

Chapter 9

EE 2520

Jan - June 2024

9.1 Introduction

Material Deposition and Removal in IC Fabrication

- Material **deposition** and **removal** are essential processes throughout integrated circuit (IC) manufacturing.
- Various materials involved:
 - **Insulators** (e.g., SiO_2 , Si_3N_4).
 - **Semiconductors** (e.g., silicon, polysilicon).
 - **Conductors** (e.g., aluminum, tungsten, copper).
- Deposition typically covers the entire wafer surface in a **blanket form**.
- Some deposition methods can be **selective** and deposit only in targeted areas.
- Deposition processes will be covered in detail in **Chapter 10**.

2. Material Removal Methods

- Selective material removal is generally accomplished through:
 - **Lithography-defined masks** that expose specific regions.
 - Followed by **etching** to remove material from these exposed regions.
- Material removal can also be done via:
 - **Chemical-Mechanical Polishing (CMP)**.

3. Chemical-Mechanical Polishing (CMP)

- CMP uses a combination of:
 - **Chemical etching**.
 - **Mechanical polishing**.
- Initially developed to:
 - **Planarize back-end structures** by producing flat wafer surfaces.
- CMP is now used in:
 - Both **back-end** and **front-end** processing.
 - Especially important for shrinking device geometries and **high-resolution lithography**.
- As device geometries shrink:
 - The **depth of focus** in lithography decreases.
 - CMP ensures flat surfaces for successful lithographic pattern transfer.
- CMP will be discussed further in **Chapter 11**.

4. Etching as the Pattern Transfer Mechanism

- Etching plays the key role of:
 - Transferring mask designs into **physical structures** on the wafer.
- Defines critical IC features such as:
 - **Doped regions.**
 - **Isolation structures.**
 - **Gates.**
 - **Interconnects.**
- Without precise etching:
 - Mask patterns cannot be faithfully realized on the wafer.
 - Device integrity and performance would be compromised.
- Modern etch machines are among the **most advanced processing equipment**, second only to lithography tools.

5. Isotropic vs. Directional Etching Concepts

- Two key etching mechanisms:
 - (a) **Isotropic etching:**
 - Material removal occurs **uniformly in all directions** (both vertical and lateral).
 - Typical of most **wet etchants**.
 - Often leads to **undercutting** beneath the mask.
 - (b) **Directional (anisotropic) etching:**
 - Etches **primarily in the vertical direction**.
 - Minimizes lateral etching.
 - Commonly associated with **dry or plasma etching**.
- Important to note:
 - While wet etching is typically isotropic, in some specific cases wet etch profiles may exhibit **directionality**.

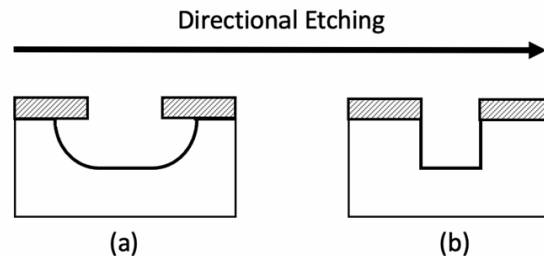


Figure 1: Schematic illustration of isotropic and directional etching profiles

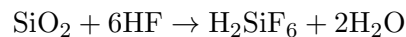
9.2 Wet Etching

1. Key Features of Wet Etching

- **Wet etching** involves the removal of materials using liquid chemical solutions.
- Two main advantages:
 - (a) **Simplicity**:
 - Etching is performed by simply **immersing the wafer** into a chemical bath.
 - The process targets only the **exposed regions** defined by the lithography mask.
 - (b) **Selectivity**:
 - Chemical reactions allow for **high selectivity** between the target material and the underlying or masking materials.
 - Enables **uniform and reproducible** material removal.

2. Example: Silicon Dioxide (SiO₂) Etching with Hydrofluoric Acid (HF)

- **Hydrofluoric acid (HF)** is commonly used for etching SiO₂.
- The overall chemical reaction is:



- Features of HF-based oxide etching:
 - **High selectivity** against silicon and silicon nitride.
 - Widely used for etching **thermal oxide** and cleaning native oxide layers.

3. Buffered Oxide Etch (BOE)

- **Buffered Oxide Etch (BOE)** is created by adding **ammonium fluoride (NH₄F)** to HF.
- Purpose of buffering:
 - Prevents **depletion of fluoride ions**.
 - Maintains **uniform etch rates**.
 - Reduces **mask lifting** during oxide etching.
- Typical etch rate:
 - About **100 nm/min** for thermal oxide.

4. Dilute HF for Thin Oxide and Native Oxide Removal

- For very thin oxide layers or **native oxide** on silicon:
- A **diluted HF solution** (e.g., 100:1 HF) is used.
- Etch rate:
 - Approximately **1 nm/min**.
- Offers excellent control for fine oxide removal.

5. Etching of Silicon Using HF with Oxidizers

- Silicon does not etch readily in HF alone.
- Adding an **oxidizer like nitric acid (HNO₃)**:
 - Forms a thin chemical oxide on the silicon surface.
 - The oxide is then etched away by HF.
- **Acetic acid (CH₃COOH)** is used as a buffering agent:
 - Limits nitric acid dissociation.
 - Ensures uniform oxide formation and etching.
- This mixture is commonly referred to as the “**isotropic silicon etch**”.

6. Selectivity in Wet Etching

- Selectivity S defines the ratio of etch rates between two materials:

$$S = \frac{r_1}{r_2}$$

where:

- r_1 = Etch rate of the target material.
- r_2 = Etch rate of the masking or underlying material.
- **High selectivity** minimizes damage to masks and underlying structures.

7. Etch Profiles and Anisotropy in Wet Etching

- Despite high selectivity, **wet etching is typically isotropic**.
- Isotropic etching causes:
 - **Lateral undercutting** beneath the mask.
 - Profiles that may appear **semi-circular** if etched to full film thickness.
- Profile shape is sensitive to:
 - **Etch time**.
 - Mask positioning.
 - Over-etching may increase verticality but does not imply true anisotropy.

8. Anisotropy Definition and Calculation

- Anisotropy A quantifies the directionality of the etching process:

$$A = 1 - \frac{r_{\text{lat}}}{r_{\text{vert}}}$$

where:

- r_{lat} = Lateral etch rate.
- r_{vert} = Vertical etch rate.
- Interpretation:

- $A = 0$: Completely isotropic etching.
- $A = 1$: Perfectly anisotropic etching.
- $A < 0$: Vertical rate is smaller than lateral rate (rare but possible).
- For purely chemical (wet) etching:
 - $A = 0$ due to equal rates in all directions.

9. Anisotropy Behavior with Etch Time

- Over time, if the target layer is fully removed:
 - r_{vert} may approach zero (perfect selectivity stops etching on underlying layer).
 - Finite selectivity means r_{vert} decreases but remains non-zero.
- The anisotropy A may become **negative** if the vertical rate becomes much smaller than lateral rate.

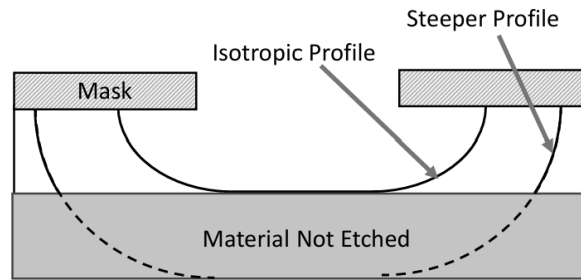


Figure 2: Schematic of isotropic wet etching profile

9.3 Basics of Dry or Plasma Etching

1. Motivation for Dry Etching

- **Wet etching** often leads to:
 - Significant **lateral etching** (isotropic profiles).
 - Enlargement of the etched area beyond the mask dimensions.
- For accurate pattern transfer, **directionality** is essential.
- **Dry or plasma etching** was developed to:
 - Provide more **anisotropic (directional) etching**.
 - Enable faithful mask pattern transfer into underlying layers.

2. Role of Ions and Neutrals in Plasma Etching

- The **directionality** of plasma etching comes from:
 - **Ions** accelerated perpendicularly toward the wafer surface by electric fields in the plasma sheath.

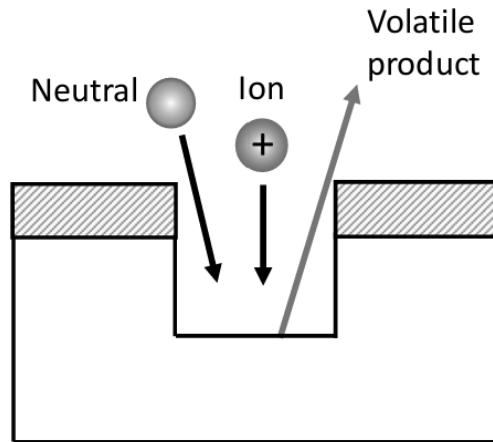


Figure 3: Schematic of directional etching in a plasma system

- **Neutral species** may also contribute chemically:
 - But they do not provide directionality.
- Requirement for etching:
 - Etch byproducts must be **volatile** so that they do not redeposit and block the surface.

3. Plasma: The Fourth State of Matter

- A **plasma** is a partially ionized gas consisting of:
 - Ions.
 - Electrons.
 - Neutral atoms or molecules.
 - Excited molecules.
 - Free radicals (highly reactive neutral species with unpaired electrons).
- Termed the **fourth state of matter** by W. Crookes in 1880.
- In thermal equilibrium, plasma temperatures can be extremely high (e.g., stars).
- Semiconductor processing uses **non-thermal, low-pressure, weakly ionized plasmas**:
 - Ion and electron densities $n_i \approx n_e$.
 - Ionization levels 10^{-4} to 10^{-6} of the neutral gas density.

