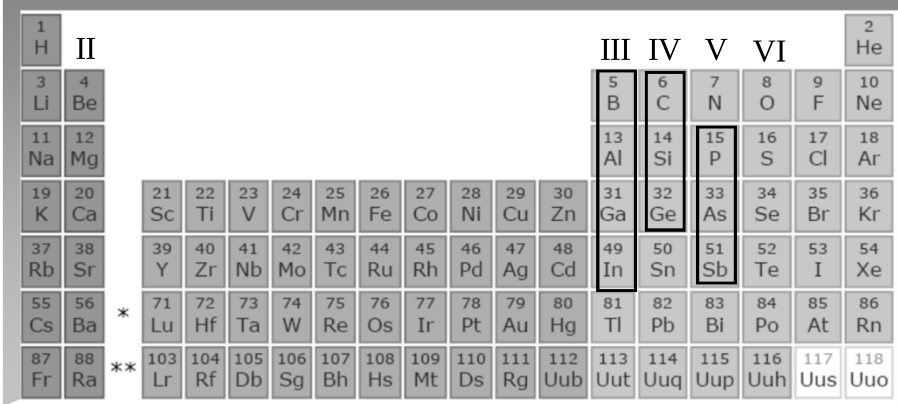
The Crystal Structure of Solids

Outline:
- ➢Semiconductor Materials
- ➢Types of Solids
- ➢Space Lattices
- ➢Atomic Bonding
- ➢Imperfections and Impurities in Solids
- ➢Growth of Semiconductor Materials

Periodic table



redrawing from web elements

A list of some semiconductor materials

Elemental semiconductors		
Si	Silicon	→ 25%
Ge	Germanium	
Compound semiconductors		
AlP	Aluminum phosphide	
AlAs	Aluminum arsenide	
GaP	Gallium phosphide	
GaAs	Gallium arsenide	→ optical devices high speed
InP	Indium phosphide	
Ternary (three-element)		
$Al_XGa_{1-X}As$		→ lattice electrical properties

TYPES OF SOLIDS

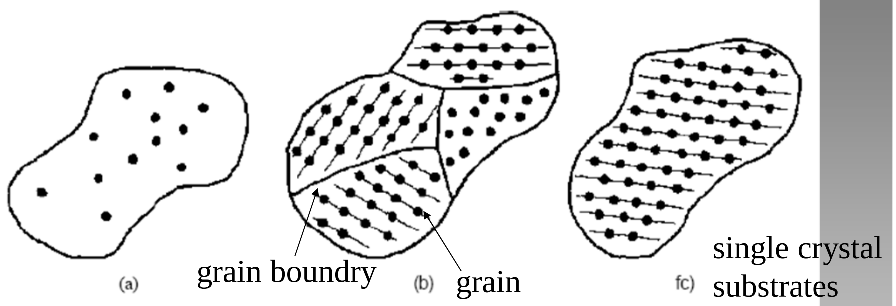
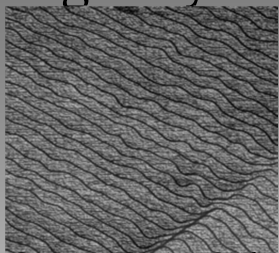


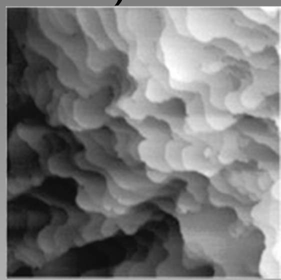
Figure 1.11 Schematics of three general types of crystals: (a) amorphous, (b) polycrystalline, (c) single crystal.

