Solid State Electronics (26331)

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Introduction:


Objective: To learn the basics of semiconductor (SC.) materials, devices, and related applications

Goals: Text book is designed to acheive the following:
1- to provide students with a sound understanding for existing SC. Devices
2- most interestingly is to give the basic tool with which the students can later learn about newly developed materials, devices, and applications
Introduction:

Why this course is important?

It is directly related to high technological applications such as:

- Cell-phone towers
- Airplane
- Satellite
- Cell-phones
- Computers

Silica sand ($\text{SiO}_2$)

Si wafer

Microprocessor
Introduction:

Course Contents
• Ch.1 Semiconductor Materials
• Ch.2 Atoms and Electrons
• Ch.3&4 Energy Bands and Charge Carries in Semiconductors
• Ch.5 p-n Junction
• Ch.6, 7, 8, &10 Devices
  □ Field-Effect Transistors
  □ Bipolar Junction Transistors
  □ Optoelectronics Devices
  □ Microwave and power Devices
• Ch.9 Integrated Circuits Fabrication Overview
Ch. 1: Crystal Properties and Growth of Semiconductors

Objectives: 1- Describe what is Semiconductor

2- Perform simple calculations about crystals

3- Understand epitaxial crystal growth in solids and thin films

4- Learn about crystal defects

The transport of charge through a metal or a semiconductor depends not only on the properties of the electron but also on the arrangement of atoms in the solid. This gives an argument why there is a change in electrical properties between different SC. materials
1.1 Semiconductor materials

What are semiconductors?
1) Materials with electrical conductivity in between conductors and insulators

- Conductors
  - Metals (silver, gold, etc)
  - \(\rho = 10^{-6}-1\ \text{ohm.cm}\)

- Semiconductors
  - Silicon, germanium,
  - \(\rho = 10^{-2}-10^6\ \text{ohm.cm}\)

- Insulators
  - Ceramics (quartz, alumina)
  - \(\rho > 10^7\ \text{ohm.cm}\)

2) The conductivity of a semiconductor materials can be varied over orders of magnitude by changes in a) temperature, b) optical excitation, c) electrical excitation and d) impurity content (by doping)
3) Type of semiconductor
1.1 Semiconductor materials

3) Semiconductor materials are found in column IV and neighboring columns of the periodic table as shown below.
1.1 Semiconductor materials

4) Types of semiconductors (table 1-1)

a) **Elemental Sc.** composed of single species of atoms (most commonly Si and Ge)

b) **Compound Sc.** Compounds of binary (two elements - table 1-1), ternary (three elements- like GaAsP), or quaternary (four elements- like InGaAsP) elements semiconductor

*Table 1-1* shows: (a) where semiconductors occur in the periodic table; (b) elemental and compound semiconductors.

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<thead>
<tr>
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<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
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<td>(a)</td>
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<td>B</td>
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<td>Zn</td>
<td>Ga</td>
<td>Ge</td>
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<td>Se</td>
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<td></td>
<td>Cd</td>
<td>In</td>
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<td>Sb</td>
<td>Te</td>
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<table>
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<tr>
<th>(b)</th>
<th>Elemental</th>
<th>IV compounds</th>
<th>Binary III–V compounds</th>
<th>Binary II–VI compounds</th>
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<tbody>
<tr>
<td></td>
<td>Si</td>
<td>SiC</td>
<td>AlP</td>
<td>ZnS</td>
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<td></td>
<td>Ge</td>
<td>SiGe</td>
<td>AlAs</td>
<td>ZnSe</td>
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<td>AlSb</td>
<td>ZnTe</td>
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<td>GaN</td>
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<td>GaSb</td>
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<td>InP</td>
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<td>InAs</td>
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<td>InSb</td>
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</table>
5) Applications of semiconductor compounds:

a) The elemental semiconductor Ge and Si is now used for the majority of diodes, rectifiers, transistors, integrated circuits, and infrared and nuclear radiation detectors.

b) III-V compounds such as GaN, GaP, and GaAs are common in light-emitting diodes (LEDs).