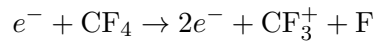
4. Plasma Generation for Semiconductor Processing

- Achieved by applying **electric fields** to accelerate free electrons.
- Free electrons gain enough energy to:
 - Ionize neutral gas molecules or atoms.
 - Sustain the plasma through **collisions and secondary ionization**.

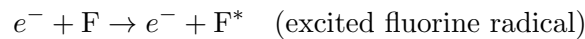
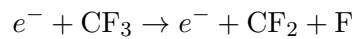
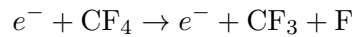
- Example: Fluorescent light bulbs or neon signs.
- In these systems:
 - Electron temperatures $T_e \approx 11,000$ K.
 - Overall plasma remains **weakly ionized** with low total heat transfer.

5. Example Reaction: Dissociation of CF_4 in Plasma

- Using CF_4 gas as an example for silicon etching.
- **Dissociative ionization:**



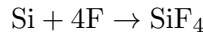
- **Neutral dissociation and excitation** reactions:



- **Free radicals** like F, CF_3 , CF_2 are highly reactive due to unpaired electrons.

6. Chemical Reaction with Silicon

- Key chemical etch reaction:



- SiF_4 is volatile and can be pumped away, completing the etch process.
- Note: **Copper cannot be etched** this way because it forms no volatile byproducts.

7. Role of Ions and Radicals in Etch Directionality

- Neutral radicals alone produce **isotropic etching**.
- Directionality is achieved through:
 - **Ion bombardment** across the plasma sheath.
 - Ions like CF_3^+ impact the surface perpendicularly.
- Ion impact:
 - Enhances etching by **activating or breaking surface bonds**.
 - Helps remove inhibitors like fluorocarbon films (e.g., CF_2 , CF_3 layers).

8. Competitive Processes in Plasma Etching

- Key competing effects:
 - **Deposition of inhibitors** (e.g., carbon-rich fluorocarbon layers).
 - **Ion-enhanced etching** (removal of these inhibitors).
 - Balance between:
 - * **Etchants.**

- * **Inhibitors.**
- * **Ion bombardment.**
- Example:
 - Fluorocarbon layer ≈ 0.5 nm thick.
 - May require ion activation to enable continued etching.
 - Oxygen can be added to promote volatile CO or CO₂ byproduct formation, removing carbon contamination.

9.3.1 The Plasma Sheath and Ion Energies

1. Importance of Ion Energies in Plasma Etching

- Ion energy plays a critical role in:
 - Determining the **etch directionality**.
 - Driving the chemical reactions at the wafer surface.
- In a plasma etching system:
 - **Ion bombardment energy** contributes to the formation of anisotropic etch profiles.
- Understanding ion energies requires a basic understanding of:
 - Plasma temperatures.
 - Plasma potentials.
 - Sheath formation.

2. Energy Descriptions in Plasma Physics

- Plasma energy is often described using the concept of **temperature**.
- For plasma particles:
 - **Ion temperature** T_i .
 - **Electron temperature** T_e .
- Energy in joules:

$$E \text{ (J)} = kT$$

where:

- $k = 1.38 \times 10^{-23}$ J/K (Boltzmann constant).
- T is temperature in kelvin.

3. Energy in Electron-Volts (eV)

- Often, plasma energies are expressed in **electron-volts (eV)**:

$$E \text{ (J)} = qV$$

where:

- $q = 1.6 \times 10^{-19}$ C (elementary charge).

- V is the potential in volts.
- Conversion between temperature and energy:

$$1 \text{ eV} \approx 11,600 \text{ K}$$

- Example:
 - Room temperature $\approx 297 \text{ K} \approx 0.026 \text{ eV}$.

4. Plasma Characteristics Relevant to Etching

- Plasma in etching systems is typically **weakly ionized**.
- Densities:
 - Neutral gas density \gg ion and electron densities $n_i \approx n_e$.
- Energy levels:
 - Electrons: **higher temperature** (higher energy).
 - Ions: **lower temperature** (slower to respond).
- Electrons respond quickly to the **RF electric field**.
- Heavy ions respond more slowly, but are accelerated across the plasma sheath.

5. Ion Energy Distribution

- Despite low average ion temperature T_i , a significant fraction of ions:
 - Acquire **high kinetic energies** due to **sheath acceleration**.
- These high-energy ions are crucial for:
 - Breaking surface bonds.
 - Enhancing the etch rate.
 - Producing anisotropic profiles.

6. Plasma Potential and Ion Acceleration

- In a plasma:
 - Electron and ion densities are equal $n_e = n_i$.
 - Plasma behaves like a conductor: electric field $E = 0$ in the bulk.
- Near the plasma boundary (sheath region):
 - Electrons, being lighter, escape more easily to the walls.
 - Plasma builds up a **positive DC potential** V_P relative to the grounded walls.
- This potential:
 - **Confines electrons** within the plasma.
 - **Accelerates ions** toward the wafer through the sheath.
- Ion energy from the sheath acceleration:

$$E_{\text{ion}} \approx qV_P$$

where:

- V_P is the plasma potential.



Figure 4: Energy distributions of electrons, ions, and neutrals in a low-pressure capacitive plasma discharge (Adapted from Figure 9.6).

7. Energy Relations

- Energies in plasma can be represented as:

$$E = kT \quad \text{or} \quad E = qV$$

- Important conversions:
 - $1 \text{ eV} = 11,600 \text{ K}$.
 - Room temperature $297 \text{ K} \approx 0.026 \text{ eV}$.
- Plasma ions are **heated and accelerated across the sheath** despite having low T_i .
- This **ion bombardment energy** is key to achieving:
 - Directional etching.
 - Effective surface reaction activation.

9.3.2 Plasma Sheath Formation

1. Concept of Plasma Sheath

- In plasma etching systems, the **glowing plasma** does not extend all the way to the chamber walls.
- A **dark region**, known as the **plasma sheath**, forms naturally at all surfaces surrounding the plasma.
- The sheath plays a critical role in:
 - **Isolating** the plasma from chamber surfaces.
 - **Accelerating ions** toward the wafer surface.
 - Supporting the **electric fields** needed for anisotropic etching.

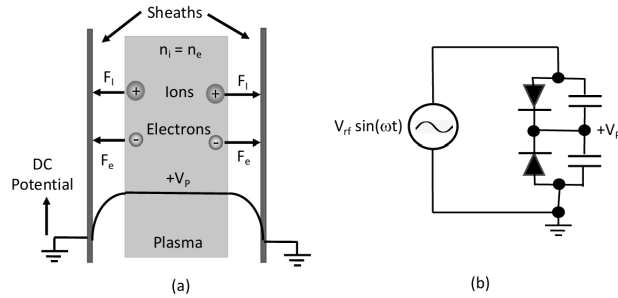


Figure 5: a) Plasma and sheath region, with electric field and ion and electron fluxes indicated (after Lieberman [9.3]). (b) shows a simple circuit model for a typical high-frequency RF plasma.

2. Origin of Sheath Formation

- In the plasma bulk:
 - Ion and electron densities are approximately equal: $n_i = n_e$.
 - Plasma behaves like a **conductor** with $\mathcal{E} = 0$.

- At the plasma edges:
 - Electrons, being much lighter than ions, escape more rapidly to the walls.
 - The loss of electrons builds up a **positive plasma potential** V_P relative to the grounded walls.
- This potential confines electrons and prevents continuous electron loss.
- Ions are accelerated across the sheath toward the walls to balance the charge loss.

3. Basic Plasma Dynamics in Sheath Formation

- Electron mass m is much smaller than ion mass M :

$$\frac{m}{M} \ll 1$$

- Electron temperature T_e is much higher than ion temperature T_i :

$$T_i \ll T_e$$

- Electron **thermal velocity** is much higher than ion velocity:

$$v_{e, \text{ thermal}} \gg v_{i, \text{ thermal}}$$

- Rapid electron escape leads to sheath formation to maintain flux balance:

$$\Phi_i = \Phi_e$$

where:

- Φ_i : Ion flux.
- Φ_e : Electron flux.

4. Estimation of Plasma Potential V_P

- Assuming a **Boltzmann distribution** for the electron energy:

$$n_e \sim \exp\left(-\frac{qV_P}{kT_e}\right)$$

- To confine electrons, the plasma potential V_P must be a few times kT_e/q :

$$V_P \approx \text{a few} \times \frac{kT_e}{q}$$

- This positive potential allows ions to gain significant energy for bombardment:

$$E_{\text{ion}} \approx qV_P$$

5. Plasma Sheath Structure

- The sheath is an **electron-depletion region**:
 - Contains mostly positive ions.
 - Electrons are repelled, creating a net positive charge in the sheath.
- The **electric field** across the sheath:
 - May be several **kV/cm**.
 - Responsible for **ion acceleration** toward surfaces.
- The sheath region appears **dark** (no glow):
 - Few electron-neutral collisions.
 - Minimal excited species to emit light.

6. Equivalent Circuit Representation

- The sheath behaves like a **capacitor**:
 - Supports the sheath voltage.
 - Most RF current is displacement current across the sheath capacitance.
- Electron and ion currents balance:

$$I_{\text{ion}} = I_{\text{electron}}$$

- Diode-like behavior in the equivalent circuit:
 - Electrons flow easily only when the sheath potential allows.
 - Reverse-biased conditions limit the electron current.

7. Role of RF Fields and Sheath Behavior

- When RF power is first applied:
 - Electrons escape rapidly to the walls.
 - Plasma develops a **positive DC potential** to confine electrons.
- In steady state:
 - Ions respond to the DC sheath field and are continuously accelerated.
 - Electrons follow the **RF oscillations** but flow to the electrode only during certain phases of the cycle.