In general, the electrical properties of a single-crystal are superior to those of a nonsingle-crystal material, since grain boundaries tend to degrade the electrical characteristics.

single crystal (wafers, substrates)

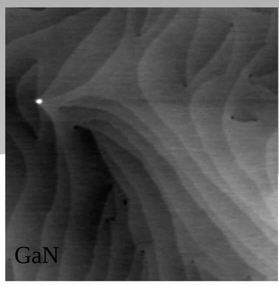


Strontium Titanium Oxide (001)



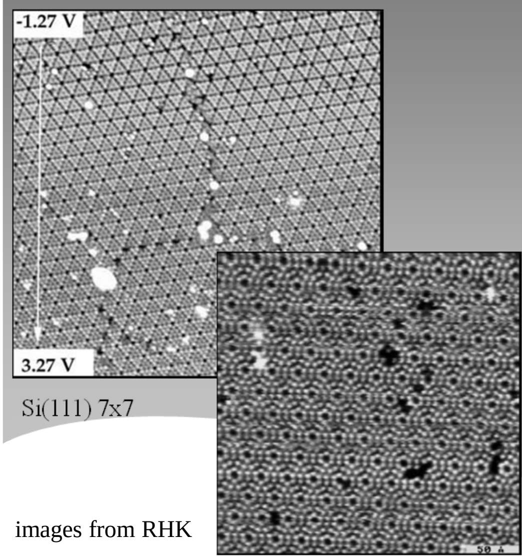
mono atomic steps on Sapphire wafer surface.(3x3μm) The height of each atomic step is 0.57nm.

images from PSIA



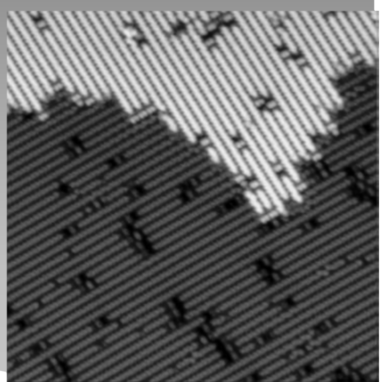
GaN

Si surface



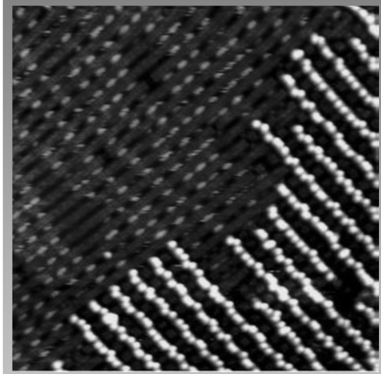
Si(111) 7x7

images from RHK



Si(100) surface dimer reconstruction

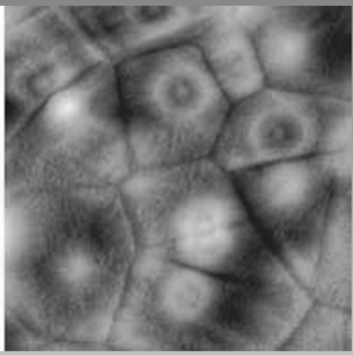
GaAs surface



It shows a GaAs(001) surface with two different surface reconstructions in an area of 40x40 nm2: in the lower right part of the image a (2x6) reconstruction is seen with a zig-zag pattern of As dimer rows consisting of groups of 4 atoms. In the upper left part a (4x2) reconstruction is present with double rows of atoms which are resolved in the image.

images from RHK

Polycrystal

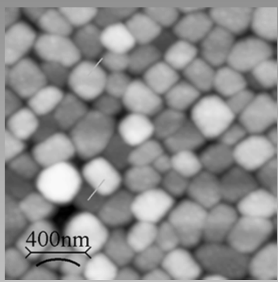


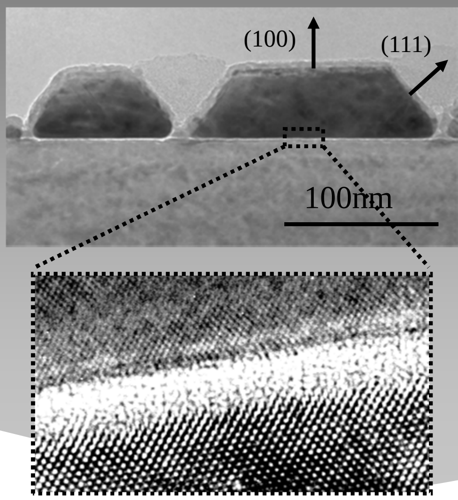
PZT (30/70) (70nm thick) film grown on ITO covered glass

images from Veeco

Textures

織構, 晶粒具優選方向





Unit Cell

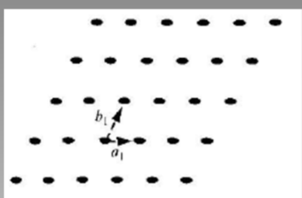


Figure 1.2 | Two-dimensional representation of a single-crystal lattice.

