

5.5.1. Introduction

The fabrication of integrated circuits involves deposition of many layers above silicon substrate. These layers include dielectric, semiconductor and metals. So, thin film deposition is a foundational process in the manufacturing of microelectronic devices, enabling the formation of ultra-thin layers of material with precise characteristics on a substrate. The technique is essential for building integrated circuits, transistors, memory storage devices, and various semiconductor components. By carefully depositing controlled layers of conductive, insulative, or semiconductor materials, thin film deposition provides the layered architecture needed in modern electronic devices. The choice of deposition method whether chemical or physical depends on various factors such as the desired film properties, the materials involved, and the thermal or structural constraints of the substrate. This controlled deposition process has become indispensable in advancing the microelectronics industry, enabling higher density and more efficient devices with each technological generation.

2. Historical Development

Thin film deposition techniques generally fall into two main categories: Chemical Vapor Deposition (CVD) and Physical Vapor Deposition (PVD), each using distinct approaches to form thin films on silicon wafers. In both methods, the wafer is placed in a specialized chamber where film-forming materials are delivered in the gas phase. In CVD, reactant gases are introduced, which undergo chemical reactions on the substrate surface, producing a solid film layer. PVD, by contrast, relies on physical processes to generate atoms or molecules that travel through a low-pressure gas environment and condense onto the substrate. PVD techniques include "evaporation," where a source material is heated until it vaporizes, and "sputtering," where energetic ions from a plasma bombard the source material, ejecting atoms that deposit onto the substrate. PVD is often referred to as "vacuum deposition" due to its reliance on very low-pressure conditions, essential for transporting atoms to the wafer surface. While CVD is extensively used in the integrated circuit industry for its high-quality silicon and dielectric films with good conformal coverage, PVD is preferred for depositing a wide range of metals and alloys, which can be challenging to deposit using CVD alone.

5.3. Chemical Vapor Deposition (CVD)

Chemical Vapor Deposition (CVD) is a versatile and widely used thin film deposition process where gaseous precursors are introduced into the deposition chamber react on a heated substrate to form a solid film. CVD relies on thermally or plasma-activated chemical reactions, enabling the deposition of a variety of materials, including metals, dielectrics, and semiconductors. The process involves a gas-phase reaction where volatile compounds of the material to be deposited decompose or react on the substrate's surface, resulting in the desired thin film. CVD allows excellent control over film thickness and composition, making it ideal for forming conformal layers in complex structures. With flexibility in precursor choices and process conditions, CVD can achieve high purity and uniformity, making it essential for creating semiconductor layers, insulating films, and conductive pathways in microelectronics.

In general, CVD process can be explained by the following steps, as it is schematically illustrated in figure 5.1.

1. Transport of reactants convected to the deposition
2. Transport of reactants by diffusion from the main gas stream through the boundary layer to the wafer surface.

3. Adsorption of reactants on the wafer surface.
4. Surface processes, including chemical decomposition or reaction, surface migration to attachment sites (such as atomic-level ledges and kinks), site incorporation, and other surface reactions.
5. Desorption of byproducts from the surface.
6. Transport of byproducts by diffusion through the boundary layer and back to the main gas stream.
7. Transport of byproducts by forced convection away from the deposition region.

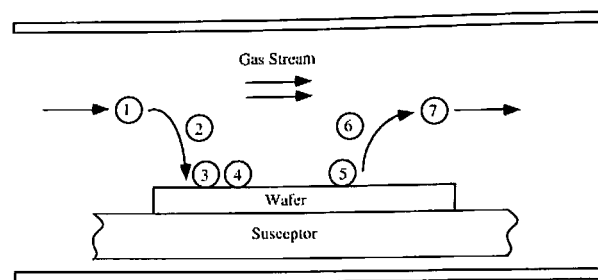


Figure 5.1 Steps involved in a CVD process.

In general, CVD Thin film process has two different rate-limiting steps in the process of film growth on the substrate. **Mass transfer control** (or **diffusion control**) and **surface reaction control**.