8. Summary of Plasma Sheath Formation

- Plasma sheaths form **naturally** due to electron mobility and plasma dynamics.
- They play a key role in:
 - **Confining electrons**.
 - **Accelerating ions** to drive anisotropic etching.
- Sheath voltage directly determines the **ion bombardment energy**:

$$E_{\text{ion}} = qV_P$$

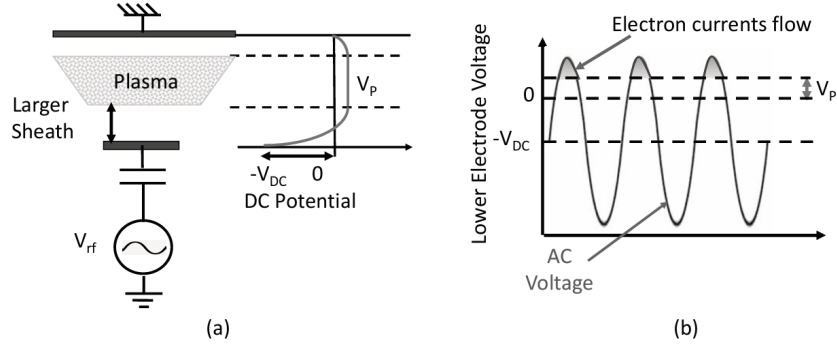


Figure 6: Schematic of the higher DC field on the smaller electrode. An additional DC sheath bias (-VDC) is created by the system to maintain the same current at the smaller electrode.

- Essential for achieving:
 - **High anisotropy.**
 - **Effective surface activation** during plasma etching.

9.4 Plasma Chemistry

1. Overview of Plasma Chemistry in Etching

- Plasma chemistry plays a crucial role in the **etching mechanism**.
- Involves complex interactions between:
 - **Electrons.**
 - **Ions.**
 - **Neutral molecules.**
 - **Free radicals** (highly reactive neutrals).
- Plasma reactions are mostly **inelastic electron-neutral collisions**:
 - Transfer electron kinetic energy into **internal energy** of the molecules.

2. Major Types of Plasma Reactions

(a) **Excitation:**

- Electron collision raises a molecule to an **excited state**.
- The excited state decays by emitting **characteristic light**.
- Example: Oxygen plasma glows blue.

(b) **Dissociation:**

- A gas molecule splits into two **neutral radicals** with unpaired electrons.
- These free radicals are highly reactive.

(c) **Ionization:**

- Collision produces a **positive ion** and a **secondary electron**.
- Maintains the plasma by sustaining electron density.

(d) **Dissociative Ionization:**

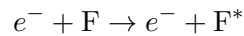
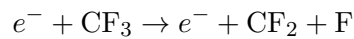
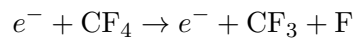
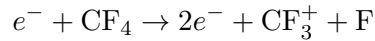
- A combined reaction where ionization and dissociation occur simultaneously.

(e) **Recombination:**

- Electrons recombine with positive ions.
- Acts as a loss mechanism for sustaining plasma density.

3. Example: CF_4 Plasma Chemistry

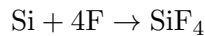
- Example reactions in a CF_4 discharge:



- Resulting species:
 - Free radicals like F , CF_3 , CF_2 .
 - Excited fluorine F^* .
 - Positive ions like CF_3^+ .

4. Role of Radicals and Etch Byproducts

- Free radicals are:
 - Electrically neutral.
 - Highly reactive due to unpaired electrons.
- Etching occurs via chemical reactions such as:



- Key requirement for etching:
 - **Reaction products must be volatile** (e.g., SiF_4).
 - Otherwise, byproducts will redeposit and block the etching process.

5. Reaction Probabilities and Cross-Sections

- The likelihood of plasma reactions depends on:
 - **Collision cross-section.**
 - **Densities** of the reacting species.
 - **Electron energy (temperature).**
- Electron-neutral collisions:
 - Allow electrons to gain energy over multiple RF cycles.
 - Lead to the **high-energy tail** in the electron energy distribution.

6. Weak Ionization and Dissociation Preference

- Dissociation energy threshold (E_{diss}) is generally lower than ionization energy (E_{iz}):

$$E_{\text{diss}} < E_{\text{iz}}$$

- Therefore, **dissociation reactions dominate** over ionization in low-temperature plasmas.
- Result:
 - High **neutral and radical densities**.
 - Relatively low **charged species densities**.
- This is why low-pressure plasmas are typically **weakly ionized**.

7. Plasma Emission Spectroscopy

- Optical emission spectra provide:
 - Direct information about **plasma species**.
 - Characteristic emission peaks for radicals, ions, and byproducts.
- Example:
 - Complex spectrum from CF_4/O_2 plasma (Fig. 9.10(b)).
 - Allows **process monitoring** and end-point detection.

8. Complexity of Real Plasma Systems

- Actual plasma chemistry involves:
 - Chains of secondary and tertiary reactions.
 - Interaction of etch byproducts with the plasma.
- Etch products themselves may participate in:
 - Additional dissociation.
 - Excitation.
 - Ionization.
- This feedback loop can significantly affect:
 - Etch rate.
 - Etch uniformity.
 - Profile shape.

9.4.1 Choosing a Plasma Chemistry

1. Criteria for Selecting Plasma Source Gases

- The primary consideration when choosing a plasma chemistry is:
 - The **volatility of the reaction byproducts**.
- Reaction products must be **volatile** to avoid:

- Redeposition on the wafer surface.
- Inhibition of further etching.
- Volatility is typically indicated by:
 - Low **boiling points**.
 - High **vapor pressures**.

2. Guidelines for Gas Selection

- **Fluorine-based chemistries** (e.g., SF_6 , CF_4):
 - Suitable for silicon etching.
 - Form highly volatile byproducts like SiF_4 .
- **Chlorine-based chemistries** (e.g., Cl_2 , BCl_3):
 - Effective for etching metals like Al.
 - Require volatile chlorides to avoid residue.
- **Bromine-based chemistries**:
 - Sometimes used for specific applications where chlorides or fluorides are ineffective.

3. Example: Si vs. Cu Etching

- **Silicon**:
 - Reacts with fluorine to form volatile SiF_4 .
 - Hence, fluorine-based plasmas are effective for Si etching.
- **Copper**:
 - Does not form volatile byproducts with F, Cl, or Br.
 - Cannot be etched effectively using conventional halogen chemistries.

4. Vapor Pressure and Boiling Point Considerations

- Table 9.3 provides boiling points of common halide compounds (fluorides, chlorides, bromides).
- Lower boiling points suggest higher volatility, making those chemistries suitable for etching.
- Example from Table 9.3:
 - SiF_4 : highly volatile (favorable).
 - CuCl , CuF_2 : not volatile at typical processing temperatures (unfavorable).

5. Strategy for Plasma Chemistry Selection

- Use boiling point data as an **initial screening tool**.
- Select source gases that produce **volatile etch byproducts**.
- Ensure compatibility with:
 - Etch material.
 - Mask materials.
 - Underlying layers.

6. Summary

- Plasma gas selection depends primarily on:
 - Ability to form **volatile etch products**.
- Boiling point and vapor pressure data offer practical guidance.
- **No single gas works universally** — careful material-specific optimization is required.

9.5 Plasma Etching Mechanisms

1. Overview of Plasma Etching Mechanisms

- Plasma etching mechanisms cover a spectrum:
 - (a) **Purely chemical etching**.
 - (b) **Purely physical etching**.
 - (c) **Ion-enhanced (mixed-mode) chemical etching**.
- Mixed-mode processes are the most widely used in semiconductor fabrication.
- Figure 9.12 provides a schematic overview of these different etching regimes.

9.5.1 Purely Chemical Plasma Etching (Isotropic Plasma Etching)

1. Introduction

- Although plasma etching is often associated with directional profiles, **isotropic plasma etching** is useful in several applications.
- Example: **Photoresist stripping** and selective layer removal.
- Plasma etching avoids problems associated with wet etching:
 - **Toxic chemicals** like hot sulfuric acid are not required.
 - Eliminates issues of **wettability** and **surface tension** at small dimensions.

2. Mechanism of Isotropic Plasma Etching

- Plasma contains:
 - Free radicals (highly reactive neutrals with unpaired electrons).
 - Neutrals and ions.
- In isotropic etching:
 - **Free radicals dominate** the etch process.
 - Ion bombardment is **minimized or eliminated**.
- Typical system: **Barrel etcher**.
 - Wafers are surrounded by a grounded metal grid.
 - Grid captures bombarding ions, allowing only radicals to reach the wafer.

3. Example: Oxygen Plasma for Photoresist Stripping

- Photoresist materials are **carbon-based polymers**.
- Oxygen plasma forms volatile products like:
 - **CO**, **CO₂**, and **H₂O**.
- Advantages:
 - Effective for **removing hardened resist**.
 - Common in **high-dose implant masks** and advanced stripping processes.

4. Selectivity and Process Benefits

- Isotropic plasma etching shares selectivity characteristics with wet etching:
 - High selectivity between the photoresist and underlying layers.
 - Example: Oxygen plasma strips resist without affecting Si, SiO₂, or Si₃N₄.
- Applications include:
 - **Gate-all-around FET fabrication** — selective removal of SiGe in alternating Si/SiGe stacks.
 - **MEMS membrane formation** — isotropic undercutting of layers.

9.5.2 Purely Physical Plasma Etching (Ion Milling)

1. Introduction to Ion Milling

- **Ion milling**, also called **physical sputter etching**, represents the extreme case of plasma processing where:
 - Etching occurs via **momentum transfer** from incident ions to substrate atoms.
 - No chemical reactions are involved.
- Similar to **sandblasting** at the atomic scale.
- Especially useful for materials where no volatile etch products can be formed.

