



Wafer fabrication and Silicon epitaxy





Recap

- Introduction to IH2655
- Brief historic overview
- Moore's Law and the ITRS (International Technology Roadmap for Semiconductors)
- From Geometrical to Material-based scaling
- Process Flow: CMOS (Complementary Metal Oxide Semiconductor)



Lecture 2: Wafer Fabrication and Silicon Epitaxy





Lecture 2: Wafer Fabrication and Silicon Epitaxy

Outline

- The Silicon Crystal
- Silicon Wafer Fabrication
- Silicon Epitaxy

The Silicon Crystal

Silicon has a *Diamond Cubic Lattice Structure*

Two merged FCC lattices (Face < Centered Cubic)

Shifted by $\frac{1}{4}$ of a_0 in each crystal direction

Bulk properties are isotropic

Number of surface atoms on the wafer depends on crystal plane

- Highest on Si {111}
- Lowest on Si {100}
- Influence on oxidation rate
- Influence on channel mobility...



The Silicon Crystal: Defects

0-D or Point defects :

- V vacancy (neutral, single- or double-• charged, see further Plummer p133-138)
- I interstitial or interstitialcy •

1-D defect: dislocation

2-D defect: Stacking fault

3-D defect: Precipitates

e.g. oxygen precipitation

Surface defects

• e.g. dangling bonds

Defects are mobile

- Stress
- Diffusion



Figure 3-4 Simple 2D representation of some of the common defects found in crystals. V and I are point defects, the edge dislocation represents a typical line defect, the stacking fault is an area defect, and the precipitate is a volume defect.

The Silicon Crystal: Doping

Doping: controlled substitution of lattice atoms

- n-type (electron donor)p-type ("hole donor")



See Lecture 6 on diffusion and ion implantation

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- The Silicon Crystal
- Silicon Wafer Fabrication
- Silicon Epitaxy

Silicon Wafer Fabrication

Goal: Single crystal silicon wafers

- Raw material: Quartzite (SiO2, sand), then refined to
- Metallurgical Grade Silicon (MGS)
 - Furnace with coal / coke and SiO₂ @ ~ 2000°C
 - Main reaction: 2 C (solid) + 2 SiO₂ (solid) \rightarrow Si (liquid) + 2 CO
 - Significant power needed: ~ 13 kWh/kg
 - End result: 98% Silicon
- Electronic Grade Silicon (EGS)
 - MGS + HCI (gas) \rightarrow SiH₄ (silane)
 - \rightarrow SiCl₄ (silicon tetracloride)
 - \rightarrow SiHCl₃ (trichlorosilane)...
 - Boiling purifies SiHCl₃
 - Chemical Vapor Deposition (CVD) on silicon rod (nucleation surface)
 - Reaction: 2 SiHCl₃ (gas) + 2 H₂ (gas) \rightarrow 2 Si (solid) + 6 HCl (gas)
 - Resulting poly-crystalline silicon (polysilicon) has only part per billion (ppb) impurities (10¹³ – 10¹⁴ /cm³)

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Silicon Wafer Fabrication: Czochralski Method

Starting material: electronic Grade Si (EGS)



Loading the high purity poly-Si

Si Melting point: ~1420°C Pulling process: 1-3 days Power: tens of kW



Seed
Single crystal silicon
Quartz crucible
Water cooled chamber
Heat shield
Carbon heater
Graphite crucible



Silicon Ingot

Silicon Wafer Fabrication: Czochralski Method

1-3 days



Seed Down

Seed Pulling

Shoulder

Si Crystal Growth

- Seed determines Silicon crystal orientation
- Dash method for moving dislocations to the surface at onset of pulling.
- Oxygen dissolves from quartz crucible; **impurity level:** ~10¹⁸ cm⁻³ !
 - Si-O-Si bindings resulting in higher mechanical strength (+)
 - Oxygen donors (SiO₄). 10^{16} cm⁻³ form at 400-500°C (-)
 - Bulk precipitation (SiO₂ clusters; can be controlled by gettering) (-)
- Carbon: from graphite susceptor and ESG, impurity level 10¹⁵-10¹⁶ cm⁻³

Silicon Wafer Fabrication: Float-Zone Method

- No crucible, crystal formed in Ar atmosphere
- RF coil induces large currents in Silicon → resistive heating → melting and recrystalization
- Low oxygen content (no crucible)
- High-resistivity possible
- Controlled doping:
 - Doped poly-silicon rod
 - Doped seed
 - Controlled gas ambient
- More difficult to scale up in wafer diameter
- Applications in power devices, detectors...