c) II-VI compound semiconductors such as ZnS (Fluorescent materials) are usually used in television screens.

d) Light detectors are commonly made with InSb, CdSe, or other compounds such as PbTe and HgCdTe.

e) Microwave Gunn diode, is usually made of GaAs or InP.

f) Semiconductor lasers are made using GaAs, AlGaAs, and other ternary and quaternary compounds.
1.1 Semiconductor materials

6) The most important characteristics for semiconductor compounds that distinguish them from each other and from metals and insulators is the energy band gap ($E_g$)

$E_g$ determines the wavelengths of light that can be absorbed or emitted by the semiconductor. The following equation show the relation between the photon energy $E$ in ev and its wavelength $\lambda$ in nm.

$$E(ev) = \frac{hc}{\lambda} = \frac{1240(ev.nm)}{\lambda(nm)}$$

$E_g$ for different Sc. Materials can be found in appendix III of the text book.

As a result of the wide variety of semiconductor band gaps, light-emitting diodes and lasers can be constructed with wavelengths over a broad range of the infrared and visible portions of the spectrum.

7) The optical and electronic properties of semiconductor materials are strongly affected by impurities, which may be added in precisely controlled amounts by a process called *doping*.
1. Crystalline Solids

Crystalline – periodic arrangement of atoms: definite repetitive pattern

Non-crystalline or Amorphous – random arrangement of atoms.

The periodicity of atoms in crystalline solids can be described by a network of points in space called lattice.
1.1 Crystal Lattices

Properties such as mechanical, electrical and optical are intimately tied to crystal type.

1.2.1 Periodic structure

A **crystalline solid** *(single crystal solid)* is composed of atoms arranged in a periodic fashion (repeated throughout the entire solid in 3D).

2) Other solids are composed of many small regions of single-crystals. They are called **polycrystalline solids**.

3) Some solids have no periodic structure at all. They are called **amorphous solids**.
1) **Crystal lattice:** Periodic arrangement of points (in 3D space) making up the crystal. Note: Each point may have a single atom or multiple atoms in an arrangement called **basis** to get the crystal.

2) Always, arrangement of atoms or a volume called **unit cell** can be moved in space (regularly repeated) by unit **lattice constant** in each direction to create the entire crystal lattice. Note: Lattice constant: Smallest distance between periodically arranged atoms in each direction.

3) The smallest unit cell is called **primitive cell**; it has lattice points (shared between 4 primitive cells) at the corners (as for figure shown) ➔ effective number of lattice points for each primitive cell is unity (one).

4) The primitive cell can be represented by primitive vectors (vectors represents the primitive cell) \( \mathbf{a}, \mathbf{b}, \) and \( \mathbf{c} \) (for 3D lattice). It can be translated by integer multiple of primitive vectors according to

\[
\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}
\]

where \( u, v, \) and \( w \) are integers.
The figure above shows an example of a crystal lattice. It shows a two-dimensional arrangement of atoms called a rhombic lattice, with a *Two dimension primitive* cell ODEF. The primitive cell is translated to a new primitive cell identical to the original (O'D'E'F) by \( r = 3a + 2b \)

5) In many lattices, however, the primitive cell is not the most convenient to work with. It is more convenient and simpler to choose to work with a larger rectangular *unit cell*, PQRS with lattice point T at the center (a so-called *centered rectangular* lattice), rather than the smallest primitive cell, ODEF. A unit cell allows lattice points not only at the corners, but also at the face center (and body center in 3-D) if necessary.
Crystal Systems

- The space lattice points in a crystal are occupied by atoms.
- The position of any atom in the 3D lattice can be described by a vector \( \mathbf{r}_{\mu\nu\omega} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \), where \( u, v \) and \( w \) are integers.