In Chemical Vapor Deposition (CVD), the growth of thin films can be influenced by two primary mechanisms: mass transfer control (or diffusion control) and surface reaction control. Each mechanism plays a crucial role in determining the rate and quality of the film deposition process. Recognizing which mechanism dominates allows for better process optimization in CVD applications, ultimately leading to improved material properties and performance in various applications such as microelectronics.

a. Mass Transfer Control (Diffusion Control)

Definition: In mass transfer control, the rate of film growth is limited by the transport of reactant species from the gas phase to the surface of the substrate where the deposition occurs. This means that the concentration of reactants at the surface is not sufficient to sustain a higher reaction rate.

Mechanism:

- **Diffusion Process:** The reactant gas molecules must diffuse through a boundary layer that forms near the substrate surface. This layer can be influenced by factors such as temperature, pressure, and flow rates.
- **Concentration Gradient:** A concentration gradient is established, where the concentration of reactants is higher in the bulk gas phase than at the surface. The diffusion of these molecules into this boundary layer and then to the surface limits the overall reaction rate.
- **Factors Affecting Mass Transfer:**
 - **Gas Flow Rate:** Higher flow rates can reduce the thickness of the boundary layer, enhancing mass transfer.
 - **Temperature:** Increasing temperature can increase molecular velocity, improving diffusion rates.

- **Pressure:** Higher pressures can increase the concentration of reactants in the gas phase, affecting diffusion.

Implications for CVD:

- When diffusion is limiting, increasing the temperature or adjusting flow rates may enhance deposition rates.
- This situation often leads to non-uniform film thickness if mass transfer limitations are significant, especially in large-scale systems or complex geometries.

b Surface Reaction Control

Definition: In surface reaction control, the rate of film growth is limited by the chemical reactions occurring at the surface of the substrate rather than by mass transfer processes. Here, sufficient reactants are available at the surface, but the reaction kinetics are slow.

Mechanism:

- **Surface Reactions:** The reactant species adsorb onto the substrate surface and undergo chemical reactions to form a solid film. The rate of these reactions determines how quickly material is deposited.
- **Reaction Kinetics:** Factors such as activation energy, temperature, and catalyst presence affect how quickly these reactions occur.
- **Factors Affecting Surface Reaction Rates:**
 - **Temperature:** Higher temperatures typically increase reaction rates due to greater kinetic energy.
 - **Catalysts:** The use of catalysts can lower activation energy barriers and enhance reaction rates.
 - **Surface Coverage:** If too many reactant molecules occupy active sites on the surface, it can lead to saturation and inhibit further reactions.

Implications for CVD:

- When surface reactions are limiting, increasing temperature or using catalysts may significantly enhance deposition rates.
- This scenario often results in better film uniformity and quality since sufficient reactants are available at the surface for reaction.

In Summary, understanding whether a CVD process is limited by mass transfer or surface reactions is critical for optimizing deposition conditions:

- **Mass Transfer Control (Diffusion Control):** Limited by how quickly reactants can reach the substrate surface. Enhancing gas flow rates or temperatures can improve deposition rates but may lead to non-uniform films.
- **Surface Reaction Control:** Limited by how quickly chemical reactions occur at the substrate surface. Increasing temperature or using catalysts can improve reaction rates and lead to higher-quality films.

Thin films deposited by CVD may be doped during the deposition process. This is

common for oxides, polysilicon, and epitaxial silicon. A gaseous source of the desired dopant is mixed with the other source gases, often along with hydrogen which acts as a carrier gas and a diluent. Common dopant source gases are arsine (AsH_3), phosphine (PH_3), and diborane (B_2H_6). The same steps occur in the incorporation of the dopants as occur in the thin film deposition, including mass transport and surface reactions. The surface reactions include (1) dissociation of the hydride gas, (2) lattice site incorporation and (3) burying of dopants atoms by the other atoms in the film. It is believed that these are the limiting steps for doping of Si during epitaxial growth, and not the mass transport through the boundary layer.

