

# Theory of Semiconductor Devices (반도체 소자 이론)

## Lecture 2. The Crystal Structure of Solids

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## Semiconductor Materials

- ✓ Semiconductors are a group of materials having conductivities between those of metals and insulators.
- ✓ Two general classifications
  - Elemental : Silicon or Germanium
  - Compound : binary, ternary, ...

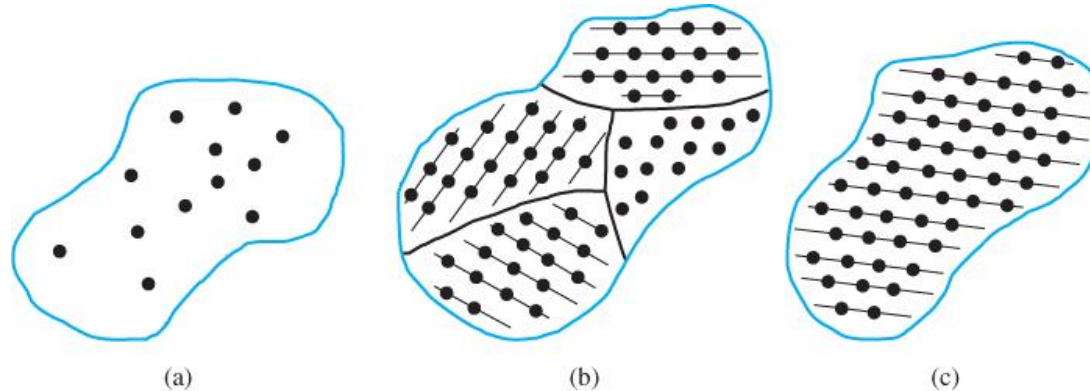
**Table 1.1** | A portion of the periodic table

III	IV	V
5 <b>B</b> Boron	6 <b>C</b> Carbon	
13 <b>Al</b> Aluminum	14 <b>Si</b> Silicon	15 <b>P</b> Phosphorus
31 <b>Ga</b> Gallium	32 <b>Ge</b> Germanium	33 <b>As</b> Arsenic
49 <b>In</b> Indium		51 <b>Sb</b> Antimony

**Table 1.2** | A list of some semiconductor materials

Elemental semiconductors	
Si	Silicon
Ge	Germanium
Compound semiconductors	
AlP	Aluminum phosphide
AlAs	Aluminum arsenide
GaP	Gallium phosphide
GaAs	Gallium arsenide
InP	Indium phosphide

## Types of Solids : depending on the size of ordered region within material



**Figure 1.1** | Schematics of three general types of crystals: (a) amorphous, (b) polycrystalline, (c) single.

When the atoms in the material are arranged in a *regular* manner with a three-dimensional ***periodicity*** that extends throughout a given volume of the solid, the material is considered to be a ***single crystal***.

The periodic arrangement of atoms is interrupted *randomly* along two-dimensional sections that can intersect, dividing a given volume of solid into a number of smaller single-crystalline regions or grains. (can be as small as several atomic spacings)

There is *no* periodicity in the arrangement of atoms (the periodicity is of the same size as the atomic spacings)

## Why single crystal?

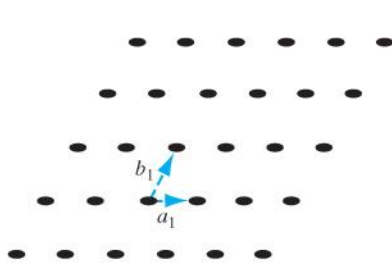
- Although semiconducting properties are observed in all three classes of solids, we will *restrict* our attention to semiconducting materials in *single*-crystalline form .
- Theoretically, when we consider that the spacing between nearest-neighbor atoms in a solid is typically several angstroms ( $1\text{\AA} = 10^{-8} \text{ cm}$ ) , we find that there are  $10^{22}$  to  $10^{23}$  atoms per cubic centimeter. *If* this enormous number of atoms were arranged *randomly* in the material, it would be very difficult to construct a useful physical theory of semiconductor behavior.
- In single crystals , however, the theoretical problems are reduced to *manageable size* and we find that many of the important properties of solids are actually determined by the *periodicity* of the atoms.
- Practically, the use of single crystals greatly *simplifies* a number of the processing steps (etching, diffusion, etc.) used in the fabrication of semiconductor devices and permits the high device yields that are characteristic of modern integrated-circuit technology.
- Also, charge carriers in single crystals exhibit properties that are very useful in device operations.
- Thus, most useful semiconductor devices are fabricated with single-crystalline material.