![Diagram of a unit cell](image)

Unit Cell

The three unit vectors, \( a, b, c \) can define a cell as shown by the shaded region in Fig.(a) This cell is known as unit cell (Fig. b) which when repeated in the three dimensions generates the crystal structure.
Crystal Systems

Bravais Lattice

The unit vectors $a$, $b$ and $c$ are called lattice parameters. Based on their length equality or inequality and their orientation (the angles between them, $\alpha$, $\beta$ and $\gamma$) a total of 7 crystal systems can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as Bravais lattices, can be generated.
**Crystal Systems**

1. **Cubic:** \( a = b = c, \quad \alpha = \beta = \gamma = 90^\circ \)
   - Simple cubic
   - Body-centered cubic (BCC)
   - Face-centered cubic (FCC)

2. **Tetragonal:** \( a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ \)
   - Simple Tetragonal
   - Body-centered Tetragonal (BCT)
3. Orthorhombic: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

Simple    Body-centered    Base-centered    Face-centered

4. Monoclinic: $a \neq b \neq c$, $\alpha = \gamma = 90^\circ \neq \beta$

Simple monoclinic    Base-centered monoclinic
Structure

Crystal Systems

Rhombohedral
\[ a = b = c \]
\[ \alpha = \beta = \gamma \neq 90^\circ \]

Hexagonal
\[ a = b \neq c \]
\[ \alpha = \beta = 90^\circ, \gamma = 120^\circ \]

Triclinic
\[ a \neq b \neq c \]
\[ \alpha \neq \beta \neq \gamma \neq 90^\circ \]
### Examples of materials having different crystal systems

<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>$\text{K}_2\text{S}_2\text{O}_8, \text{K}_2\text{Cr}_2\text{O}_7$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$\text{As}_4\text{S}_4, \text{KNO}_2, \text{CaSO}_4.2\text{H}_2\text{O}, \beta-\text{S}$</td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>$\text{Hg}, \text{Sb}, \text{As}, \text{Bi}, \text{CaCO}_3$</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$\text{Zn}, \text{Co}, \text{Cd}, \text{Mg}, \text{Zr}, \text{NiAs}$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$\text{Ga}, \text{Fe}_3\text{C}, \alpha-\text{S}$</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$\text{In}, \text{TiO}_2, \beta-\text{Sn}$</td>
</tr>
<tr>
<td>Cubic</td>
<td>$\text{Au}, \text{Si}, \text{Al}, \text{Cu}, \text{Ag}, \text{Fe}, \text{NaCl}$</td>
</tr>
</tbody>
</table>
The simplest unit cell is a cubic volume with lattice constant $a$; such as the three cells shown in the figure below. All three structures have different primitive cells, but the same cubic unit cell.

a) *simple cubic* structure (\textit{sc}) has an atom located at each corner of the unit cell.

b) *body-centered cubic* (\textit{bcc}) lattice has an additional atom at the center of the cube.

c) *face-centered cubic* (\textit{fcc}) unit cell has atoms at the eight corners and centered on the six faces.

**Cubic Lattices**

- Simple Cubic
- Body-centered cubic
- Face-centered cubic
Cubic Lattices

- Simple Cubic
- Body-centered cubic
- Face-centered cubic
Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c.

Thus the point located at \(\frac{a}{2}\) along x axis, \(\frac{b}{3}\) along y axis and \(\frac{c}{2}\) along z axis, as shown in the figure below, has the coordinates \( \frac{1}{2} \frac{1}{3} \frac{1}{2} \).
In crystal studying, we always refer to what is called planes and directions → we need to know what is called Miller indices

Crystal Planes

Miller Indices

Planes in a crystal are described by notations called Miller indices

- Miller indices of a plane, indicated by \( h \ k \ l \), are given by the reciprocal of the intercepts of the plane on the three axes.

- The plane, which intersects X axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices \( h = 1/1 = 1, \ k = 1/\infty = 0, \ l = 1/\infty = 0 \). It is written as \( (hkl) = (100) \).