2. Ion Milling Mechanism

- Relies on:
 - High-energy ion beams (e.g., Ar⁺ ions).
 - Ion bombardment transfers kinetic energy to surface atoms.
 - If the energy exceeds the **binding energy** of the atoms, they are ejected from the surface.
- No selectivity between mask and substrate — purely physical removal.

3. Ion Milling Yield

- Defined as:

$$\text{Yield} = \frac{\text{Number of ejected atoms}}{\text{Number of incident ions}}$$

- Yield depends on:
 - Ion energy.
 - Angle of incidence.
 - Masses of ions and target atoms.
 - Binding energy of the substrate material.

4. Angle Dependence of Sputter Yield

- Yield varies with the **angle of incidence**:
 - Maximum yield at intermediate incidence angles.
 - Lower yield at normal and grazing incidences.
- Substrate topography can influence:
 - Effective local angle of incidence.
 - Uniformity of the etch rate across patterned features.

5. Process Conditions in Ion Milling

- Typical conditions:
 - Low pressure ($\sim 10^{-5}$ Torr) to minimize ion-neutral collisions.
 - Higher sheath fields at smaller electrode areas to increase ion energies.
 - Often uses **argon ions** (Ar^+) due to chemical inertness.

6. Advantages and Limitations of Ion Milling

Advantages:

- Can etch **any material**, even those without volatile byproducts.
- Highly directional due to ion acceleration across the sheath.

Limitations:

- **No selectivity** — mask and substrate are etched equally.
- **Low etch rates** due to the purely physical process.
- Ion flux and etch rates are limited by plasma density at low pressures.
- Typically used in **research and development**, not for high-volume manufacturing.

7. Summary

- Ion milling (sputter etching) is an important technique for:
 - Non-volatile material removal.
 - Applications where chemical etching is ineffective.
- Selectivity and throughput are sacrificed for **universality and anisotropy**.

9.5.3 Ion-Enhanced Chemical Etching

1. Introduction to Ion-Enhanced Chemical Etching

- Plasma etching achieves its widespread use due to the **synergistic effect** between:
 - **Ion bombardment.**
 - **Chemical etching** by neutral species (free radicals).
- The synergy between these two mechanisms leads to:
 - Enhanced etch rates.
 - Anisotropic profiles.
 - Good selectivity between mask and substrate.

2. Experimental Demonstration of Synergistic Effects

- Classic experiment by Coburn and Winters (1979):
 - Compared silicon etch rates under three conditions:
 - (a) **Chemical gas alone (XeF_2)** — slow etch.
 - (b) **Ion bombardment alone (Ar^+)** — slow etch.
 - (c) **Both combined** — **dramatic increase** in etch rate.
- The enhancement is not additive but **synergistic**.

3. Mechanism of Synergy

- Ions provide:
 - **Surface bond breaking.**
 - Activation of surface atoms.
- Radicals (neutrals) provide:
 - **Chemically reactive species.**
 - React with the activated surface to form **volatile etch products**.
- The combined process allows:
 - Etching at areas exposed to ion bombardment.
 - Suppressed etching at areas without ion exposure (sidewalls), leading to anisotropy.

4. Misconceptions and Nomenclature

- The term **Reactive Ion Etching (RIE)** is commonly used.
- However, ions themselves are often **inert** (e.g., Ar^+).
- The enhanced etching arises from:
 - **Ion activation.**
 - **Reactive radicals**, not reactive ions.
- More accurate terms:
 - **Ion-enhanced etching.**
 - **Ion-assisted etching.**

5. Dependence on Ion and Radical Fluxes

- Etch rate is a function of:
 - Ion flux.
 - Neutral radical flux.
- Both fluxes must be balanced to:
 - Maximize etch rate.
 - Maintain anisotropy.

6. Saturation Behavior of Ion-Enhanced Etching

- Controlled experiments using:
 - Argon ion beam.
 - Molecular Cl_2 or atomic Cl flux.
- Observation:
 - Etch rate increases initially with chlorine flux.
 - Saturation occurs when the **chlorine flux far exceeds ion flux**.
- Physical explanation:
 - Maximum adsorption of chlorine on the surface.
 - Beyond saturation, excess chlorine does not enhance the etch rate further.

7. Challenges in Plasma Etching Control

- In simple parallel-plate plasma systems:
 - Increasing RF power increases both:
 - * **Ion energy**.
 - * **Radical generation**.
 - Difficult to **independently control ion and radical fluxes**.
- More sophisticated systems (e.g., inductively coupled plasma, ECR plasma) can:
 - Provide **independent control** over ion energy and radical density.

8. Summary

- Ion-enhanced chemical etching:
 - Provides the optimal combination of:
 - * **High anisotropy**.
 - * **Good selectivity**.
 - * **Enhanced etch rates**.
- It is the dominant etching technique in modern semiconductor fabrication.

9.5.4 Ion-Enhanced Inhibitor Etching

1. Concept of Ion-Enhanced Inhibitor Etching

- A specialized form of ion-enhanced etching where:
 - **Inhibitor layers** play a key role in controlling the etch profile.
 - Ions remove the inhibitor from specific regions (e.g., horizontal surfaces).
 - Chemical etching proceeds only where the inhibitor has been removed.
- This approach enables:
 - Highly **anisotropic etching profiles**.
 - Protection of **sidewalls** by retaining the inhibitor there.

2. Typical Chemistries for Inhibitor Etching

- Fluorine-based systems such as:
 - CF_4 , CHF_3 , C_2F_6 , C_4F_8 .
- These gases form:
 - **Carbon-rich fluorocarbon layers** that act as inhibitors.
 - Deposition of a $(\text{CF}_2)_n$ -like polymer, similar to Teflon.

3. Process Control via F/C Ratio

- **Fluorine-to-carbon (F/C) ratio** determines:
 - Selectivity.
 - Etch rate.
 - Profile control.
- Lower F/C ratios:
 - Increase carbon deposition (more inhibitor formation).
 - Improve selectivity by slowing etch rates of silicon relative to SiO_2 .
- Example: CF_4 vs. C_4F_8 :
 - CF_4 : higher F/C ratio, aggressive etching.
 - C_4F_8 : lower F/C ratio, more inhibitor deposition.

4. Role of Additives (H_2 , O_2) in Chemistry Control

- **Hydrogen additions:**
 - React with fluorine to form HF.
 - Reduce free F radical concentration, promoting deposition.
- **Oxygen additions:**
 - React with CF_x species (e.g., CF_3 , CF_2).
 - Prevent recombination with F radicals, increasing free fluorine concentration.
 - Shift process toward etching by removing inhibitors.

5. Selectivity Control Example

- Table 9.4 shows etch rates for:
 - Si.
 - SiO₂.
 - Si₃N₄.
- Lower F/C ratios increase selectivity:
 - More carbon inhibits silicon etching.
 - Oxygen in SiO₂ helps remove the carbon layer, allowing oxide etching.

6. Bosch Process (Deep Reactive Ion Etching)

- Uses **alternating cycles** of:
 - (a) **Polymer deposition** (e.g., with C₄F₈).
 - (b) **Ion bombardment removal** of the inhibitor from horizontal surfaces.
 - (c) **Isotropic silicon etching** with SF₆.
- Enables **deep silicon etching** with vertical sidewalls.
- The sidewalls remain protected by the polymer layer, preventing lateral etching.

7. Process Complexity and Considerations

- Deposition species may originate from:
 - Etch gas breakdown.
 - Mask material outgassing.
- Control of:
 - Gas flows.
 - Power levels.
 - Pressure.
 - Ion energies.
- Accurate process tuning is critical to:
 - Control inhibitor thickness.
 - Maintain profile shape.
 - Balance between etching and deposition.

8. Summary

- Ion-enhanced inhibitor etching combines:
 - **Directional ion bombardment**.
 - **Chemistry-based selectivity** via inhibitors.
- Techniques like the **Bosch process** leverage this mechanism for:
 - **MEMS fabrication**.
 - **Through-wafer etching**.
 - Other high-aspect-ratio applications.

9.6 High-Density Plasma Etching

1. Introduction to High-Density Plasma (HDP) Etching

- **High-Density Plasma (HDP) etching** represents an advanced form of plasma etching designed to:
 - Provide **higher plasma densities**.
 - Improve **etch rates** and **anisotropy**.
- In HDP systems, the plasma density is significantly higher than in traditional RIE systems.
- The electron density typically reaches:

$$10^{11} - 10^{12} \text{ electrons/cm}^3.$$

2. Methods of Plasma Generation in HDP Systems

- Two common techniques for high-density plasma generation:
 - **Inductively Coupled Plasma (ICP)**:
 - * Uses a **coil outside the chamber** to inductively couple RF energy into the plasma.
 - **Electron Cyclotron Resonance (ECR) Plasma**:
 - * Uses **microwave power** and a **magnetic field** to confine and energize electrons.
- Both methods decouple:
 - **Plasma generation power** (for plasma density).
 - **Bias power** (for ion energy and directional control).

3. Features and Benefits of High-Density Plasma Etching

- Advantages of HDP etching:
 - **Higher etch rates**.
 - **Excellent anisotropy**.
 - **Better sidewall profile control**.
 - Enhanced **selectivity** due to independent control of plasma density and ion energy.
- Suitable for:
 - **Deep trench etching**.
 - **Via formation in high-aspect ratio structures**.
 - **MEMS and advanced CMOS fabrication**.

4. Challenges and Limitations of HDP Etching

- Potential issues include:
 - **Complex reactor design**.