## Assumption of perfect crystal

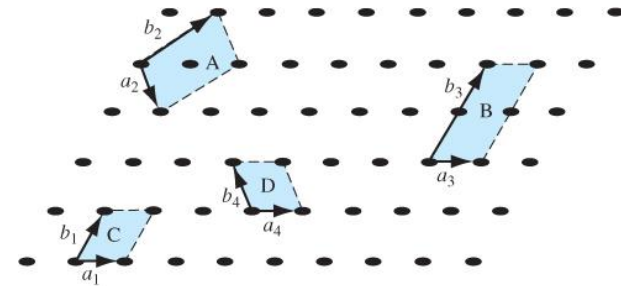
- We consider in detail the crystal structures of the most important semiconductors.
- The approach we take is to assume that the material is *perfectly* periodic with no deviations from its periodicity. This, of course, is an *idealization* since even a perfect single crystal must have surfaces, and some of the most useful physical properties of semiconductors are obtained by introducing defects into the crystal structure doping.
- It is, therefore, worthwhile to examine the assumption of perfect periodicity.
- Considering the surface atoms, if the material has  $10^{23}$  atoms in a centimeter cube, only about 1 atom in  $10^8$  is on the surface.
- In many applications, *intentionally added* impurities produce the dominant deviation from perfect periodicity. Typically, this doping would result in at most 1 impurity atom in  $10^3$ .
- Thus, in most instances, it is *reasonable* initially to treat the material analytically as a *perfect* crystalline structure and later to introduce small *perturbations* to account for deviations from periodicity.

**Lattice** : The periodic arrangement of atoms in the crystal

**Unit cell** : A small volume of the crystal that can be used to reproduce the entire crystal



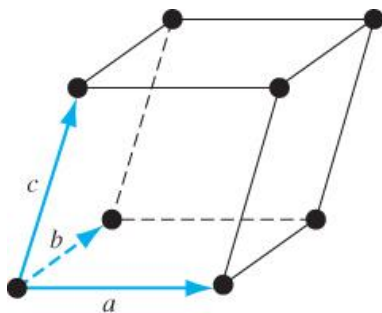
**Figure 1.2** | Two-dimensional representation of a single-crystal lattice.



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

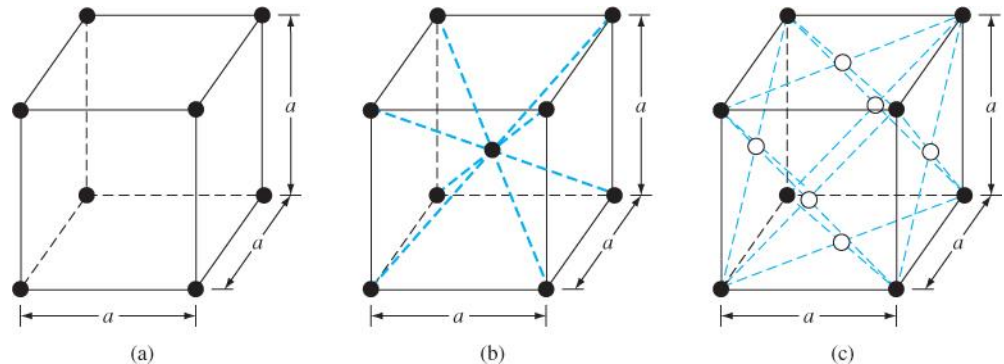
**Primitive cell** : the smallest unit cell that can be repeated to form the lattice

A generalized primitive unit cell in 3-D



**Figure 1.4** | A generalized primitive unit cell.

Basic Crystal Structures

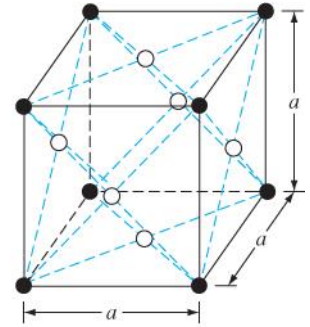
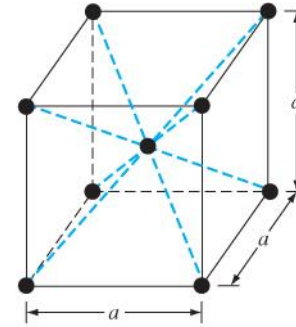
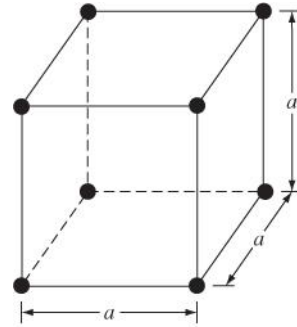