Silicon Wafer Fabrication: Czochralski Method Doping

Dopant incorporation: Segregation coefficient $k_0 = C_{Solid}/C_{liquid}$

Typically $K_0 < 1 \rightarrow$ preference for liquid phase

CZ ingot doping concentration is a function of time, or position in the ingot

FZ process: dopants prefer to remain in the liquid float zone



Silicon Wafer Fabrication: Wafer Shaping

- Single crystal ingot ground into uniform diameter (e.g. 300mm)
- Notch or Flat added
- Wafer Sawing
 - Slicing into wafers by an inner saw or a wire saw
- Wafer Lapping
 - Removes surface roughness from saw cuts and process damages
 - Mechanical lapping with alumina or silicon carbide abrasive
- Wafer Edge Rounding
- Wafer Etching
 - Mechanical damages induced during previous processes are removed by chemical etching
- Laser Scribing
- Wafer Polishing
 - Chemical-Mechanical Polishing (CMP) process yield flat surface using colloidal silica
- Wafer Cleaning and Inspection
 - Wafers are cleaned and inspected to be polished wafers



Silicon Ingot





http://product-category.com

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Silicon Wafer Fabrication: Wafer Shaping

- Single crystal ingot ground into uniform diameter (e.g. 300mm)
- Notch or Flat added
- Crystal orientation



- Wafer Sawing
- Slicing into wafers by an inner saw or a wire saw



http://serve.me.nus.edu.sg/nanomachining/waf er_preparation.htm



Structure of a wire saw machine



saw machine Wire saw machines http://www.sumcosi.com/english/products/process/step_02.html

Mikael Östling

Silicon Wafer Fabrication: Wafer Shaping

http://www.sumcosi.com/english/products/process/step 02.html

wafer

- Wafer Lapping
- Removes surface roughness from saw cuts and process damages
- Removes sub-surface damage from sawing \rightarrow Lapping damage
- precise thickness uniformity, flatness and parallelism
- Mechanical lapping with alumina or silicon carbide abrasive





cutting tool

- Wafer Edge Rounding
- Improved resistance to thermal stress
- Reducing particles, chip breakage and lattice damage^L
- Avoid build-up of photoresist at the wafer edge
- "Mechanical edge contouring"

red

Kr

edge

- diamonds

Silicon Wafer Fabrication: Wafer Shaping

Laser Scribing

http://www.sumcosi.com/english/products/process/step_02.html

- Wafer Etching
- Mechanical damages induced during previous processes removed by chemical etching (Lecture 3)
- Wafer Polishing
- Chemical-Mechanical Polishing (CMP) process yield
 flat surface using colloidal silica



• cracks, ridges and valleys after lapping



- Wafer Cleaning and Inspection
- Wafers are cleaned and inspected before
- shipping





Polisher

Silicon Wafer Fabrication: Gettering

Capture defects at locations far away from the device region. Damaged region will act as "sink" for unwanted elements. Metals diffuse as interstitials (>> diffusivity than dopants) Metals need defects to become trapped:

- Dislocations
- Stacking faults
- Grain boundaries
- Precipitates (e.g. O₂)

PSG captures alkali ions (Phosphosilicate Glas)

General Stategy

- 1. Free impurities
- 2. Diffuse to gettering site
- 3. Trap at gettering site



Silicon Wafer Fabrication: Gettering

Extrinsic gettering:

Treatment on backside of wafer, e.g. n⁺doping Deposition of poly silicon on back side

Intrinsic gettering:

Intentional SiO₂ precipitation inside bulk CZ silicon Requires dedicated thermal cycling:



Idea:

Active devices on insulating oxide to reduce leakage currents High quality silicon crystal isolated from bulk



Example: Bulk vs. SOI Transistor



- Reduced leakage to the bulk
- Improved isolation between devices
- Smaller junction capacitance





- Reduced leakage to the bulk
- Improved isolation between devices
- Smaller junction capacitance
- Enable 3-D structures (e.g. FinFET)
- Microelectromechanical Systems (MEMS)



Silicon Wafer Fabrication: Wafer Size Scaling



Issues with transition to 450mm: vibrational effects gravitational bending (sag) Flatness crystal ingots 3 times heavier (1 ton!) 2-4 times longer cooling 2 x process time



http://technologyinside.com



Source: Covalent Materials (formerly Toshiba Ceramics)

Silicon Wafer Fabrication: Summary

- Czochralski (CZ) Method
- Float Zone (FZ) Method
- From Ingot to Wafer
- Gettering
- Silicon-on-Insulator (SOI)

PS: For a short video of the wafer production process see: http://www.siltronic.com/int/en/press/film/film-overview.jsp **Lecture 2: Wafer Fabrication and Silicon Epitaxy**

Outline

- The Silicon Crystal
- Silicon Wafer Fabrication
- Silicon Epitaxy



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Epitaxy					
	Outline:				
	Definition and terminology				
	Chemical vapor deposition				
	CVD process and source gases				
	Grove model:				
	 Mass-transfer or surface-reaction controlled growth rate 				
	Gas flow and pressure in CVD				
	Chlorine in Si CVD				
	Doping				
	Autodoping				
	Defects and characterization				
	Reactor types				
	Batch				
	Single-wafer				
	• MBE				
	Applications of Si epitaxy				
	• HT epitaxy: Si				
	LT epitaxy: SiGe				
	 Selective epitaxy: Si and SiGe 				



S.M. Sze: Semiconductor Devices 1985

S-M.Sze ed: VLSI Technology 1988

Chang and S.M. Sze: ULSI Technology 1996

S. Wolf and R.N. Tauber: Silicon Processing for VLSI vol. 1 1986

J. Plummer, Silicon VLSI Technology 2000

Epitaxy: Definition

Growth of single-crystalline layer on a single-crystalline substrate (bulk)

Epitaxal layer thickness: From one single atom layer up to ca 100 μm

Homoepitaxy : Si on Si

Heteroepitaxy : e.g. SixGe1-x on Si

Doping level can vary substantially between the layer and bulk

Advantages of epitaxy:

High purity monocrystalline silicon films for the device region

Lower temperature compared to implantation + diffusion → much more abrupt doping profiles

Large interval of thicknesses, doping profiles, and band gap engineering \rightarrow ideal for creating "artificial" semiconductor structures, e.g.

- HBTs (Heterojunction Bipolar Transistors, H. Kroemer, Nobel Prize 2000)
- HEMTs (High electron mobility transistor, based on 2-DEG)

Epitaxy: Terminology for Silicon Epitaxy

Conventional, or high-temperature (HT) epitaxy

- T > 1000°C
- On blanket or patterned substrate wafers

Low-temperature (LT or LTE) epitaxy

- T < 1000°C
- Usually on patterned substrate wafers

Selective epitaxy

• always on patterned substrates

Terminology for Chemical Vapor Deposition (CVD) Silicon-Germanium (SiGe) epitaxy

Selective epitaxial growth: SEG

Non-selective epitaxial growth: NSEG

Heteroepitaxy (SiGe on Si)

Strained growth conditions, so-called pseudomorphic growth

 h_c = critical thickness

Unstrained \rightarrow dislocation network which are adverse for device operation



Silicon Epitaxy: Terminology

Technology of choice for Si epitaxial growth in production environment:

Chemical Vapor Deposition (CVD) sometimes denoted Vapor Phase Epitaxy (VPE) •Hydrogen (H_2) carrier gas •Reactants: SiCl₄, SiHCl₃, SiH₄, + dopant gases (AsH₃, B₂H₆...) HCI for selective growth and/or chamber cleaning $\cdot N_2$ for purge **Chemical Vapor Deposition** Heating (ca.1200°C) (CVD) method **Epitaxial Furnace** $SiHCl_{s}(G) + H_{s}(G)$ Chamber Adsorption of Si **Desorption of** (2)Wafer byproducts Migration to arowth site Rotation Infra-Red Lamp http://www.sumcosi.com

Epitaxy: CVD Reactor Types

Basic Si CVD types (both batch and single-wafer rectors)



Substrates

Epitaxy: CVD Process

- 1. Transport of reactants to the deposition region
- 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: migration, decomposition, reaction, site incorporation
- 5. Desorption of byproducts from surface
- 6. Transport of byproducts through the boundary layer
- 7. Transport of byproducts from the deposition region



Figure 9-5 Steps involved in a CVD process. Numbered steps are explained in text.

(Plummer Fig 9-5 p 514)

Fig. 19 Schematic representation of arsenic doping and growth processes.¹²

(Sze Fig 19 p323)

Si CVD sources and basic reactions for HT epitaxy

Silicon tetrachloride: Si Trichlorosilane (TCS): Si Dichlorosilane (DCS): Si Silane: Sil

$$\begin{array}{l} \text{SiCl}_4 + \text{H}_2 \\ \text{SiHCl}_3 + \text{H}_2 \\ \text{SiHCl}_2 \\ \text{SiH}_4 \end{array}$$

 $\Leftrightarrow Si + 4HCI$ $\Leftrightarrow Si + 3HCI$ $\Leftrightarrow Si + 2HCI$ $\Rightarrow Si + 2H_2$

(~1200°C) (~1150°C) (~1100°C) (~1050°C)

HT epitaxy: TCS or DCS LT epitaxy: DCS or silane

TABLE 1Epitaxial growth of silicon in hydrogen atmosphere

Chemical deposition	Nominal growth rate(µm/min)	Temperature range(°C)	Allowed oxidizer level (ppm)
SiCl ₄	0.4-1.5	1150-1250	5-10
SiHCI	0.4-2.0	1100-1200	5-10
SiHaCia	0.2-1	1050-1120	<5
SiH4	0.2–0.3	950-1250	<2

(Sze VLSI Table I p. 65)

The Grove Model for Epitaxial Growth Growth limited by mass-transfer or surface reaction



Fig. 20 Model of the epitaxial-growth process.



Assume:

Steady state: $F_1 = F_2 = F$ Growth rate $n = F/C_a$ where $C_a = number of Si atoms/cm^3$

The Grove Model for Epitaxial Growth Growth limited by mass-transfer or surface reaction

Steady state: $F_1 = F_2 = F$ Growth rate $n = F/C_a$ where $C_a =$ number of Si atoms/cm³



EMICONDUCTOR-

 $C_q = yC_t$ where y is the mole fraction and C_t is the total number of gas molec/cm³ \rightarrow

$$v = \frac{k_s h_g}{k_s + h_g} \left(\frac{C_t}{C_a}\right) y$$

 $k_{s} \text{ small} \rightarrow \text{Surface reaction controlled} \quad v \cong k_{s} \left(\frac{C_{t}}{C_{a}}\right) y \quad ; \quad C_{s} \rightarrow C_{g}$

 $h_g \text{ small} \rightarrow \text{ Mass-transport controlled} \quad v \cong h_g \left(\frac{C_t}{C_a}\right) y \quad ; \quad C_s \rightarrow 0$

k_s: surface reaction constant

h_g: vapor mass transfer coefficient (cm/s)



h_a: vapor mass transfer coefficient (cm/s)

CVD Epitaxy in the Mass-Transport Controlled Regime

Gas flow rate

Laminar gas flow with velocity v above a boundary layer with thickness δ



CVD Epitaxy in the Surface Reaction Controlled Regime

Deposition not (very) sensitive to geometrical arrangement of wafers in reactor. However, low growth rates!