- **Higher equipment cost.**
- Managing **ion-induced damage** and **charging effects**.
- Requires precise control over:
 - **Ion flux.**
 - **Ion energy.**
 - **Etchant gas flow rates.**

9.7 Etching with the Chlorides and Bromides

1. Overview of Chloride and Bromide Etching Chemistries

- While fluorine-based etching is commonly used for silicon, **chloride** and **bromide** chemistries offer:
 - Better **anisotropy**.
 - Selective etching of metals like **aluminum**, where fluorides fail due to non-volatile byproducts.
- Applicable source gases:
 - **Chlorides:** Cl_2 , HCl , CCl_4 , freons ($\text{CH}_x\text{Cl}_y\text{F}_z$).
 - **Bromides:** HBr , Br_2 .

2. Profile Control and Anisotropy

- Bromine chemistries exhibit superior anisotropy:

Vertical to lateral etch ratio $\approx 100 : 1$ (Br-based) vs. $< 10 : 1$ (F-based)

- Mixtures of **Cl_2** and **HBr** are commonly used to:
 - Optimize etch **selectivity**.
 - Improve **profile anisotropy**.
- Small additions of **O_2** assist in:
 - **Carbon residue removal.**
 - Further enhancement of selectivity.

3. Application Examples

Silicon Etching:

- Fluorine-based chemistries produce **tapered profiles** due to lateral etching.
- Tapering arises because:
 - The chemical component continuously acts laterally.
 - The top of the feature is exposed longer, leading to undercutting.
- Sometimes tapered profiles are desired to:

- Improve **step coverage** in deposition.
- Minimize **stress concentration** in trench corners.
- Another method to create a tapered profile:
 - Allow **mask erosion** during the etch process.

Aluminum Etching:

- Fluorides are ineffective due to non-volatile byproducts.
- **Chloride or bromide chemistries** are essential.

Compound Semiconductor Etching:

- For GaAs, GaP, GaSb:
 - Chlorine chemistries with **argon bombardment** (Ar/Cl₂, Ar/BCl₃).
 - Increasing Ar concentration improves **anisotropy**.
- For AlGaAs and AlN:
 - Chlorine-based chemistries are mandatory for volatile byproduct formation.

4. Advanced Etching for Device Applications

- GaAs-based devices (HEMTs, HBTs) require:
 - **Through-wafer etching** to improve electrical performance.
 - Fast etch rates (e.g., 10 $\mu\text{m}/\text{min}$) with high selectivity.
- Example: Through-wafer etching with:
 - 100 μm diameter holes.
 - 20:1 selectivity over photoresist masks.
- **High-density plasmas** (e.g., ICP systems) enable:
 - Independent control of radical density and substrate bias.
 - Flexible process tuning.

5. Plasma Process Tuning

- Key parameters (adjustable independently in ICP systems):
 - **Substrate bias**.
 - **Radical density**.
- Control over these parameters allows:
 - Wide range of process outcomes.
 - Adjustments between isotropic and anisotropic regimes.

6. Summary

- Chloride and bromide etching chemistries:
 - Provide **high anisotropy** (especially bromine-based).
 - Are essential for metals like **aluminum** and compound semiconductors.
- Process flexibility is achieved by:
 - Adjusting **ion energies** and **radical densities**.
 - Using **high-density plasma tools**.
- These techniques enable etching of advanced structures such as:
 - Deep vias.
 - Through-wafer contacts.
 - High aspect ratio features.

9.8 Plasma Etching Anomalies

1. Introduction to Etching Anomalies

- Plasma etching processes may exhibit several **anomalies** due to the complex interplay between:
 - **Ion trajectories**.
 - **Plasma chemistry**.
 - **Trench geometry**.
- Understanding these effects is crucial for:
 - Process control.
 - Yield improvement.
 - Maintaining profile accuracy.

2. Common Etching Anomalies

a) Bowing:

- Characterized by **curved or flared sidewalls**.
- Caused by:
 - **Broad ion energy/angular distributions**.
 - Ion collisions in the sheath due to high pressure.
- Solutions:
 - Lower the operating pressure (increase mean free path).
 - Increase sheath bias to better align ion trajectories (but risk substrate damage).
 - Increase **sidewall inhibitor deposition** to protect sidewalls.
 - Use **ICP high-density plasma** tools for better ion control.

b) Microtrenching:

- Occurs as **enhanced etching at the bottom corners of trenches**.
- Caused by:
 - **Off-axis ion scattering** from sidewalls.
 - Ions do not fully stick on sidewall impact; they scatter toward trench corners.
- Results in:
 - Localized increased etch rate at trench bottoms.
 - Potential profile distortion and device reliability issues.

c) Aspect-Ratio-Dependent Etching (ARDE):

- Also known as **RIE lag**.
- Etch rate decreases with:
 - Increasing **aspect ratio** (depth/width) of the feature.
- Causes:
 - (a) **Ion depletion**: Ions may stick on the sidewalls of narrow trenches.
 - (b) **Neutral depletion**: Neutrals may recombine on sidewalls, reducing flux at the trench bottom.
- More pronounced in:
 - Narrow trenches.
 - High aspect ratio structures.

3. Solutions and Process Adjustments

- Reduce pressure to:
 - **Minimize ion collisions** in the sheath.
 - Promote **directional ion trajectories**.
- Adjust gas flows and chemistry to:
 - Control sidewall recombination.
 - Optimize radical and ion flux balance.
- Use **high-density plasma sources** (e.g., ICP) for independent control of:
 - Radical generation.
 - Ion energies.

4. Summary

- Plasma etching anomalies such as:
 - Bowing.
 - Microtrenching.
 - ARDE.
- Result from complex interactions between:
 - Ion angular distribution.
 - Feature geometry.

- Plasma chemistry.
- Careful adjustment of plasma conditions and process design is essential to:
 - Suppress these anomalies.
 - Ensure high fidelity pattern transfer.

9.9 Etch simulations

9.9.1 Moving Boundaries

1. Importance of Moving Boundary Problems in Etch Simulations

- Etching, deposition, and oxidation processes require modeling of **moving interfaces**.
- Surface evolution is driven by:
 - Local **etch rate** or **deposition flux**.
 - Normal velocity of the surface at each point.
- Key challenge: Accurate numerical representation of the boundary’s movement as features evolve.

2. Governing Equation for Boundary Movement

- For a surface point at position x , the normal velocity is:

$$\frac{dx}{dt} = V_R(x, t)$$

where:

- $V_R(x, t)$ is the normal velocity at that point.
- Requires solving this ordinary differential equation (ODE) at each surface point.

3. Explicit vs. Implicit Methods

- Two primary numerical approaches:
 - (a) **Explicit Methods:**
 - Treat the surface as a connected string of points.
 - Points move explicitly according to local velocities.
 - Requires careful point reconnection and redistribution.
 - Vulnerable to **topological changes** like self-intersections or feature merging.
 - (b) **Implicit Methods (Level-Set Methods):**
 - Surface represented as a contour line where $\phi = 0$.
 - Evolution governed by:

$$\frac{\partial \phi}{\partial t} + V_R |\nabla \phi| = 0$$
 - Robust to **complex topological changes**.
 - Easily generalizable to 3D simulations.

4. Challenges in Explicit Methods

- Analogous to:
 - A string of buoys floating on water, connected by flexible lines.
 - As they move, new points may need to be added or removed.
- Difficulties arise when:
 - Two etch fronts collide.
 - Self-intersections occur.
 - Extending to three-dimensional simulations.

5. Benefits of the Level-Set Method

- Introduced in the late 1980s for moving boundary problems.
- Handles:
 - **Surface merging.**
 - **Surface splitting.**
 - Complex **topological evolutions.**
- Uses higher-dimensional PDEs but simplifies handling of:
 - Geometric complexities.
 - Boundary reconnections.

6. Summary

- Moving boundary modeling is critical in etch simulations.
- **Explicit methods** offer simplicity but suffer from instability with complex geometries.
- **Implicit (level-set) methods** offer robustness and generality, especially for:
 - Two-dimensional.
 - Three-dimensional etch profile simulations.

9.9.2 Ion and Neutral Profiles

1. Introduction to Angular Distributions

- In plasma etching, the arrival directions of:
 - **Ions** (typically accelerated across the sheath).
 - **Neutrals** (radicals, unaffected by electric fields).
- Understanding their **angular distributions** is essential for predicting:
 - Etch profiles.
 - Anisotropy.

2. Behavior of Neutrals vs. Ions

- **Neutrals:**
 - Broad angular distribution.
 - Randomized directions due to multiple gas-phase collisions.
 - Not affected by electric fields.
- **Ions:**
 - Gain energy from crossing the sheath.
 - Exhibit **directional fluxes** (nearly vertical).
 - Distribution depends on sheath voltage and plasma pressure.

3. Mathematical Representation of Angular Flux

- Described using a **cosine power law**:

$$F = F_0(\cos \theta)^n$$

where:

- F_0 : Isotropic flux.
- θ : Angle relative to the surface normal.
- n : Power-law exponent (determines directionality).

4. Interpretation of the Power-Law Exponent n

- $n = 1$: Ideal **cosine distribution** (common for neutrals).
- $n > 1$: Increasingly **directional flux** (common for ions).
- **Higher sheath voltages** lead to higher n values (sharper ion directionality).
- **Lower n values** may cause:
 - Broader ion spread.
 - Bowing in the etched profiles.

5. Simplified Modeling Approach

- Although detailed Monte Carlo simulations can estimate these distributions:
 - Most practical etch simulators use the simple $(\cos \theta)^n$ model.
- Benefits of the cosine power law approach:
 - Computationally efficient.
 - Provides reasonable accuracy for flux distribution modeling.

6. Summary

- Ion and neutral flux profiles critically impact:
 - Etch profile shapes.
 - Directionality and anisotropy.
- Representing angular distributions using a cosine power law simplifies modeling while capturing the essential physics.