5.3.1 Atmospheric Pressure Chemical Vapor Deposition (APCVD)

Atmospheric Pressure Chemical Vapor Deposition (APCVD) is a CVD process conducted at atmospheric pressure, using thermal energy to drive chemical reactions on the substrate surface. In APCVD, precursor gases are introduced into a reaction chamber at atmospheric pressure, where they flow over a heated substrate. The heat induces reactions between the gas molecules, leading to a solid thin film on the substrate surface while by-products are removed through continuous gas flow. APCVD is advantageous due to its simplicity and cost-effectiveness, though it can suffer from non-uniform film thickness due to gas-phase reactions that occur outside of the substrate surface. This technique can be used to deposit silicon dioxide (SiO_2) and silicon nitride (Si_3N_4) thin films. Nowadays, the APCVD systems are no longer commonly used in microelectronics.

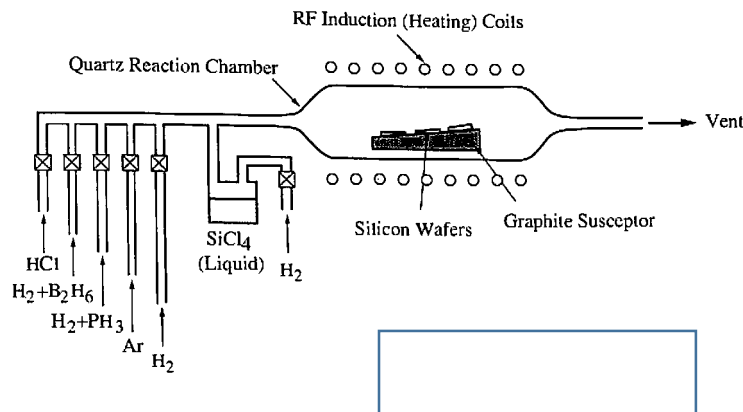


Figure 5.2 An atmospheric CVD system for depositing silicon thin film.

5.3.2 Low-Pressure Chemical Vapor Deposition (LPCVD)

Low-Pressure Chemical Vapor Deposition (LPCVD) is a refinement of the CVD process that operates in a low-pressure environment, reducing unwanted gas-phase reactions and improving film uniformity and adhesion. LPCVD involves the introduction of precursor gases into a low-pressure chamber, allowing for greater control over the reaction kinetics and reducing collisions between gas molecules in the bulk phase. This method achieves better thickness uniformity and step coverage, critical for microelectronic structures with small geometries. LPCVD typically utilizes gases such as silane (SiH_4) or phosphine (PH_3) and can achieve high-purity silicon films with fewer defects. The controlled environment of LPCVD provides films with consistent characteristics, making it ideal for semiconductor fabrication, though the requirement for vacuum equipment can add to operational costs.