**Figure 1.5** | Three lattice types: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic.

- (a) SC : simple cubic
- (b) BCC : body-centered cubic
- (c) FCC : face-centered cubic

Different Volume density  
of atoms !!

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



**Volume, conventional cell**

**Lattice points per cell**

**Volume, primitive cell**

**Lattice points per unit volume**

**Number of nearest neighbors**

**Nearest-neighbors distance**

**Number of second neighbors**

**Second neighbor-distance**

**Packing fraction**

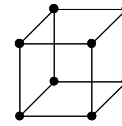
**Table 1.2 (Solid State Physics, Kittel)**

## UNIT CELL GEOMETRY

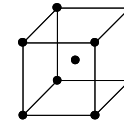
## CUBIC SYSTEM

$$a = b = c \quad \alpha = \beta = \gamma = 90^\circ$$

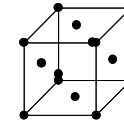
Many metals, Al, Cu, Fe, Pb. Many ceramics and semiconductors, NaCl, CsCl, LiF, Si, GaAs



Simple cubic



Body centered cubic

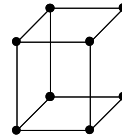


Face centered cubic

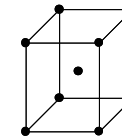
## TETRAGONAL SYSTEM

$$a = b \neq c \quad \alpha = \beta = \gamma = 90^\circ$$

In, Sn, Barium Titanate,  $\text{TiO}_2$



Simple tetragonal

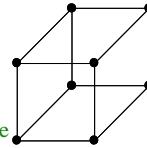


Body centered tetragonal

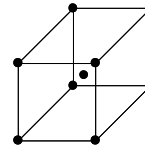
## ORTHORHOMBIC SYSTEM

$$a \neq b \neq c \quad \alpha = \beta = \gamma = 90^\circ$$

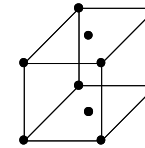
S, U, Pl, Ga ( $<30^\circ\text{C}$ ), Iodine, Cementite ( $\text{Fe}_3\text{C}$ ), Sodium Sulfate



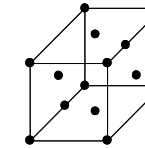
Simple orthorhombic



Body centered orthorhombic



Base centered orthorhombic

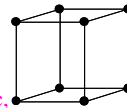


Face centered orthorhombic

## HEXAGONAL SYSTEM

$$a = b \neq c \quad \alpha = \beta = 90^\circ; \gamma = 120^\circ$$

Cadmium, Magnesium, Zinc, Graphite



Hexagonal

## RHOMBOHEDRAL SYSTEM

$$a = b = c \quad \alpha = \beta = \gamma \neq 90^\circ$$

Arsenic, Boron, Bismuth, Antimony, Mercury ( $<-39^\circ\text{C}$ )