Can be solved by reducing total pressure which affects D_G and extends surface-reaction limited region to higher T:



Silicon Epitaxy: CI-based Chemistry

- Either *deposition* or *etching* depending on T, P or concentration (mole Fraction)
- Reaction is complex, e.g. SiCl4



Silicon Epitaxy: CI-based Chemistry

Crystallinity also depends on growth rate:



Silicon Epitaxy: Doping

Doping sources: B_2H_6 (diborane), AsH₃ (arsine) and PH₃ (phosphine). *Not* standard: SbCl₅



Autodoping

Lightly doped n-epi-layer grown on n⁺ substrate \rightarrow autodoping, i.e. *unintentional doping from substrate, susceptor, adjacent wafers etc.*



(Chang Fig 16 p. 120)

Defects in Epitaxial Layers



FIGURE 20

(a) Common defects occurring in epitaxial layers. Schematic representation of line (or edge) dislocation initially present in the substrate and extending into the epitaxial layer (item 1), an epitaxial stacking fault nucleated by an impurity precipitate on the substrate surface (item 2), an impurity precipitate caused by epitaxial process contamination (item 3), growth hillock (item 4), and bulk stacking faults, one of which intersects the substrate surface, thereby being extended into the laver (item 5).

(Sze VLSI Fig. 20 p 76)

- Dislocations (line defect)
- Stacking faults (area defect) visible as squares for (100) and triangles for (111)
- Precipitates (volume defect)
- Hillocks or voids (volume defects)

Substrate surface quality and cleaning prior to epitaxy are crucial, in particular LT epitaxy.

Slip in HT epitaxy:

Dislocation network caused by temperature gradient across wafer during RTA-CVD (single-wafer machines)

Epi Thin Film Characterization

Surface smoothness:

Optical microscopy Nomarski contrast microscopy Atomic force microscopy (AFM)

Film thickness and doping:

Secondary ion mass spectroscopy (SIMS) interferometer Fourier-transform Infrared Spectroscopy (FTIR) Spectroscopic Ellipsometry

Crystallographic quality:

High-resolution X-ray diffractometry for Ge content and thickness in SiGe

Electrical properties:

Film resistivity vs doping Minority carrier life time measurement Device characteristic

Destructive, non-destructive or device-based methods!





(Wolf Fig 24 p 151)

Reactor Types for Si Epitaxy

Batch reactor types Almost only for HT epitaxy (exception UHVCVD)



FIGURE 20

Types of conventional epitaxial reactors: (a) horizontal reactor; (b) vertical reactor; (c) barrel reactor. (After Pearce, Ref. 27.)

(Chang Fig. 20 p124)

Reactor Types for Si Epitaxy: Batch Type



Fig. 21 Schematic of an induction heated vertical pancake reactor. Courtesy of Microelectronic Manufacturing and Testing.



Fig. 22 Schematic of a radiantly heated barrel reactor. Courtesy of Applied Materials Inc.

Reactor Types for Si Epitaxy: Single-wafer Si Epitaxy

RTP process! Both for HT and LT epitaxy (Si/SiGe) Used for production of wafers, epi on buried layers and LT epi SiGe. Example:





Fig.1 - Top view (a) and cross section (b) of the reactor chamber, showing the geometry and the position of the heating lamps with respect to the wafer, susceptor and thermocouples (t.c.).

(ASM Epsilon 2000 at KTH)

Ultra High Vacuum CVD (UHVCVD)

LT non-selective epi method developed by IBM specially for SiGe Batch method at very low temperature 500-600°C



Schematic drawing of a UHV/CVD system. (After Meyerson, Ref. 29.)

(Chang Fig 22 p 128)

Silicon Molecular Beam Epitaxy (MBE)

Physical vapor deposition (PVD) method

Typical for thin film research for SiGe(C) epitaxy (not in production!)

