wafer's surface. When the wafer is placed inside a chamber filled with oxygen or water molecules, depending on whether dry or wet oxidation is being performed, these molecules are plentiful and ready to react with the silicon. As the temperature in the chamber is maintained between 900°C and 1200°C, thermal energy facilitates the formation of a very thin layer of silicon dioxide through a surface reaction between the silicon and the oxidizing species.

Once this initial  $\text{SiO}_2$  layer forms, subsequent oxygen or water molecules can no longer directly reach the silicon; the newly formed oxide acts as a barrier. This means that additional oxidizing

agents must diffuse through the silicon dioxide layer to access the underlying silicon, which slows the oxidation process as the oxide thickness increases. The Deal-Grove model helps us understand these dynamics, illustrating how oxidation grows over time and why the process becomes less efficient as the silicon dioxide layer thickens.

Once the initial silicon dioxide ( $\text{SiO}_2$ ) layer forms, additional oxygen or water molecules must diffuse through this layer to reach the silicon interface. To understand this process mathematically, let's visualize the structure by rotating it 90 degrees. In this view, we see the thickness of the silicon wafer and the very thin layer of silicon dioxide formed on its surface, surrounded by the ambient environment inside the furnace, which contains a high concentration of oxygen or water molecules.

Let's denote the concentration of these molecules in the ambient air as  $C_g$  and the concentration at the silicon interface as  $C_i$ . For the formation of additional  $\text{SiO}_2$  layers, these molecules need to diffuse through the existing silicon dioxide layer. When we talk about diffusion, it's crucial to specify what is diffusing and in what medium. In this case, oxygen or water molecules are diffusing through the silicon dioxide. To analyze this diffusion quantitatively, we refer to the relevant data sheets to understand the diffusion characteristics of these molecules in silicon dioxide over time.

The diffusion constant  $D$  can be expressed in a form such as  $D = D_0 e^{-\frac{E_g}{kT}}$  where  $E_g$  may vary for oxygen and water. This indicates that the diffusion rates for these molecules are different, affecting the overall oxidation process.

Now, let's focus on the process of diffusion. In the ambient environment outside the silicon wafer, there are abundant oxygen and water molecules. These molecules reach the surface and must diffuse through the silicon dioxide layer. At this stage, a surface reaction occurs, where the reactants interact to form silicon dioxide.

However, while the ambient has an infinite supply of reactants, the bottleneck in the process lies in the diffusion of these molecules to the surface and their subsequent reaction. To model this, we can identify two types of flux occurring within the oxide layer. Let's denote the flux due to diffusion as  $F_1$  and the flux due to the surface reaction as  $F_2$ .

Outside the silicon dioxide layer, if we consider only oxygen, the diffusion flux  $F_1$  is significantly high, allowing us to treat it as a constant. Therefore, we can focus on modeling  $F_1$  (the diffusion flux) using Fick's Law, which relates the flux to the concentration gradient. This law states that the diffusion flux is proportional to the gradient of concentration, providing a framework to understand how oxygen molecules move through the silicon dioxide layer to participate in the oxidation process.

Fick's Law states that the diffusion flux  $F_1$  is proportional to the concentration gradient, represented mathematically as  $F_1 = -D \frac{\partial C}{\partial x}$ . Here,  $D$  is the diffusion constant, which varies with temperature, meaning it is not a fixed value. The negative sign in the equation is significant; it indicates that diffusion occurs from regions of higher concentration to regions of lower concentration, similar to how water flows from higher to lower elevations. This negative sign ensures that the concentration gradient is correctly accounted for, as a positive concentration gradient would imply an unrealistic movement of particles against the gradient.

The second flux,  $F_2$ , corresponds to the surface reaction and is defined by the equation  $F_2 = K_s \cdot C_i$ , where  $K_s$  is the surface reaction coefficient and  $C_i$  is the concentration at the interface. The value of  $K_s$  depends on various material properties, including the orientation of the silicon and other factors.

In addition to considering spatial variables, we must also incorporate time into our model. The final equation describes the rate of change of silicon dioxide formation as a function of the flux and  $N_i$ , which represents the number of oxygen atoms incorporated during the silicon dioxide formation process. This approach provides a comprehensive understanding of the oxidation dynamics over time.

In our discussion,  $F$  can represent either  $F_1$  or  $F_2$ . The key point is that, at equilibrium, these two fluxes must balance each other. Consider a scenario where the diffusion flux  $F_1$  is higher than the reaction flux  $F_2$ . In this case, as more molecules accumulate at the interface, the concentration gradient decreases, leading to a reduction in  $F_1$  until it matches  $F_2$ . Conversely, if the temperature is elevated significantly, causing  $C_1$  to approach zero as soon as molecules reach the interface and react to form silicon dioxide, the concentration gradient will increase. This, in turn, will cause  $F_1$  to rise until it balances with  $F_2$ .

Ultimately, at equilibrium,  $F_1$  equals  $F_2$ . We now have a differential equation that accounts for both spatial dimensions and time. By solving this equation alongside the previously defined parameters, including the diffusion constant  $D$  and the surface reaction coefficient  $K_s$ , we can determine the thickness  $x$  of the silicon dioxide layer formed during the oxidation process. We will delve deeper into the Deal-Grove model and tackle related problems in the next lecture. Thank you for your attention.