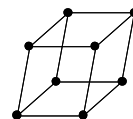


Rhombic

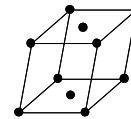
## MONOCLINIC SYSTEM

$$a \neq b \neq c \quad \alpha = \beta = 90^\circ; \gamma \neq 90^\circ$$

$\alpha$ -Selenium, Phosphorus, Lithium Sulfate, Tin Fluoride



Simple monoclinic

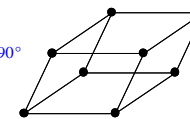


Base centered monoclinic

## TRICLINIC SYSTEM

$$a \neq b \neq c \quad \alpha \neq \beta \neq \gamma \neq 90^\circ$$

Potassium dichromate



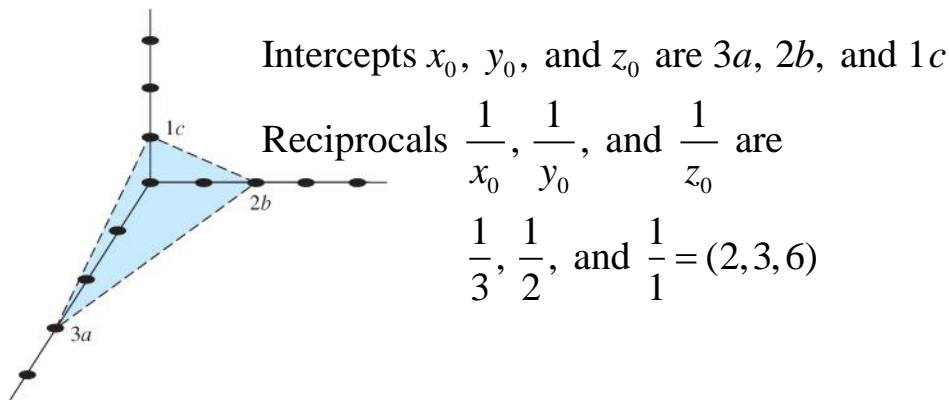
Triclinic

The seven crystal systems (unit cell geometries) and fourteen Bravais lattices.



## Crystal Planes and Miller Indices

- Since semiconductor devices are built on or near the semiconductor surfaces, the orientations and properties of the surface crystal planes are important.
- A convenient method of defining the various planes in a crystal is to use Miller indices. These indices are determined by first finding the intercepts of the plane with the three basis axes in terms of the lattice constants (or primitive cells), and then taking the reciprocals of these numbers and reducing them to the smallest three integers having the same ratio.



**Figure 1.6** | A representative crystal-lattice plane.

## Crystal Planes and Miller Indices

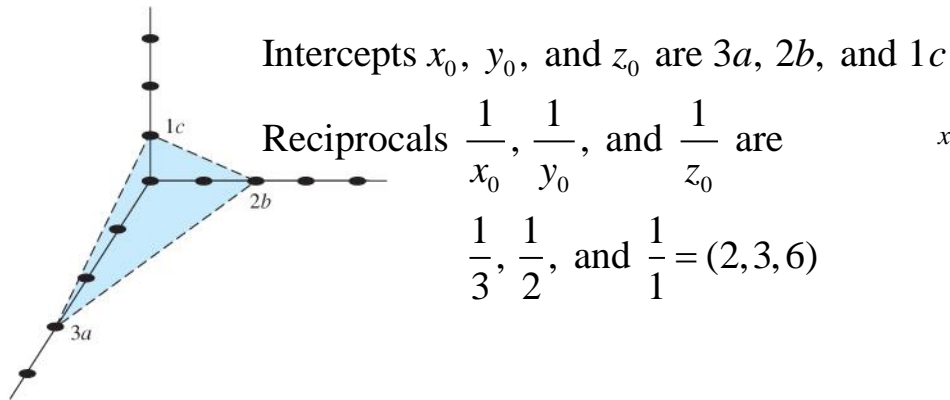
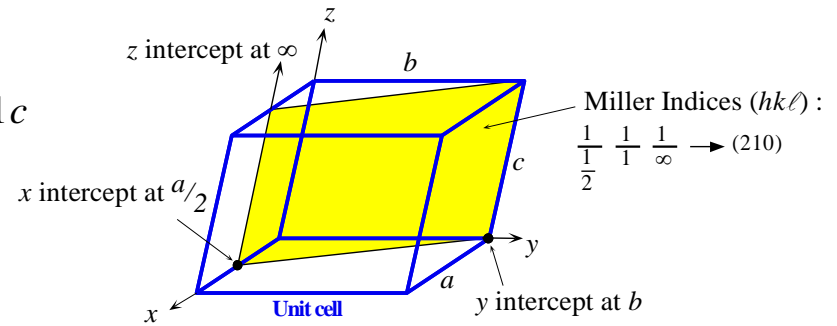


Figure 1.6 | A representative crystal-lattice plane.