- Miller indices of some other planes in the cubic system are shown in the figures in the next slide.
To find the Miller Indices of a plane, follow these steps:

- Determine the intercepts of the plane along the crystal axes
- Take the reciprocals
- Clear fractions
- Reduce to lowest terms and enclose in brackets ()

Ex: Intercepts on a, b, c : \( \frac{3}{4}, \frac{1}{2}, \frac{1}{4} \) (h k l) = (4/3, 2, 4) = (2 3 6)

- If plane intercept the origin, for example plane parallel to y-z axis and intercept x at 0 \( \rightarrow \) intercepts are: 0, \( \infty \), \( \infty \). taking reciprocals we will have (\( \infty 00 \)) plane. This is forbidden in miller indices \( \rightarrow \) we take parallel plane that intercept x- axis at 1 \( \rightarrow \) it will have miller indices (100)
Crystal Planes

Planes can also have negative intercept e.g. 1, -1/2, 1

\( h k l = 1 -2 1 \). This is denoted as \((121)\)

Family of planes \(\{hkl\}\)

Planes having similar indices are equivalent, e.g. faces of the cube (100), (010) and (001). This is termed as a family of planes and denoted as \(\{100\}\) which includes all the (100) combinations including negative indices. Some other equivalent planes are shown in the next slide.

All planes family with - ve indices are

\[\{100\} \equiv (100) (010) (001) (\bar{1}00) (0\bar{1}0) (00\bar{1})\]
Structure

Equivalent Planes

Note the shift of origin from blue to red circle for the negative indices
The interplanar spacing (space between same planes of same miller indices) in a crystal can be calculated as follows:

\[ d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \]

For example: the interplanar spacing between (111) planes is \( d_{111} = \frac{a}{\sqrt{3}} \)

The angle \( \phi \) between two planes \((h_1k_1l_1)\) and \((h_2k_2l_2)\) can be calculated from the relation:

\[ \cos \phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}} \]
Example:

Calculate the angle between the (111) and (200) planes.

From the above,

\[ \cos \phi = \frac{(1 \times 2) + (1 \times 0) + (1 \times 0)}{\sqrt{1+1+1\sqrt{4} + 0 + 0}} \]

\[ \cos \phi = \frac{1}{\sqrt{3}} \]

which produces the result, \( \phi = 54.75^\circ \).
Crystal Directions

The directions in a crystal are given by specifying the coordinates \((u, v, w)\) of a point on a vector \((r_{uvw})\) passing through the origin. \(r_{uvw} = ua + vb + wc\). It is indicated as \([uvw]\). For example, the direction \([110]\) lies on a vector \(r_{110}\) whose projection lengths on x and y axes are one unit (in terms of unit vectors \(a\) and \(b\)).

Directions of a form or family like \([110]\), \([101]\), \([011]\) are written as \(<110>\)

<100> and <110> family  <111> family
Crystal Directions

- The line which passes through $uvw$ will also pass through $2u2v2w$ and $\frac{1}{2} u \frac{1}{2} v \frac{1}{2} w$. Hence $[uvw]$, $[2u2v2w]$ and $[\frac{1}{2} u \frac{1}{2} v \frac{1}{2} w]$ are same and written as $[uvw]$.

- Fractions are converted into integers (as shown in the figure below) and reduced to lowest terms.

Point coordinates are
$\frac{1}{2}, \frac{1}{2}, 1 \rightarrow$ direction is $[112]$
Also $0, 1, \frac{1}{2} \rightarrow [021]$
Crystal Directions

To determine a direction of a line in the crystal:

- Find the coordinates of the two ends of the line and subtract the coordinates (Head – Tail) OR draw a line from the origin parallel to the line and find its projection lengths on x, y and z axis in terms of the unit vectors $a$, $b$ and $c$.

- Convert fractions, if any, into integers and reduce to lowest term.

- Enclose in square brackets $[uvw]$
Coordination number

Coordination number is the number of nearest neighbor to a particular atom in the crystal.

The coordination number of BCC crystal is 8.

BCC coordination number $Z = 8$

The body centered atom is in contact with all the eight corner atoms. Each corner atom is shared by eight unit cells and hence, each of these atoms is in touch with eight body centered atoms.
Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell

\[
\text{APF} = \frac{\text{Volume of atoms}}{\text{Volume of unit cell}}
\]

Packing Fraction = \(\frac{\text{volume of atoms in the unit cell}}{\text{volume of unit cell}}\) × 100%

Theoretical density \(\rho = \frac{m}{V} = \frac{\text{mass of atoms in the unit cell}}{\text{volume of unit cell}}\)

Atomic weight (A) ~ \(N_A\) of atoms or molecules
mass of atoms in the unit cell (??) ~ n (no. of atoms in unit cell)
Theoretical Density

Theoretical density calculation from crystal structure.