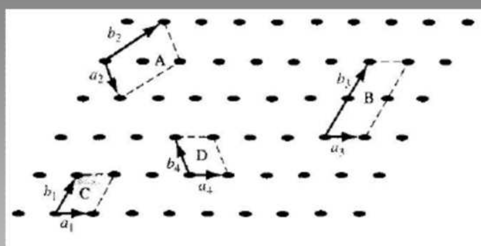


Figure 1.3 | Two-dimensional representation of a single-crystal lattice showing various possible unit cells.

A *unit cell* is a small volume of the crystal that can be used to reproduce the entire crystal. A unit cell is not a unique entity.

Primitive Cell

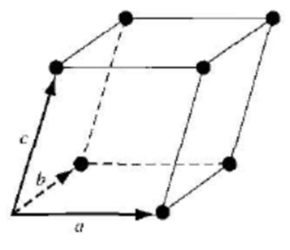


Figure 1.4 | A generalized primitive unit cell.

A *primitive cell* is the smallest unit cell that can be repeated to form the lattice. In many cases, it is more convenient to use a unit cell that is not a primitive cell. Unit cells may be chosen that have orthogonal sides, for example, whereas the sides of aprimitive cell may be nonorthogonal.

Lattice vector

Every equivalent lattice point in the three-dimensional crystal can be found using the vector

$$\bar{r} = p\bar{a} + q\bar{b} + s\bar{c}$$

where *p*, *q*, and *s* are integers.

Basic Crystal Structures

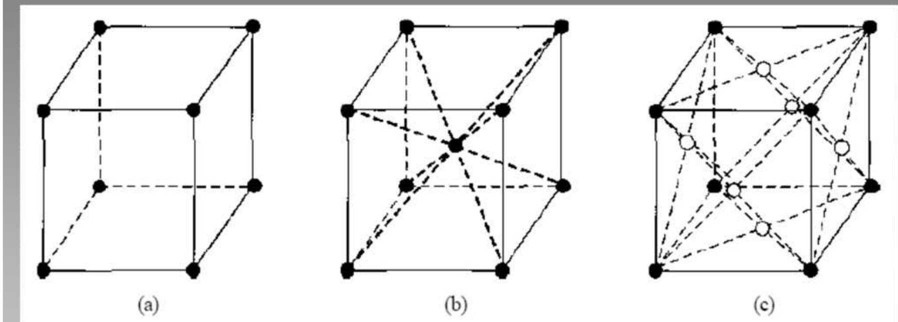
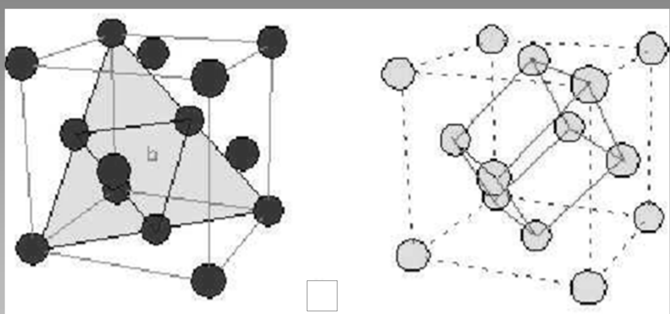


Figure 1.5 I Three lattice types: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic.

FCC structure



(left) 面心結構之晶胞（非原始晶胞）
(right)原始晶胞（該體積為(a)的1/4）

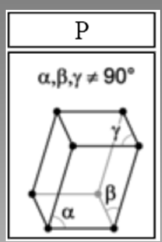
Crystal

Crystal = lattice + basis

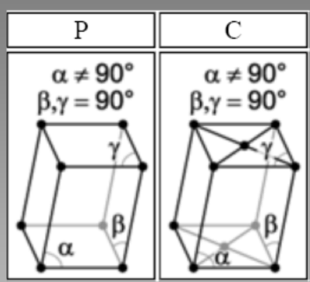
↙ periodic points　　↘ a set of atoms

The crystal structure consists of the same group of atoms, the *basis*, positioned around each and every lattice point. This group of atoms therefore repeats indefinitely in three dimensions according to the arrangement of one of the 14 Bravais lattices.