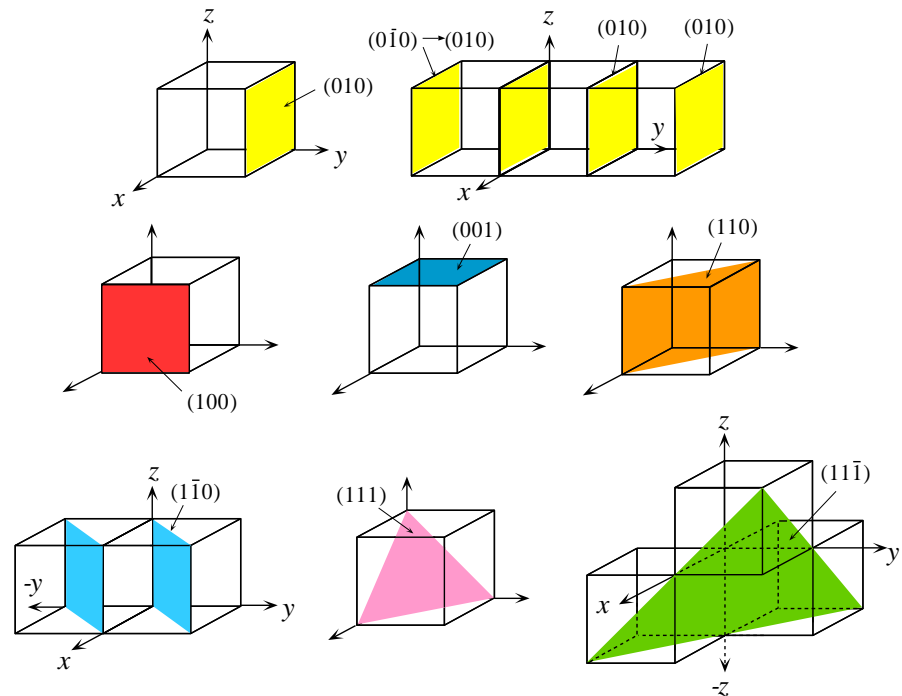


(a) Identification of a plane in a crystal

## Family of Planes

$$\left. \begin{matrix} (100), (010), (001), \\ (\bar{1}00), (0\bar{1}0), (00\bar{1}) \end{matrix} \right\} \Rightarrow \{100\}$$

- ✓ The distance between nearest equivalent parallel planes
- ✓ The surface concentration of atoms



(b) Various planes in the cubic lattice

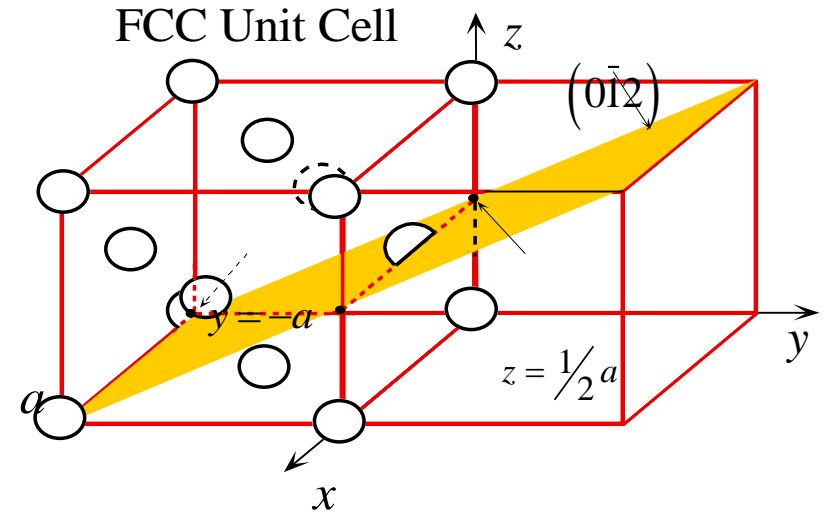
Labelling of crystal planes and typical examples in the cubic lattice

## Examples

Intercepts  $x_0$ ,  $y_0$ , and  $z_0$  are  $\infty$ ,  $-1a$ , and  $\frac{1}{2}a$