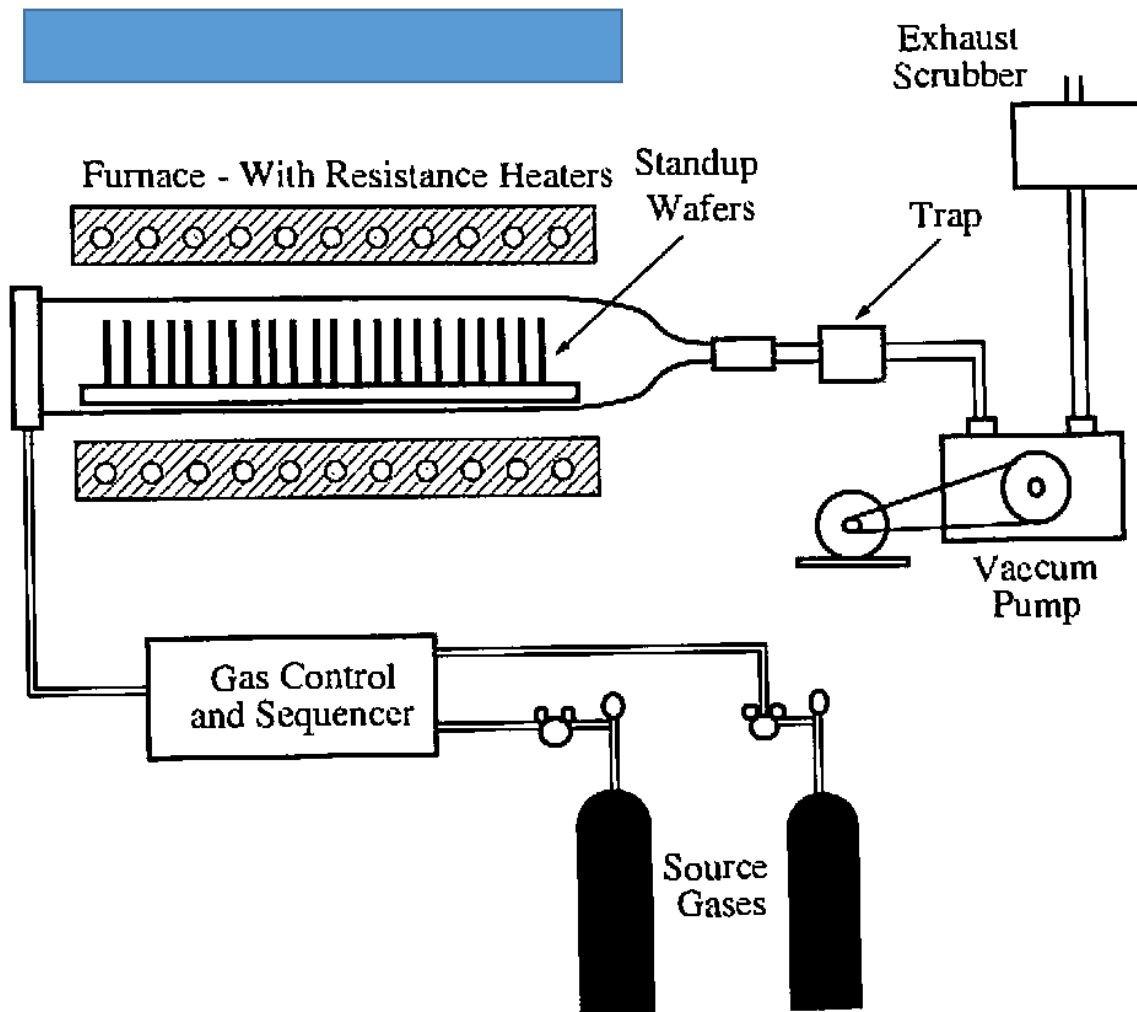


Figure 5.3 Low pressure Chemical Vapor Deposition reactor.

5.3.3 Plasma-Enhanced Chemical Vapor Deposition (PECVD)

Plasma-Enhanced Chemical Vapor Deposition (PECVD) addresses the limitations of conventional CVD by enabling deposition at lower temperatures, thanks to the energy provided by a plasma source. Plasmas are highly ionized gases that, by adding energy to reactant gases, allow deposition even at room temperature, though dielectric materials are typically deposited between 200°C and 350°C. This lower temperature benefits temperature-sensitive substrates and enables fine-tuning of film properties, such as composition and stress, though it can also lead to unwanted byproduct incorporation.

A typical PECVD setup places wafers on a heated electrode plate, with reactant gases like silane and oxygen introduced through inlets. An electric field generates a glow discharge plasma, creating ions and free radicals. These reactive species adsorb onto the wafer surface, interact, and react to form a solid film, aided by ion bombardment which enables deposition at lower temperatures than non-plasma CVD. Reaction byproducts are then exhausted through outlet ports.

Due to the complexity of plasma reactions, PECVD films may have nonstoichiometric compositions (e.g., Si-rich or O-rich SiO_2) or byproducts (e.g., H_2 , O_2), potentially causing issues like outgassing or cracking. PECVD generally provides good coverage over non-planar

surfaces, similar to high-temperature CVD. For small, high-aspect-ratio features, however, additional methods may be necessary for optimal coverage.

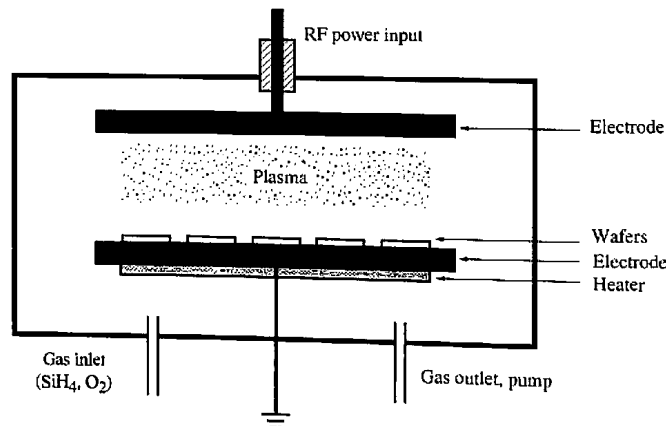


Figure 5.4 Typical PECVD equipment configuration.