Theoretical density, \[ \rho = \frac{nA}{V_c N_A} \]

- \( n \) = number of atoms in the unit cell
- \( A \) = atomic weight (Molecular weight \( \rightarrow \) mass of 1 mole for material)
- \( V_c \) = volume of unit cell
- \( N_A \) = Avogadro’s number \( (6.023 \times 10^{23} \text{ atoms/mol}) \)

Calculate the theoretical density of Al.

Al is FCC, lattice parameter, \( a = 4.05 \text{ Å} \), \( n = 4 \).

Atomic weight of Al is 26.98 g/mol

\[ \rho = \frac{4 \times 26.98}{(4.05 \times 10^{-8})^3 \times 6.023 \times 10^{23}} = 2.697 \text{ g/ cc} \]
Structure

Example, for Fcc lattice of lattice constant $a$, Find

a) The coordination number

b) Number of atoms per unit cell

c) The nearest neighbor distance

d) Radius of each atom (assume atoms are spheres)

e) Volume of each atom

f) Packing fraction

g) Density of GaN which has an fcc structure, lattice constant ($a = 4.5 \text{ Å}$), atomic weight ($\mu_{\text{Ga}} = 69.7 \text{ g/mol, } \mu_{\text{N}} = 14 \text{ g/mol}$) and Avogadro’s number ($N_A = 6.02 \times 10^{23} \text{ particles/mole}$).
Structure

a) Coordination number = 12

b) Atoms per cell = 1 (corners) + 3 (faces) = 4

c) Nearest neighbor distance = $\frac{1}{2}a\sqrt{2}$

d) Radius of each sphere = $\frac{1}{4}a\sqrt{2}$

e) Volume of each sphere = $\frac{4}{3}\pi\left[\frac{1}{4}a\sqrt{2}\right]^3$

f) Maximum fraction of cell filled =
   No. of spheres X vol. of each sphere
   / total vol. of each cell = 74%

FCC Unit Cell

g) $\rho = \frac{m}{V} = \frac{nm_{GaN}}{a^3} = \frac{4\mu_{GaN}}{a^3N_A} = \frac{4(69.7+14)}{(4.5\cdot10^{-8})^3 6.02\cdot10^{23}} \frac{g\text{mol}^{-1}}{cm^3\text{mol}^{-1}} = 6.1 \frac{g}{cm^3}$. 
The Diamond Lattice

Many important semiconductors have the arrangement of diamond structure
Like: Elemental SC’s (Si, Ge, C - diamond structure)
Like: Compound SC’s (III-V compounds - GaAs, InP - zinc blend structure)

Diamond Lattice, can be treated as two interpenetrating FCC sub-lattices

Zincblende Lattice

Basic FCC

Two interpenetrating FCC - diamond or zinc blend structure
The Diamond Lattice

Diamond structure is an fcc lattice with a basis of two atoms displaced by \( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \) \( \rightarrow \) two interpenetrating fcc (two fcc sites displaced by \( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \)). Diamond structure is fcc lattice with extra atoms placed at \( \frac{a}{4}, \frac{b}{4}, \frac{c}{4} \) from each atom. Single fcc diamond structure looks like.

- If the two fcc sites have same type of atoms \( \rightarrow \) it is called diamond structure like Si, Ge, C
- If each fcc site have different type of atom \( \rightarrow \) zincblend structure like GaAs \( \rightarrow \) Ga occupy 1\(^{st}\) site and As occupy the 2\(^{nd}\) site
Useful features for III-V compounds (zinc blend structure):

- Ability to vary the mixture of elements on each fcc site to get new compounds

  - Ternary compounds like AlGaAs (Al from column III substitute Ga: \(\text{Al}_x\text{Ga}_{1-x}\text{As}\)) with \(x\) ranges from 0 (GaAs) to \(x=1\) (AlAs)

  - Quaternary compounds like AlGaAsP (Al substitute Ga and P from column V substitute As): \(\text{Al}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{P}_y\)

- The ability of changing the compound gives a semiconductors of very wide range of applications
Bulk Crystal Growth

To get effective Semiconductor devices and integrating circuits, the semiconductor must be highly pure (less than 1 ppm) single crystal.