9.9.3 Sticking Coefficients

1. Introduction to Sticking Coefficient Concept

- Not every incoming **etchant species** (ion or neutral) reacts immediately upon striking the surface.
- The **sticking coefficient** (S_C) quantifies:
 - The probability that an incoming species sticks (adsorbs) to the surface at the point of incidence.
- Defined as:

$$S_C = \frac{F_{\text{reacted}}}{F_{\text{incident}}}$$

where:

- F_{reacted} = Flux of species that reacts or sticks.
- F_{incident} = Total incoming flux at the surface.

2. Typical Sticking Coefficient Values

- **Ions:** Typically modeled with $S_C = 1$ (perfect sticking).
- **Neutrals:** Often have $S_C \ll 1$ (low sticking probability).
- Neutrals may bounce several times (re-emission) before eventually sticking.
- Example:
 - $S_C = 0.1 \rightarrow$ On average, the molecule bounces 10 times before sticking.

3. Angular Independence of Re-emission

- Surprisingly, bounced molecules:
 - Lose memory of their original incidence angle.
 - Re-emit according to a **cosine distribution** ($n = 1$).
- Similar to:
 - Photon scattering or molecular collisions in gases.

4. Equation for Sticking Coefficient

$$S_C = \frac{F_{\text{reacted}}}{F_{\text{incident}}}$$

where:

- $0 \leq S_C \leq 1$.
- Higher velocity ions \rightarrow Higher sticking (often assumed $S_C = 1$).
- Slower, low-energy neutrals \rightarrow Lower sticking.

5. Role of Sticking Coefficient in Profile Evolution

- Sticking and re-emission behavior affects:
 - Etching inside **shadowed regions** (under mask or trench overhangs).
 - Etch **uniformity and directionality**.
- With $S_C = 1$:
 - Shadowed regions receive little to no etch flux.
- With $S_C < 1$:
 - Re-emitted species allow etching into shadowed areas.

6. Summary

- The sticking coefficient S_C :
 - Quantifies the interaction between incoming species and the wafer surface.
 - Influences etch profile shapes, especially in high-aspect-ratio and shadowed regions.
- Accurate modeling of S_C is essential for realistic etch simulations.

9.9.4 Viewing Angles and Shadowing

1. Introduction to Viewing Angles in Etching

- The **angular distribution** of incoming species (ions and neutrals) impacts the local etch rate at each surface point.
- Due to mask geometries and trench features, certain areas may be **shadowed** from direct flux.
- Each point on the etched structure has a **viewing angle** that determines how much of the incoming flux is accessible.

2. Shadowing Effect and Its Impact

- Shadowing occurs when:
 - Physical structures block direct paths of incoming flux to certain surface regions.
- Effect of shadowing:
 - Reduced etch rate in shadowed regions.
 - Increased anisotropy.

3. Calculation of Viewing Angles

- At any point i on the surface:
 - Determine the solid angle over which flux can directly reach point i .
- Geometrically analyze:
 - Direct flux from the plasma.
 - Re-emitted flux from other surface points g .

4. Influence of Sticking Coefficient on Shadowing

- If $S_C = 1$:
 - No re-emission \rightarrow purely direct flux determines the etch rate.
- If $S_C < 1$:
 - Re-emission from surrounding points helps supply flux to shadowed regions.
 - Enhances etching beneath overhangs or masked areas.

5. Summation of Flux Contributions

- The total flux at point i is the sum of:
 - **Direct flux** from the plasma.
 - **Re-emitted flux** from all other surface points g .
- View factor calculation is required between each pair of points i and g .

6. Practical Implementation in Etch Simulators

- Geometric calculations of viewing angles are embedded into modern plasma etch simulators.
- Etch rate at each surface point is updated based on:
 - Accessible flux.
 - Re-emission pathways.

7. Summary

- **Viewing angles** determine how much of the incoming etchant flux reaches each surface point.
- **Shadowing** reduces etch rates in obstructed regions.
- Re-emission (when $S_C < 1$) mitigates shadowing effects and allows more isotropic etching.
- Accurate simulation of viewing angles is essential for predicting realistic etch profiles.

9.9.5 Linear Combination of Isotropic and Directional Etching

1. Concept of Mixed Etching Profiles

- Etch profiles can often be approximated as a combination of:
 - (a) **Isotropic etching** — driven primarily by neutral species.
 - (b) **Anisotropic (directional) etching** — dominated by ion bombardment.
- This approach allows the generation of a wide variety of etch profiles by adjusting the relative contributions.

2. Mathematical Model

- Total etch rate at each surface point is given by:

$$\text{Etch Rate} = \frac{1}{N} (S_C K_I F_I + K_A F_A)$$

where:

- N = Density of atoms in the material being etched (atoms/cm³).
- S_C = Sticking coefficient for the isotropic species (neutrals).
- F_I = Flux of isotropic species (neutrals).
- F_A = Flux of anisotropic species (ions).
- K_I = Relative etch rate constant for isotropic etching.
- K_A = Relative etch rate constant for anisotropic etching.

3. Physical Interpretation of Parameters

- **Neutral species:**
 - Contribute to isotropic etching.
 - May have low sticking coefficients ($S_C \ll 1$).
- **Ion species:**
 - Typically have $S_C = 1$ (perfect sticking).
 - Contribute to anisotropic (directional) etching.

4. Application in Profile Generation

- Simulators use this linear combination to:
 - Rapidly generate etch profiles.
 - Approximate profiles from purely isotropic to purely directional etching.
- Useful for:
 - Isolation structures.
 - Device structure simulations where full plasma physics may not be necessary.

5. Limitations of This Model

- Does not capture detailed **etch physics** like:
 - Ion-enhanced chemical etching (IECE).
 - Surface coverage effects.
- Primarily used for:
 - Fast prototyping.
 - Preliminary device layout testing.

6. Summary

- Simple yet effective approach to estimate etch profiles.
- Balances between:
 - Isotropic chemical etching (neutrals).
 - Directional physical etching (ions).
- Acts as a foundation for more sophisticated etch models.

9.9.6 Ion-Enhanced Chemical Etching (IECE)

1. Concept of Ion-Enhanced Chemical Etching

- IECE is the most significant mechanism behind anisotropic plasma etching.
- Combines:
 - **Chemical etching** by neutral species (e.g., F-radicals).
 - **Ion-assisted desorption** of the byproduct molecules.
- Unlike sputter-based ion milling, ions do not physically dislodge substrate atoms:
 - They **enhance desorption** of reaction products like SiF_x .

2. Reaction Mechanism and Desorption Process

- Surface reaction:
$$\text{Si} + \text{F-radical} \rightarrow \text{SiF}_x \text{ (adsorbed byproduct)}$$
- Removal of SiF_x occurs via:
 - (a) **Natural desorption** (thermal).
 - (b) **Ion-enhanced desorption** (ion bombardment).
- Key concept:
 - Ions help remove the adsorbed byproducts, exposing fresh Si for further reaction.
 - Ions do not directly sputter silicon atoms.

3. Surface Coverage Model

Without ion bombardment:

$$\theta_s = \frac{J_R}{J_R + d_0}$$

where:

- θ_s = Steady-state surface coverage.
- J_R = Neutral flux.
- d_0 = Natural desorption rate of the byproducts.

With ion bombardment:

$$\theta_s = \frac{J_R}{J_R + J_I + d_0}$$

where:

- J_I = Ion flux.

4. Etch Rate Expression

- The etch rate of silicon is given by:

$$R_{\text{etch}} = \frac{J_R S_C}{x} (1 - \theta_s)$$

where:

- S_C = Sticking coefficient of neutrals.
- x = Number of F atoms in one SiF_x molecule.

5. Simulation Example

- Figure 9.35 shows:
 - Pure chemical etching profile.
 - Ion-enhanced etching profile.
- Matches well with experimental observations (e.g., Coburn and Winters experiment).

6. Key Features of IECE

- **Selectivity:** Driven by the chemistry of the radicals.
- **Anisotropy:** Result of the directional ion bombardment.
- **Etch rate enhancement:** Due to ion-assisted desorption.

7. Summary

- IECE enables:
 - Efficient anisotropic etching.
 - High etch rates via synergy between chemical reaction and physical ion assistance.
- Provides a robust foundation for modern plasma etching processes.

9.9.7 Aspect Ratio Dependent Etching (ARDE) Simulation

1. Introduction to ARDE (Reactive Ion Etching Lag)

- **Aspect Ratio Dependent Etching (ARDE)**, also known as **Reactive Ion Etching (RIE) lag**, refers to:
 - The phenomenon where **etch rate decreases** as the **aspect ratio** (depth/width) of the trench increases.
- This behavior is commonly observed in:
 - High aspect ratio vias.
 - Narrow trenches.
 - Dense pattern regions.

2. Causes of ARDE

- **Ion depletion:**
 - Ions may stick or scatter on sidewalls.
 - Leads to reduced ion flux at the trench bottom.
- **Neutral depletion:**
 - Neutrals may recombine on sidewalls.
 - Reduces the flux of reactive species at the base of narrow features.

3. Simulation of ARDE in Ion-Enhanced Chemical Etching Models

- The simulation considers:
 - Variation of neutral and ion fluxes with trench geometry.
 - Reduced access to flux at higher aspect ratios.
- Directly integrated into:
 - The **IECE** models developed in previous sections.

4. Example Simulation Results

- Simulation of a series of gaps (trenches) with varying widths.
- Observations:
 - **Wide openings** → deeper etching due to higher flux availability.
 - **Narrow openings** → shallow etching due to ARDE effects.