5.3.4 High-Density Plasma Chemical Vapor Deposition (HDP-CVD)

A newly developed version of PECVD utilizes a very high-density plasma and a separate RF bias applied on the substrate. Called HDP (High-Density Plasma) CVD this technique combines PECVD deposition with bias sputtering to obtain very good filling of narrow gaps. It is used primarily for silicon dioxide depositions. The high-density plasma can be generated by a variety of sources, including Electron Cyclotron Resonance (ECR) and Inductively Coupled Plasma (ICP). This high-density plasma results in a dense CVD silicon dioxide film at low temperatures, typically 150°C down to room temperature, and with a very low chamber pressure in the 1-10 mtorr range. In fact, there is usually no intentional heating in these CVD systems. The ion bombardment supplies enough energy to raise the substrate temperature and cooling of the wafers is often required to keep the temperature below 400°C. With a separate RF bias applied on the substrate in HDP systems, the angular dependence of ion sputtering is exploited. Sputtering—the knocking off of atoms from a solid by incident ions when the solid is electrically biased—occurs preferentially on sloped surfaces rather than on vertical or horizontal surfaces. This simultaneous sputtering of the film during its deposition can result in planarized and void-free films. This is the same idea behind the bias sputtering deposition method. Bias-sputter deposition and angle-dependent sputtering will be more fully explained in the next section. The strong directed ion component of the HDP deposition process also helps in the filling of holes, and the ion bombardment helps make the film denser.

5.4 Physical Vapor Deposition (PVD)

Physical Vapor Deposition (PVD) is a thin film deposition process that, unlike CVD, does not involve chemical reactions. Instead, PVD relies on physical mechanisms to vaporize a material, which then condenses on a substrate to form a thin film. PVD techniques include evaporation and sputtering, both of which are extensively used for depositing metallic films in microelectronics. PVD provides excellent purity in the deposited material and allows for high precision in thickness control. However, PVD methods generally lack the conformal coverage of CVD, making them less suitable for highly structured surfaces. Despite this, PVD remains popular for applications requiring high-purity metal films and protective coatings, especially in the production of integrated circuits, capacitors, and thin film transistors.

5.4.1 Evaporation

A schematic of a simple evaporator is shown in Figure 9-15. In this process the source material is heated in a vacuum chamber which has initially been pumped down to less than 10^{-5} torr. Evaporated atoms from the source condense on the surfaces of the wafers. The heater can be of the resistance type, using a tungsten filament which heats up when current passes through it. More popular for microelectronics use is an e-beam heater, in which a high-energy electron beam is focused onto the source material in a crucible using magnetic fields, e-beam heaters can achieve higher temperatures so that a wider range of materials can be evaporated. In addition, the process is cleaner since no metal filaments are used. In addition, since only the top of the source in e-beam systems is usually melted, no contamination from the crucible occurs. As a result, purer films are deposited with e-beam evaporation systems. A downside of e-beam systems is that X-rays can be emitted when an e-beam strikes Al. These X-rays can create trapped charges in gate oxides. Annealing of the film is required to remove this damage.

Evaporation as a method for thin film deposition faces several significant challenges that have largely limited its use in mainstream silicon fabrication. One primary issue is the difficulty of depositing metals with low vapor pressures, such as tungsten (W), and of achieving precisely controlled compositions in alloy or compound films. Each material has a unique vapor pressure, and differences in evaporation rates make it challenging to maintain accurate stoichiometry in multi-component films. Another key drawback of evaporation is the lack of an in situ precleaning step, which is available in sputter deposition. Without this cleaning process, residual surface contamination on wafers can lead to poor film adhesion and quality.