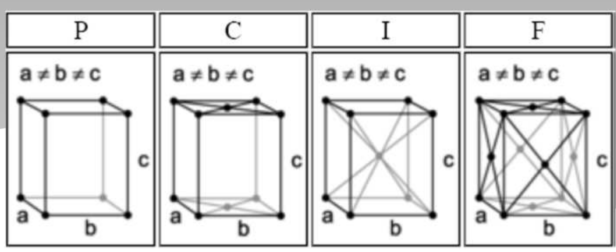
Bravais lattices



triclinic



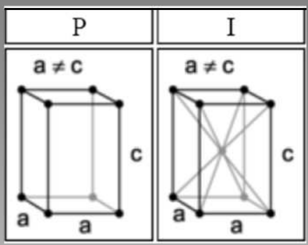
monoclinic



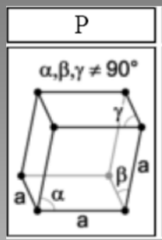
orthorhombic

From WIKIPEDIA

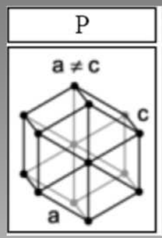
Bravais lattices



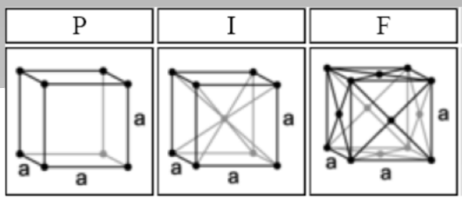
tetragonal



rhombohedral
(trigonal)



hexagonal



cubic

From WIKIPEDIA

volume of the unit cell

Crystal system	Volume
Triclinic	$abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$
Monoclinic	$abc\sin\beta$
Orthorhombic	abc
Tetragonal	a^2c
Rhombohedral	$a^3\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$
Hexagonal	$\frac{\sqrt{3}\,a^2c}{2}$
Cubic	a^3

From WIKIPEDIA

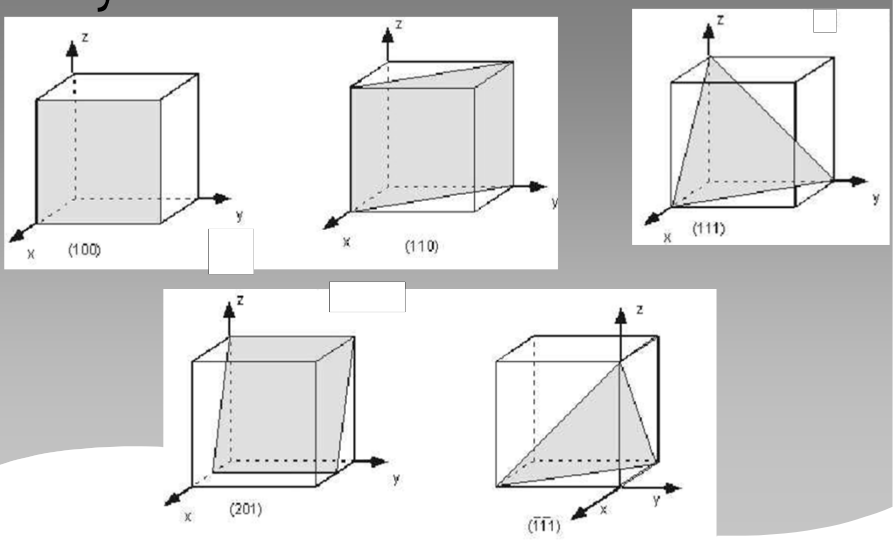
Crystal Planes and Miller Indices

Miller indices : the reciprocal of the intercepts
Why ? ➔ reciprocal lattice space
Case : 1. a plane that pass through the origin
2. a plane that is parallel an axis