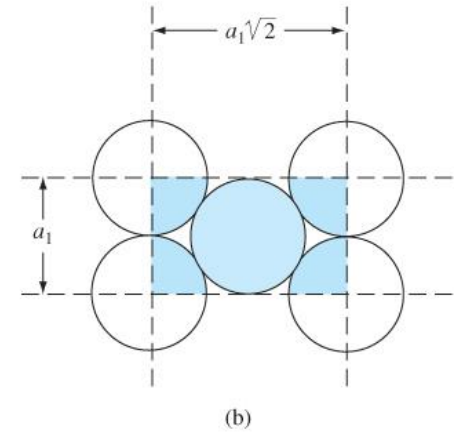
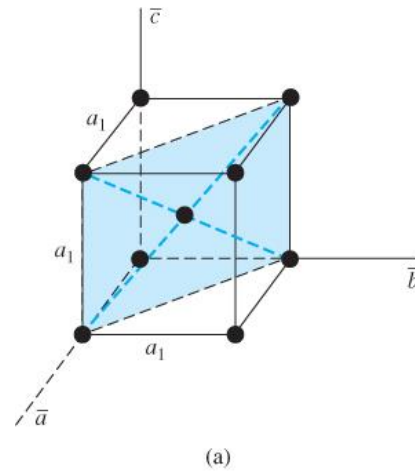
Reciprocals  $\frac{1}{x_0}$ ,  $\frac{1}{y_0}$ , and  $\frac{1}{z_0}$  are

$$\frac{1}{\infty}, \frac{1}{-1}, \text{ and } \frac{1}{\frac{1}{2}} = 0, \bar{1}, 2$$



$$\text{Surface density} = \frac{2 \text{ atoms}}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5 \times 10^{-8})^2(\sqrt{2})}$$

$$5.66 \times 10^{14} \text{ atoms/cm}^2$$



**Figure 1.9** | (a) The (110) plane in a body-centered cubic and (b) the atoms cut by the (110) plane in a body-centered cubic.

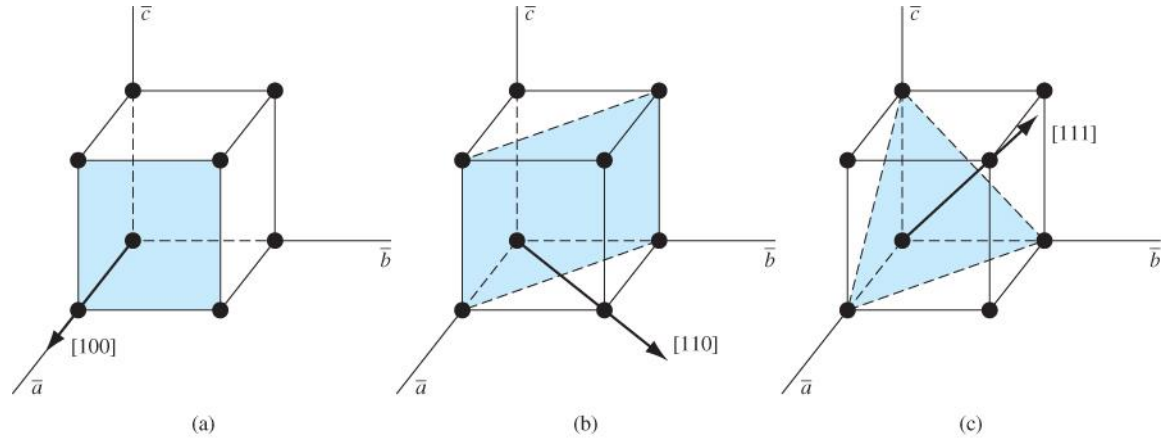
## Directions

*“Many properties, for example, the elastic modulus, electrical resistivity, magnetic susceptibility, etc., are directional within the crystal.”*