Additionally, evaporation faces challenges with step coverage. Due to the very low chamber pressures needed, evaporated atoms or molecules travel in straight-line paths from the source to the substrate surface, with minimal collisions in the gas phase. Since the evaporant arrives from a small source, the atoms reach the wafer surface at a limited range of angles. This directional deposition results in poor step coverage, especially on complex or non-planar surfaces, where shadowing effects prevent the evaporated species from adequately reaching recessed or angled areas. While rotating the planetary holders and wafers during deposition helps to increase the range of arrival angles, it only partially addresses shadowing, leading to inconsistent thickness and film uniformity in complex topographies.

Finally, evaporated films often exhibit a lower density and weaker adhesion compared to films deposited by sputtering or CVD. The lack of energetic bombardment during deposition means that atoms have limited mobility on the substrate surface, resulting in a porous, columnar microstructure. This structure can be prone to moisture absorption and mechanical instability, further impacting the film's reliability in integrated circuits.

Evaporation faces several challenges that limit its use in silicon fabrication. It struggles with depositing low-vapor-pressure metals like tungsten and with maintaining precise compositions in alloy or compound films. The process also lacks in situ precleaning, leading to potential adhesion issues. Additionally, due to the straight-line travel of atoms in low-pressure environments, evaporation results in poor step coverage, especially on complex surfaces, as shadowing limits material reach. Finally, evaporated films often have low density and weak adhesion, making them prone to porosity and mechanical instability.

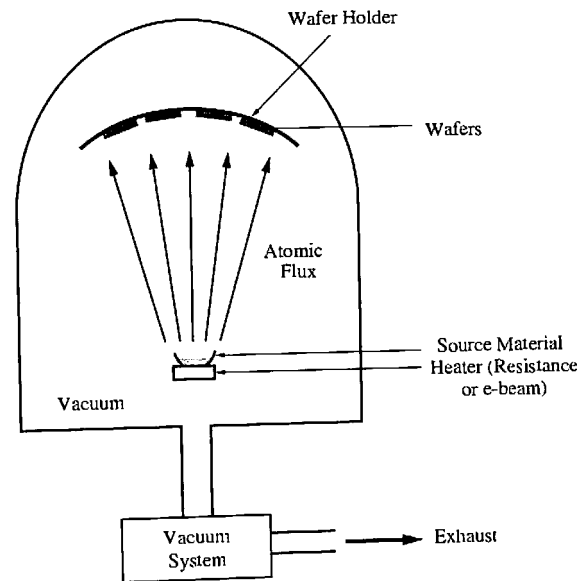


Figure 5.5 Schematic diagram of evaporation equipment.

5.4.2 Sputtering Deposition

Sputtering deposition is a PVD technique in which ions, typically from an inert gas like argon, bombard a target material, causing atoms to be ejected and deposited on the substrate. The process takes place in a vacuum chamber where plasma is created to ionize the argon, allowing high-energy ions to collide with the target. This method produces films with excellent adhesion and uniformity and enables the deposition of alloys and composite materials that would be difficult to achieve with evaporation. Sputtering is widely used for metal and dielectric films in microelectronics due to its precise thickness control, though it may require substrate cooling due to heating effects from ion bombardment.

3. Epitaxial Silicon

Epitaxial silicon deposition is a specialized thin film deposition method used to create high-quality monocrystalline silicon layers on a crystalline silicon substrate. In epitaxial growth, the deposited silicon atoms align with the atomic structure of the substrate, creating a film with minimal defects and excellent electrical properties. This process usually employs CVD at high temperatures, with silane (SiH_4) or trichlorosilane as the precursor gases. Carefully controlled temperature and pressure conditions ensure that the deposited silicon film has the same crystallographic orientation as the substrate. Epitaxial silicon is crucial in semiconductor device fabrication, as it allows for precise control over doping and layer thickness, essential for creating active layers in transistors and other devices with well-defined electrical properties.

4. Molecular Beam Epitaxy (MBE)

Molecular Beam Epitaxy (MBE) is a highly controlled thin film deposition technique that operates in ultra-high vacuum (UHV) conditions, enabling the deposition of extremely pure and precise atomic layers. The principle of MBE involves directing molecular or atomic beams onto a heated substrate, where the atoms or molecules condense to form a thin film.

MBE's ultra-high vacuum environment minimizes contamination and enables individual control over each atomic layer. This process is especially valuable in semiconductor device fabrication, where epitaxial layers