A) To obtain highly pure semiconductor like Si for instance

1. Making metallurgical grade SiO₂

\[ \text{sand} \leftarrow \text{SiO}_2 + 2\text{C} \rightarrow \text{Si} + 2\text{CO} \quad (\sim 1800 \, ^\circ\text{C}) \]

This is metallurgical grade Si (MGS).

1. Clean enough for metallurgical applications
2. Not single crystal → Polycrystalline
3. Not pure enough for electronic applications

2. MGS is refined more by reacting Si with dry HCl

\[ \text{Si} + 3\text{HCl} \rightarrow \text{SiHCl}_3 + \text{H}_2 \]

Fractional Distillation → \text{SiHCl}_3 (Boiling point of 32 \, ^\circ\text{C})

3. Converting to highly pure Electronic-grade Si (EGS)

\[ 2\text{SiHCl}_3 + 2\text{H}_2 \rightarrow 2\text{Si} + 6\text{HCl} \]

EGS is
1. (1) highly pure for electronic applications
   (2) polycrystalline
Growth of single crystal: in this step we convert EGS to single crystal Si ingot. This can be done by the

Growth Methods: Czochralski (CZ) Growth and Float Zone (FZ) Growth

Main stream growth technology for large diameter wafer

For small and medium diameter wafer less contaminations than CZ method

CZ Growth

FZ Growth

Heat to Si melting point 1412 °C
The Diamond Lattice

- CZ growth method: a seed crystal is lowered into molten Si then raised slowly while being rotating slowly → Crystal grow onto the seed. Rotating allow homogeneous solidification by averaging temperature

**Czochralski (CZ) Growth (Si)**

**Initial Control**
- Seed Crystal
- First Pull
- Pulling Speed
- Rotation Speed

**Growth Control**
- Pulling Speed
- Rotation Speed

**Final Control**
- Pulling Speed
- Rotation Speed

200 mm Si ingot
Si Wafer Production

Bulk Crystal Growth
Bulk Crystal Growth

Si Wafer production

From Ingot to Wafers

- Shaping
- Grinding
- Sawing or Slicing
- Edge Rounding
- Lapping
- Etching
- Polishing
- Cleaning
- Inspection
- Packaging
- Shipping
Bulk Crystal Growth

Doping during growth of substrate

Purpose: To change the electronic properties of the molten Electronic-grade Si (EGS), we add intentional impurities or dopants to the Si melt.

[ How does it work? The dopant atoms usually have one (or in some cases more) electrons deficient or excess compared to the atoms of the semiconductor. The excess electrons can contribute to conduction and dope the material n-type. In case of electron deficiency, “holes” are formed and they can also take part in conduction, though not as efficiently as the electrons (holes are more sluggish). ]

Distribution Coefficient ($k_d$): The ratio of the concentration of the impurity in the solid $C_S$ to the concentration in the liquid $C_L$ at equilibrium.

$$k_d = \frac{C_S}{C_L}$$

**Dependence of $K_d$:**

- Material properties
- Impurities
- The temperature of the solid-liquid interface
- Growth rate
A Si crystal is to be grown by the Czochralski method, and it is desired that the ingot contain $10^{16}$ phosphorus atoms/cm$^3$. Si density 2.33 g/cm$^3$.

(a) What concentration of phosphorus atoms should the melt contain to give this impurity concentration in the crystal during the initial growth? For P in Si, $k_d = 0.35$.

(b) If the initial load of Si in the crucible is 5 kg, how many grams of phosphorus should be added? The atomic weight of phosphorus is 31.