(a) (100) plane and [100] direction

(b) (110) plane and [110] direction

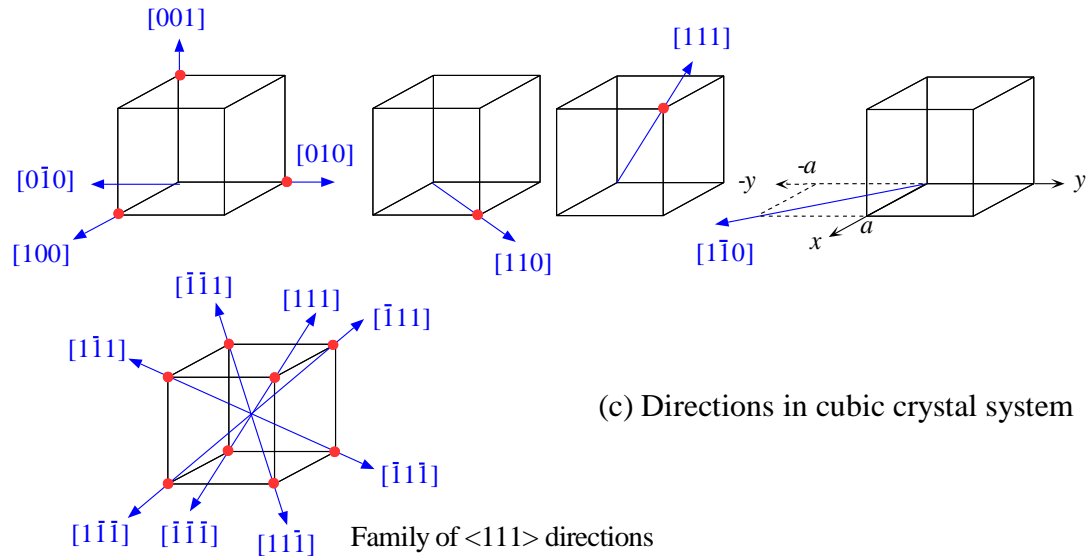
(c) (111) plane and [111] direction



**Figure 1.10** | Three lattice directions and planes: (a) (100) plane and [100] direction, (b) (110) plane and [110] direction, (c) (111) plane and [111] direction.

## Family of directions

$$\left\{ \begin{array}{l} [100], [010], [001], \\ [\bar{1}00], [0\bar{1}0], [00\bar{1}] \end{array} \right\} \Rightarrow \langle 100 \rangle$$



(c) Directions in cubic crystal system

Family of  $\langle 111 \rangle$  directions

**Table 1** Miller Indices and Their Represented Plane or Direction of a Crystal Surface

Miller Indices	Description of plane or direction
$(hkl)$	For a plane that intercepts $1/h$ , $1/k$ , $1/l$ on the $x$ -, $y$ -, and $z$ -axis, respectively.
$(\bar{h}kl)$	For a plane that intercepts the negative $x$ -axis.
$\{hkl\}$	For a full set of planes of equivalent symmetry, such as $\{100\}$ for $(100)$ , $(010)$ , $(001)$ , $(\bar{1}00)$ , $(0\bar{1}0)$ , and $(00\bar{1})$ in cubic symmetry.
$[hkl]$	For a direction of a crystal such as $[100]$ for the $x$ -axis.
$\langle hkl \rangle$	For a full set of equivalent directions.
$[hk\bar{l}m]$	For a plane in a hexagonal lattice (such as wurtzite) that intercepts $1/h$ , $1/k$ , $1/l$ , $1/m$ on the $a_1$ -, $a_2$ -, $a_3$ -, and $z$ -axis, respectively (Fig. 1g).

## Diamond structure

- Covalently bonded solids; Si, Ge, diamond, etc.
- Eight atoms in the unit cell.

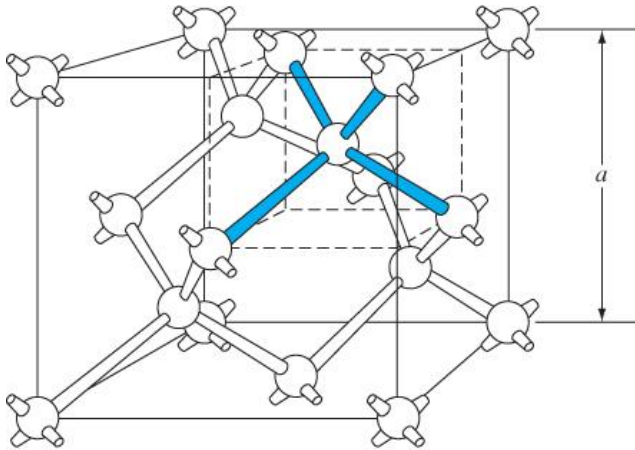


Figure 1.11 | The diamond structure.

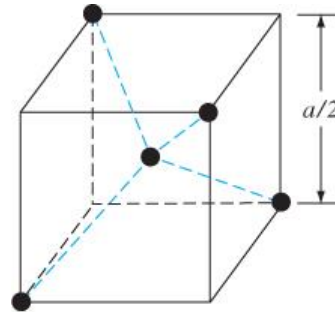


Figure 1.12 | The tetrahedral structure of closest neighbors in the diamond lattice.