- Vacuum evaporation with excellent thickness control
- Ultra-high vacuum
- Extremely low growth temperatures < 500°C
- In situ analysis of growing film
- As (arsenic) and, in particular, Ph (phosphor) dopants difficult. Often Sb (antimony) for n+



Schematic of MBE growth system. (After Konig, Kibbel, and Kasper, Ref. 54.)

(Sze VLSI Fig 23 p.80)

Applications of Si epitaxy

HT epitaxy:

- p-epi on p+ bulk in CMOS for suppression of latch-up
- n- epi on n+ buried collector layer in bipolar devices for reduced series resistance



Grahn ASM User meeting'99

Problem: *Pattern shift* during n-epi on buried layer:







- different crystal planes lead to significantly different growth rates
- geometry of a feature can influence growth rate (feature edges)
- Important to control for wafer alignment on buried layer!



(Chang p.123)

Applications of SiGe epitaxy

LT epitaxy:

SiGe epi for base in bipolars, channel for MOS



Applications of SiGe epitaxy

SiGe LT epitaxy

Typically at 550-650°C using UHVCVD, LPCVD or APCVD

Selective or non-selective growth







Figure 7. SIMS profiles of an HBT structure grown by APCVD at 900°C (collector) and 700°C (base and emitter). The box-shaped profiles allow very accurate control of the base width and dopant content. The As signal in the SiGe material is meaningless due to interference of As and GeH.

de Boer MRS 94

Silicon Selective Epitaxial Growth (SEG)

Chemistry:

Addition of HCI to DCS makes Si epi selective with **respect** to field oxide SEG is a difficult process in VLSI!

STI isolation is the preferred process choice









FIGURE 25

Schematic illustration of a typical SEG process for device isolation: (a) oxide deposition; (b) window formation; (c) epi growth; (d) n-well drive-in. (After Borland and Drowley, Ref. 57.)

Applications of Silicon Selective Epitaxial Growth (SEG)

Source-Drain regions of nanoscale MOSFETs, especially in novel structures:

- Ultra-Thin-Body-SOI MOSFETs •
- FinFETs •



M. leong et al., Silicon Device Scaling to the Sub-10-nm Regime, Science 306, 2057-2060, 2004

Applications of Epitaxy in the CMOS process

Epitaxial high-k gate dielectrics

• Potential technology for "End-of-ITRS" CMOS Technology

CMOS integration of epitaxial Gd2O3 high-k gate dielectrics





Fig. 3. HRTEM image of a crystalline Gd_2O_3 layer on Si (001) and fully silicided NiSi electrode.

H. Gottlob et al. , Solid State Electronics, 2006

Applications of Epitaxy in the CMOS process

Epitaxial high-k gate dielectrics

• Potential technology for "End-of-ITRS" CMOS Technology

CMOS integration of epitaxial Gd2O3 high-k gate dielectrics

Process step	Compatibility		Comment
	NiSi	TiN	
Acetone	√	√	
Propanol	√	✓	
MF-86 MX (developer)	√	√	
TMAH 50 °C	*	✓	* NiSi: not applicable
O ₂ Plasma (resist stripping)	√*	\checkmark	* NiSi: slight change of VFB
UVN-30 (resist)	√	√	
H ₂ SO ₄	√	×*	* Etches TiN
$H_2O_2:H_2SO_4 = 1:3$	×	×*	* Etches TiN
Forming gas annealing 30 min @ 350 °C in N2/H2	?*	√*	* NiSi: increase of NiSi resistivity
			* TiN: no effect
RTA 10 s @ 800 °C	×*	√*	* NiSi: high leakage current
0			* TiN: RTA increases CET
HBr and HBr + Cl ₂ RIE	✓	\checkmark	

Table 1 Overview of investigated process compatibility with Gd₂O₃ gate dielectric and NiSi or TiN gate electrode

H. Gottlob et al. , Solid State Electronics, 2006

Summary: Epitaxy

- Definition and Terminology
- Chemical Vapor Deposition (CVD) / Vapor Phase Epitaxy (VPE)
 - □ Grove Model: Mass-transport vs. Surface Reaction Regime
 - Reactors
 - Chemistry
- Reactor Types
- Applications