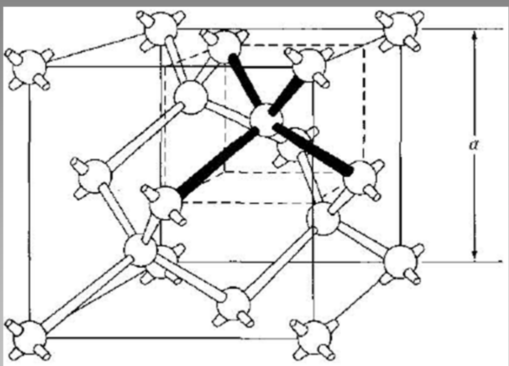
(plane), [direction], {set of plane}
Note that in the simple cubic lattices, the *[hkl]* direction is perpendicular to the *(hkl)* plane. This perpendicularity may not be true in noncubic lattices.

- the distance between nearest equivalent parallel planes
- surface concentration of atoms, number per square centimeter (#/cm^2)

Crystal Planes and Miller Indices



The Diamond Structure



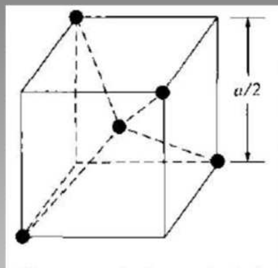


Figure 1.11 | The tetrahedral structure of closest neighbors in the diamond lattice.

Ex: diamond, Si

Zincblende structure

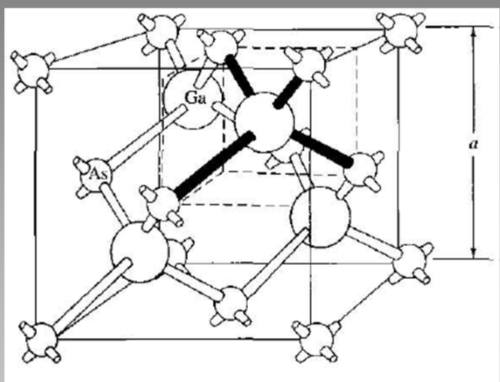


Figure 1.13 | The zincblende (sphalerite) lattice of GaAs.

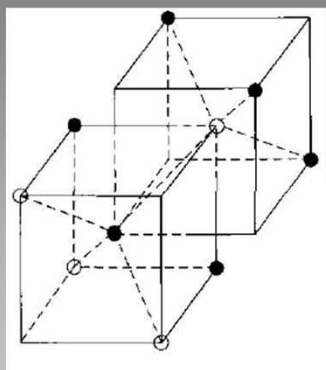


Figure 1.14 | The tetrahedral structure of closest neighbors in the zincblende lattice.

Ex: GaAs, ZnB

Atomic bonding

- Ionic bond – These oppositely charged ions then experience a coulomb attraction and form a bond referred to as an *ionic bond.*
- Covalent bond – Covalent bonding results in electrons being shared between atoms, so that in effect the valence energy shell of each atom is full.
- metallic bonding – The positive metallic ions are surrounded by a sea of negative electrons. the solid is held together by the electrostatic forces.
- *Van der Waals* bond – This nonsymmetry in the charge distribution results in a small electric dipole that can interact with the dipoles of other HF molecules.

Covalent bond

Figure 1.15 | Representation of (a) hydrogen valence electrons and (b) covalent bonding in a hydrogen molecule.

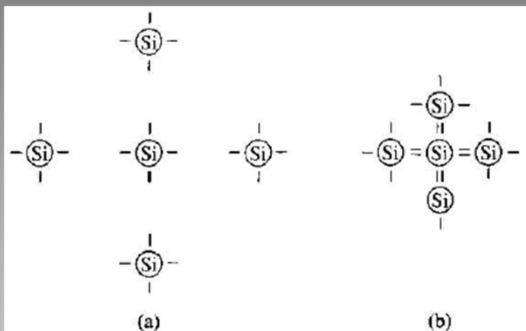
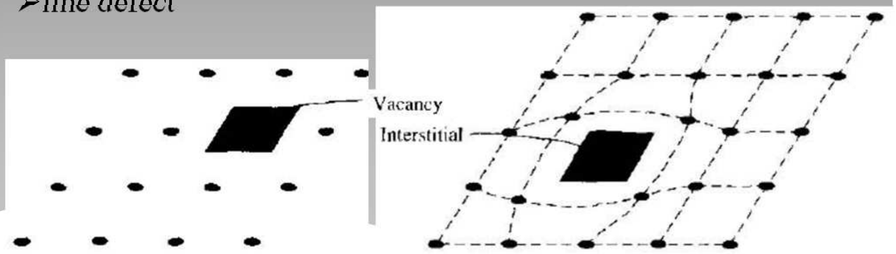