5. Physical Explanation

- Narrow trenches:
 - Restrict ion and neutral access.
 - Increase recombination and sidewall losses.
- Wide trenches:
 - Allow better ion and neutral transport to the trench bottom.

6. Summary

- ARDE is an essential factor influencing etch uniformity in micro- and nano-fabrication.
- Accurate simulation of ARDE:
 - Helps predict profile evolution.
 - Assists in process optimization for uniform etch depths.

9.9.10 Simulation Caveats

1. Introduction to Simulation Limitations

- While simulation models capture key mechanisms in plasma etching, several effects are often:
 - **Neglected.**
 - **Simplified.**
- These simplifications may lead to discrepancies between:
 - Simulated profiles.
 - Actual experimental outcomes.

2. Key Missing Effects in Simple Simulation Models

- **Ion sputtering effects:**
 - Not accounted for in many basic simulations.
 - Critical for physical etching contributions.
- **Inhibitor deposition:**
 - Important for processes like Bosch etching.
 - Can lead to **reverse ARDE** (where wide features etch slower than narrow ones).
- **Charging effects:**
 - Plasma ions may accumulate on insulating surfaces.
 - Resulting electric fields can:
 - * Distort ion trajectories.
 - * Cause anomalies like bowing.
- **Specular ion reflection:**
 - Angle of incidence equals angle of reflection.
 - May contribute to microtrenching.

3. Examples of Missed Anomalies

- Bowing and microtrenching (as discussed in Section 9.8).
- Reverse ARDE due to enhanced polymer deposition on wider features.

4. Integration of User Models

- Many modern etch simulation tools allow:
 - **User-defined models** for including additional physics.
- Facilitates inclusion of:
 - Charging effects.
 - Specular reflections.
 - Inhibitor deposition mechanisms.

5. Summary of Caveats

- Simulation models are valuable but have inherent limitations.
- Care must be taken when interpreting simulation results, particularly:
 - For high-aspect-ratio features.
 - When inhibitor deposition is critical.
 - In the presence of plasma-induced charging.
- Validation with experimental data is always recommended.

9.10 Atomic Layer Etching (ALE)

1. Introduction to Atomic Layer Etching

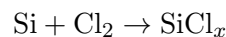
- Atomic Layer Etching (ALE) is a precision etching process that removes material in atomic-scale layers (often a single monolayer).
- It employs **sequential self-limiting reactions**:
 - Step 1: **Surface modification** to form a reactive layer (self-limited).
 - Step 2: **Removal of the modified layer** using physical or chemical means.
- Provides extremely tight control over **etch uniformity and variability**—critical for modern processes where feature tolerances are only a few atoms.
- Inspired by the similar approach in **Atomic Layer Deposition (ALD)**.

2. Working Principle of ALE

- The ALE process operates in **repeated cycles**:
 - (a) **Modification step**: Creates a saturated reactive surface layer.
 - (b) **Etch step**: Removes the modified layer, returning the surface to its pristine state.
- Prevents uncontrolled sputtering or over-etching due to self-limiting mechanisms.

3. ALE Surface Modification Example: Chlorination of Silicon

- Chlorination reaction modifies silicon by chemisorption of Cl atoms:



- The Si-Cl bond (4.2 eV) is stronger than the weakened Si-Si bond beneath the modified layer (2.3 eV).
- Follows **Langmuir adsorption kinetics**:

$$\theta(t) = 1 - \exp(-KPt)$$

where:

- $\theta(t)$: Fractional surface coverage.
 - K : Langmuir rate constant.
 - P : Partial pressure of Cl_2 .
 - t : Time.
- Adsorption is **self-limiting**—only one monolayer can form.

4. Kinetic Enhancement using Plasma Sources

- **Thermal chlorination** is slow (10s or longer).
- Plasma sources provide:
 - High concentrations of radicals.
 - Faster saturation (under 1s).
- Plasma control:
 - Low ion energy during modification to avoid simultaneous etching.
 - Use of **Inductively Coupled Plasma (ICP)** systems for independent control of ion energy and radical density.

5. ALE Etch Regimes

- Removal of the modified surface layer without damaging the underlying material.
- Techniques:
 - **Thermal desorption** (above 650 °C) — isotropic.
 - **Ion bombardment** (e.g., Ar⁺ ions with 50 eV energy) — directional.
- Selectivity achieved through:
 - Ion energy window where sputtering is minimized and desorption is maximized.
 - Avoiding high-energy sputtering which could etch unmodified layers.

6. Recent Developments and Throughput Considerations

- Studies show:
 - **Inverse relationship** between ion energy and etch time.
 - Process window depends on total **power delivered** to the surface.
- For high throughput:
 - Use high ion energy with shorter etch time per cycle.
 - Maintain selective etching without damaging underlying material.

7. Summary of Atomic Layer Etching

- ALE offers:
 - Atomic-scale precision.
 - Exceptional selectivity.
 - Control over anisotropy.
- Self-limiting steps ensure:
 - Repeatability.
 - Tight process control.
- Suitable for advanced semiconductor processes requiring atomic-level etch uniformity.

9.11 Planarization Methods – Chemical-Mechanical Polishing (CMP)

1. Introduction to CMP

- Chemical-Mechanical Polishing (CMP) is a **planarization** method combining:
 - **Chemical reactions** for material softening.
 - **Mechanical abrasion** for material removal.
- Addresses:
 - **Lithography depth-of-focus** limitations.
 - Step coverage and film uniformity.
 - Planarization of multilayer metal interconnect structures.
- Originally pioneered at IBM for oxide planarization between interconnect levels.

2. Alternative Planarization Techniques

- **Etchback processes**:
 - Deposit dielectric and sacrificial layers (e.g., photoresist).
 - Etch back both layers simultaneously with selectivity $S = 1$.
- **Spin-On-Glass (SOG)**:
 - Liquid phase material that planarizes via spin coating.
 - Converts to Si-O-Si bonds upon curing.
- Both methods provide **local planarization**, but lack the global planarity achieved by CMP.

3. Degree of Planarization (DOP)

- Defined as:

$$\text{DOP} = 1 - \frac{\Delta h_{\text{final}}}{\Delta h_{\text{initial}}}$$

where:

- Δh_{final} : Step height after planarization.
- $\Delta h_{\text{initial}}$: Initial step height before planarization.

4. CMP Mechanism and Equipment

- Wafer pressed against a rotating polishing pad.
- **Slurry** contains:
 - Abrasive particles (e.g., silica).
 - Chemical agents (oxidizers, surfactants).
- Removal occurs by:
 - (a) Surface oxidation (chemical reaction).
 - (b) Mechanical abrasion of the oxidized layer.

5. Preston's Equation for CMP

- Empirical relationship for material removal rate:

$$RR = K_P PV$$

where:

- RR : Removal rate (nm/min).
- K_P : Preston's constant (dependent on slurry, pad, material).
- P : Applied pressure.
- V : Relative velocity between wafer and pad.

6. Factors Influencing CMP

- **Pressure distribution** across wafer surface due to:
 - Pad flexibility and asperities.
 - Wafer topography.
- Nonlocal behavior:
 - Local removal rate depends on neighboring feature heights and densities.
- Chemistry influences selectivity between different materials.

7. CMP Models and Simulation (Warnock's Model)

- Local removal rate:

$$RR_i \propto K_i A_i S_i$$

where:

- K_i : Kinetic factor (geometry, slope effects).
 - A_i : Acceleration factor for protruding features.
 - S_i : Shading factor for recessed features.
- Incorporated into tools like Silvaco Athena.

8. Simulation Example and Validation

- Good agreement between:
 - Warnock's simulation.
 - Experimental CMP results.
- Simulation results shown in:
 - Figure 9.48 and Figure 9.49.

9. Summary of CMP

- CMP is the dominant method for planarization in semiconductor fabrication.
- Enables:
 - Multilevel metal integration (up to 15 levels).
 - Tight lithography process control.
- Complements etching processes by focusing on:
 - **Surface planarization.**
 - **Global topography control.**



Figure 7: Schematic of ion-enhanced inhibitor etching, showing ion removal of inhibitor on horizontal surfaces while preserving sidewall passivation (Adapted from Figure 9.20).

figures/fig9_23.png

Figure 8: Bosch process steps: alternating deposition and etch cycles for deep anisotropic silicon etching (Adapted from Figure 9.23).

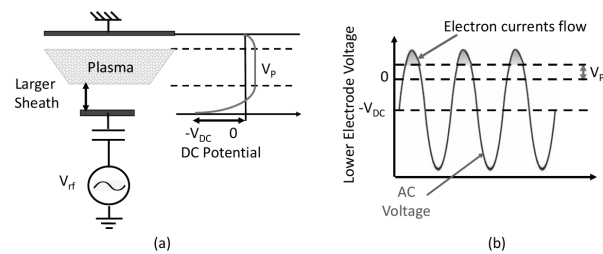


Figure 9: Schematic of an inductively coupled plasma system (ICP) that separates bulk plasma generation and the ion energy distribution using different power sources .



Figure 10: Comparison of etch profiles using fluorine, chlorine, and bromine chemistries. Bromine achieves the most anisotropic etch (Adapted from Figure 9.25).



Figure 11: Through-wafer etching in GaAs-based devices and selectivity control in high-density plasma systems (Adapted from Figure 9.26).



Figure 12: Three typical plasma etching anomalies: bowing, microtrenching, and aspect-ratio-dependent etching (ARDE) (Adapted from Figure 9.27).



Figure 13: Explicit vs. implicit approaches for moving boundary problems in etch simulations (Adapted from Figure 9.28).