(a) Assume that $C_s = k_d C_L$ throughout the growth. Thus the initial concentration of P in the melt should be

$$\frac{10^{16}}{0.35} = 2.86 \times 10^{16} \text{ cm}^{-3}$$

(b) The P concentration is so small that the volume of melt can be calculated from the weight of Si. From Appendix III the density of Si is 2.33 g/cm$^3$. In this example we will neglect the difference in density between solid and molten Si.

$$V = \frac{m}{\rho} = \frac{5000 \text{ g of Si}}{2.33 \text{ g/cm}^3} = 2146 \text{ cm}^3 \text{ of Si}$$

$$2.86 \times 10^{16} \text{ cm}^{-3} \times 2146 \text{ cm}^3 = 6.14 \times 10^{19} \text{ P atoms}$$

$$\frac{6.14 \times 10^{19} \text{ atoms} \times 31 \text{ g/mole}}{6.02 \times 10^{23} \text{ atoms/mole}} = 3.16 \times 10^{-3} \text{ g of P}$$
Bulk Crystal Growth

Silicon wafer doping and direction from flats

- Mainly [100] and [111] Si wafers are manufactured. Four different configurations to indicate each one of them.
Epitaxial Growth: The growth of a *thin crystal layer* on a wafer of a compatible crystal. The substrate crystal may be a wafer of the same material as the grown layer (*homo*-epitaxial growth), or a different material with a similar lattice structure (*hetero*-epitaxial growth).

**Purpose:** To achieve desired electrical, mechanical, or thermal properties of the *thin film material* grown. The epitaxial crystal layer usually maintains the crystal structure and orientation of the substrate.

**Methods:**
- Chemical Vapor Deposition (CVD)
- Molecular Beam Epitaxy (MBE)
- Liquid-phase epitaxy (LPE)

**Advantage over bulk (wafer) growth techniques:** The epitaxial technique can make possible controlled growth of very thin films, with well controllable doping and composition that are essential for modern day electronic devices. Some devices such as quantum mechanical ones, would not be possible without epitaxial growth.
Epitaxial Growth

Epitaxial Growth with lattice match

Homoepitaxy: The expitaxial layer grown is same as the substrate. Ex: GaAs layer grown on GaAs substrate. The main advantage here is the controlled *thickness and doping* of the epitaxial layer.

Heteroepitaxy: The expitaxial layer grown is different (and has different lattice constant, which depends on composition) from the substrate. *Advantage is tunability of the bandgap difference of adjacent layers (apart from thickness and doping) which is a big deal in device designs.*

Some examples of lattice matched *hetero*-epitaxy:

- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ on GaAs
- $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ on InP
- $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ on GaAs
- $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$ on InP or GaAs
Epitaxial Growth

Epitaxial growth with lattice mismatch (1)

Example: Growth of SiGe on Si. The lattice mismatch between SiGe and Si leads to compressive strain in the SiGe layer. Lattice constant: \( Si = 5.43\text{Å}, Ge = 5.65\text{Å} \).

Concept of critical layer thickness, \( t_c \) (for heteroepitaxial growth with lattice mismatch): Critical layer thickness is the thickness of the epitaxial layer beyond which the strain in the film will be so much as to give rise to defects and dislocations, leading to strain relaxation. Before the epitaxial films relaxes (i.e. before critical thickness is achieved), the film is called pseudomorphic — meaning it assumes the lattice constant of the film on which it is grown.

![Diagram showing pseudomorphic growth and growth with dislocations]

Advantage of lattice mismatched growth:
- The epitaxial layer formed will be under tensile or compressive strain. This can modify fundamental properties of materials such as bandgap, mobility of electrons and holes etc.

Disadvantage of lattice mismatched growth:
- Since the epitaxial layer formed will be under tensile or compressive strain, the film thickness needs to be controlled very accurately, otherwise the film will develop defects.
Review of materials covered until now

- Types of Semiconductors
- Lattice structures
- Miller indices – directions, planes
- Crystal structure (lattice + bases)
- Cubic lattices
- Diamond and Zincblende lattices
- Bulk growth of crystals
- Doping
- Epitaxial growth – Homo and hetero-epitaxy