Figure 1.16 | Representation of (a) silicon valence electrons and (b) covalent bonding in the silicon crystal.

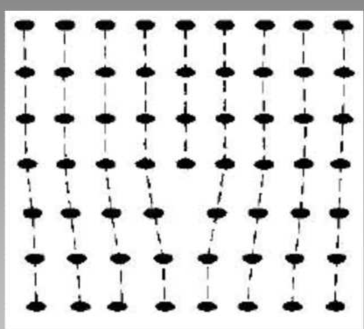
Imperfections in Solids

Imperfections tend to alter the electrical properties of a material and, in some cases, electrical parameters can be dominated by these defects or impurities.

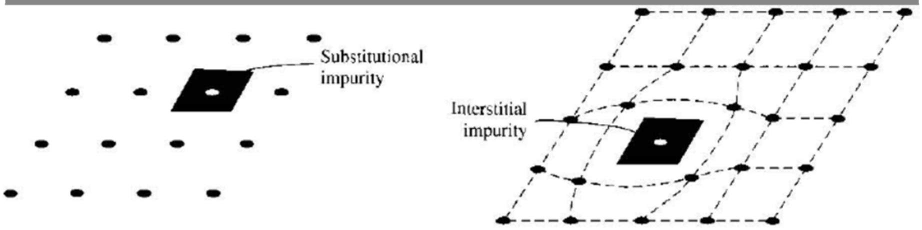
- atomic thermal vibration
- point defect
- *line defect*



Line defect



Impurities in Solids



Some impurities, such as oxygen in silicon, tend to be essentially inert; however, other impurities, such as gold or phosphorus in silicon, can drastically alter the electrical properties of the material.

Doping

- The technique of adding impurity atoms to a semiconductor material in order to change its conductivity is called *doping*. There are two general methods of doping: impurity diffusion and ion implantation.
- Impurity diffusion is the process by which impurity particles move from a region of high concentration near the surface, to a region of lower concentration within the crystal.

Ion implantation

A beam of impurity ions is accelerated to kinetic energies in the range of 50 keV or greater and then directed to the surface of the semiconductor.

- low temperature
- controlled numbers of impurity atoms can be introduced into specific regions of the crystal
- the incident impurity atoms collide with the crystal atoms, causing lattice displacement damage. ➔ thermal annealing

Doping concentration

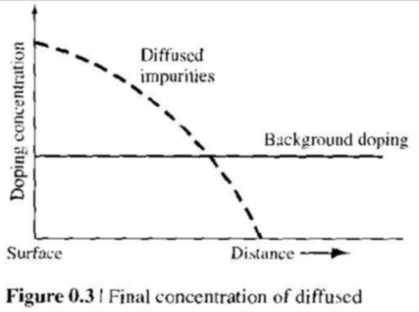


Figure 0.3 | Final concentration of diffused impurities into the surface of a semiconductor.