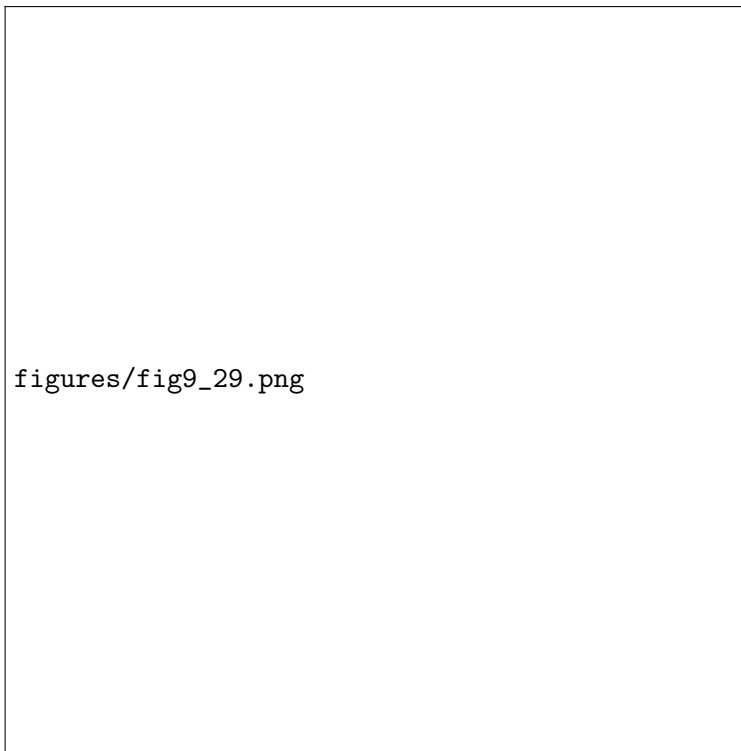


Figure 14: Schematic illustration of angular distributions for neutrals and ions approaching the wafer surface (Adapted from Figure 9.29).



figures/fig9_31.png

Figure 15: Effect of sticking coefficient on etching under shadowed regions. Low sticking ($SC \ll 1$) allows re-emission and access to these regions (Adapted from Figure 9.31).



Figure 16: Concept of viewing angles for incoming flux at different points on the etched structure (Adapted from Figure 9.32).



figures/fig9_33.png

Figure 17: Simulation results showing the transition from isotropic to directional etching profiles by varying the contribution of isotropic and anisotropic etching (Adapted from Figure 9.33).



Figure 18: Simulated etch profiles for chemical-only and ion-enhanced chemical etching processes (Adapted from Figure 9.35).



Figure 19: Simulation of ARDE: Etch depth variation for different trench widths, showing reduced etch depth for higher aspect ratio features (Adapted from Figure 9.36).



figures/fig9_37.png

Figure 20: Process window for ALE silicon etching showing the self-limiting nature of the process (Adapted from Figure 9.37).

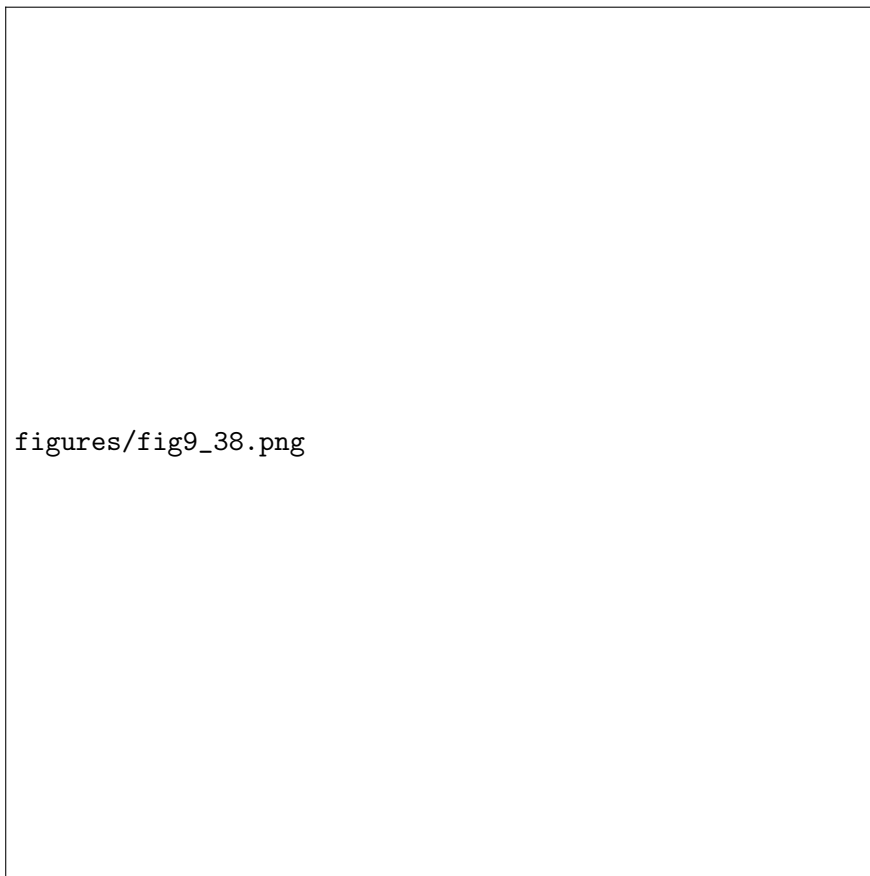


Figure 21: ALE operating as a repeated cyclic process, removing approximately one monolayer per cycle (Adapted from Figure 9.38).

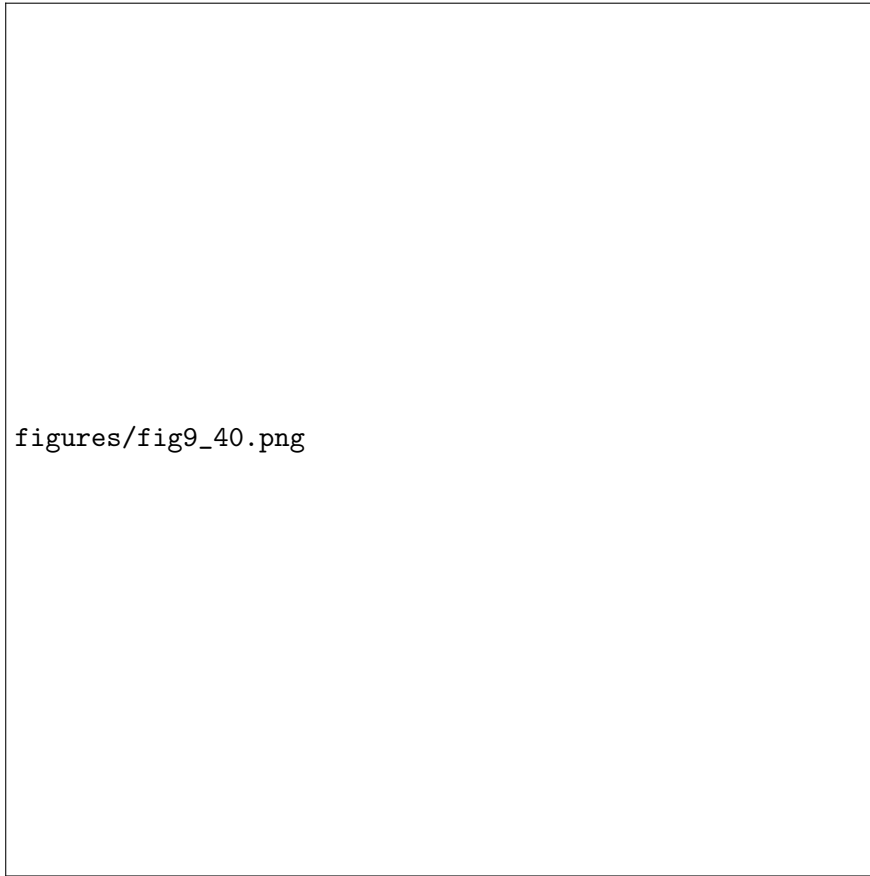


Figure 22: Ion energy window for successful ALE operation, balancing incomplete removal and sputtering (Adapted from Figure 9.40).



figures/fig9_41.png

Figure 23: CMP enabling planarization of oxide between metal interconnect levels (Adapted from Figure 9.41).



figures/fig9_44.png

Figure 24: Schematic of the CMP operation with pad rotation, wafer rotation, and slurry application (Adapted from Figure 9.44).

figures/fig9_47.png

Figure 25: Effect of local geometry on CMP rate factors K_i , A_i , and S_i (Adapted from Figure 9.47).

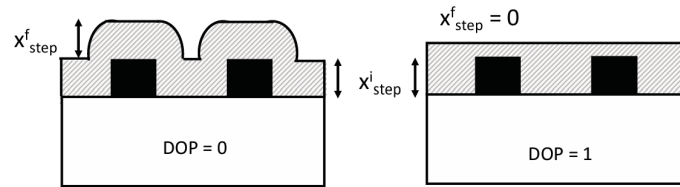


Figure 26: Example of degree of planarization (DOP).

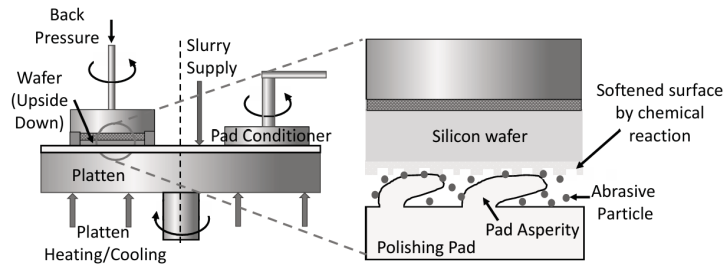


Figure 27: Illustration of CMP processes at the macroscopic and microscopic levels. The left side repeats. The right side shows an expanded, microscopic view of the polishing pad/wafer interface.