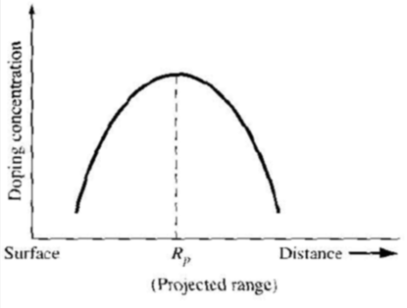
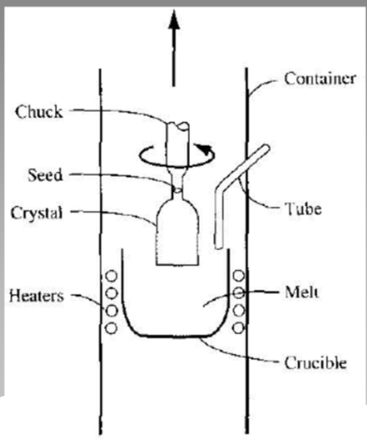
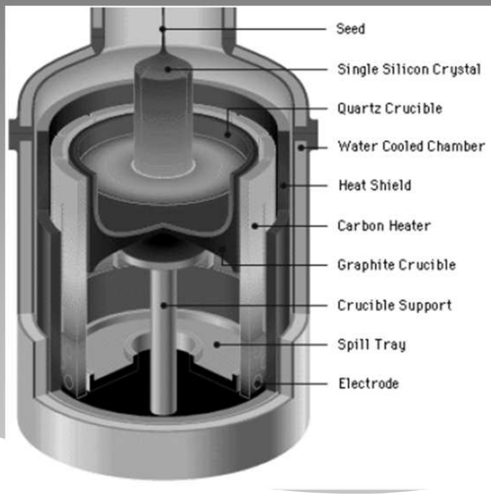


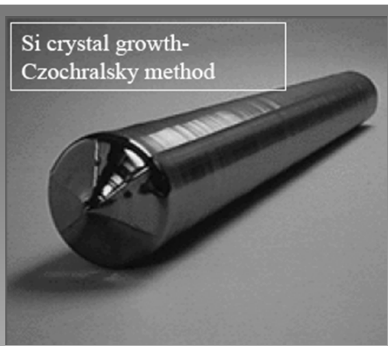
Figure 0.4 | Final concentration of ion-implanted boron into silicon.

Growth of semiconductor materials

Czochralski method

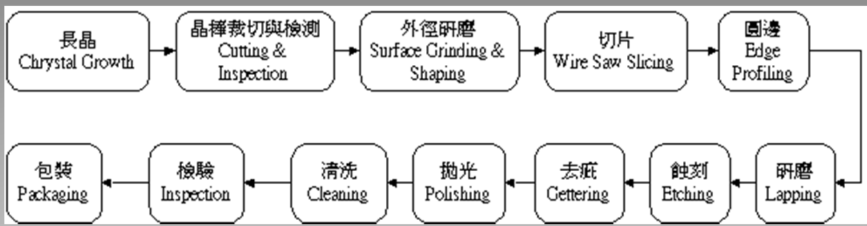




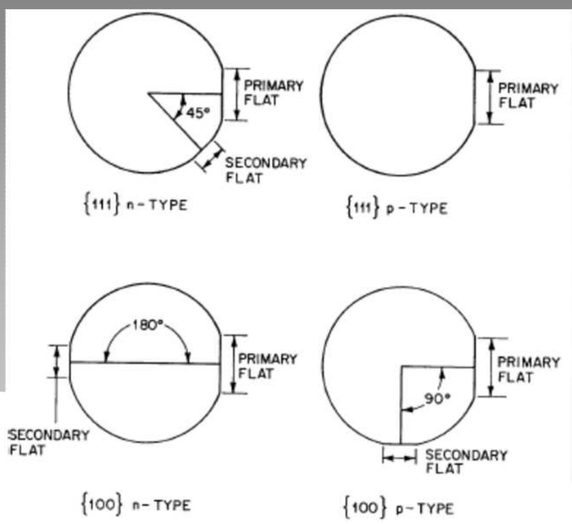


Controlled amounts of specific impurity atoms, such as boron or phosphorus, may be added to the melt so that the grown semiconductor crystal is intentionally doped with the impurity atom.

Some impurities may be present in the ingot that are undesirable. Zone refining is a common technique for purifying material.



Si Wafer shaping



(110)

(110)

Epitaxial Growth

Epitaxial growth is a process whereby a thin, single-crystal layer of material is grown on the surface of a single-crystal substrate.
homoepitaxy
Heteroepitaxy – AlGaAs on a GaAs substrate

Chemical vapor-phase deposition (CVD) – selective growth

Liquid-phase epitaxy – This technique, which occurs at a lower temperature than the Czochralski method, is useful in growing group 11I-V compound semiconductors.

molecular beam epitaxy (MBE) – optical devices such as laser diodes