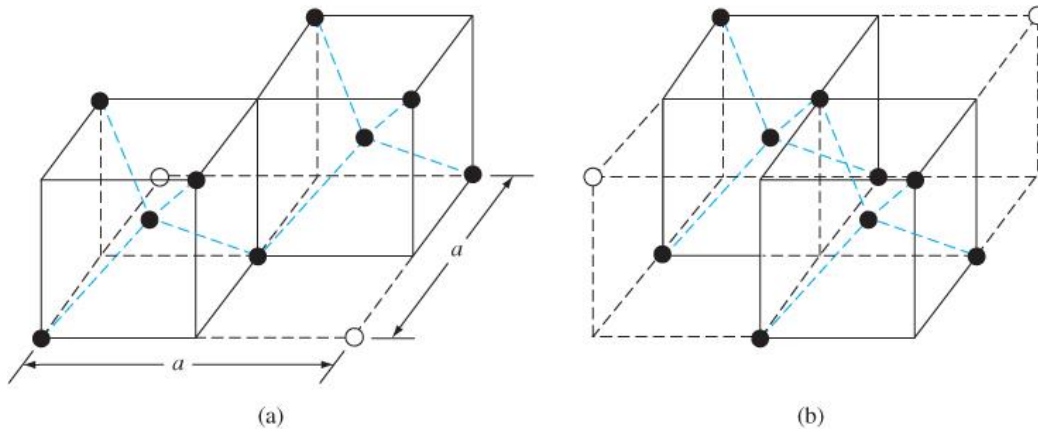
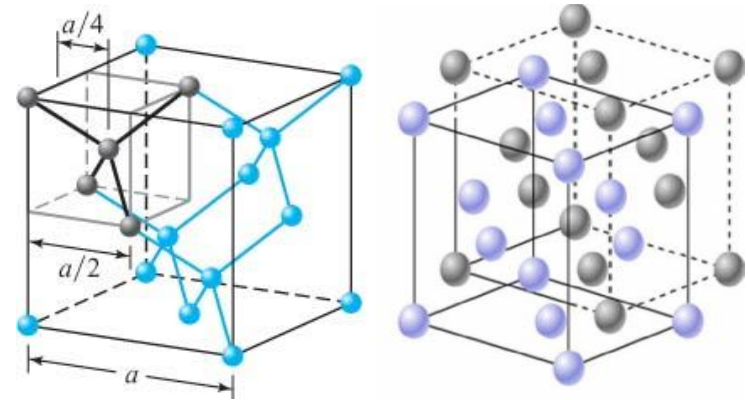


Figure 1.13 | Portions of the diamond lattice: (a) bottom half and (b) top half.

## Zincblende structure

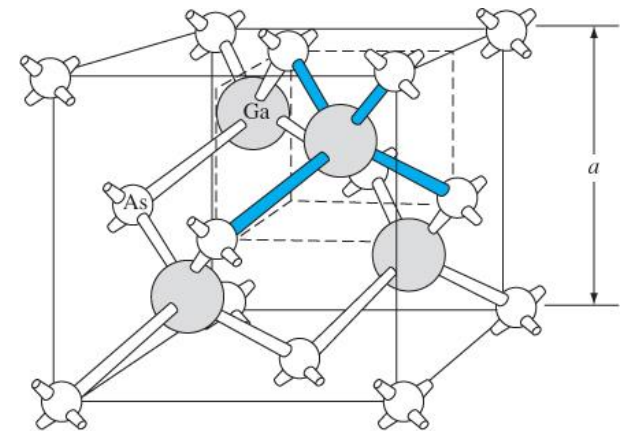
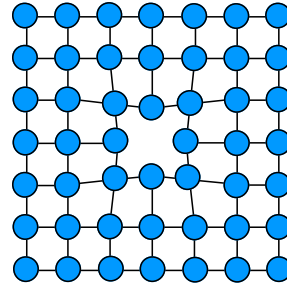


Figure 1.14 | The zincblende (sphalerite) lattice of GaAs.

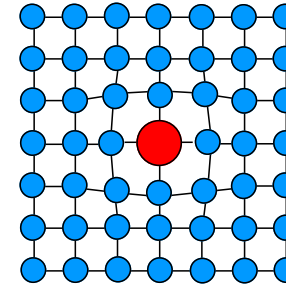
## Point defects

Vacancy



(a) A vacancy in the crystal.

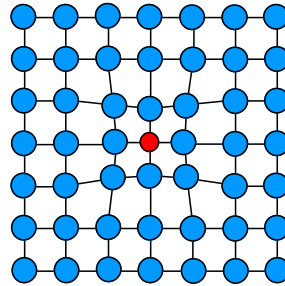
Interstitial



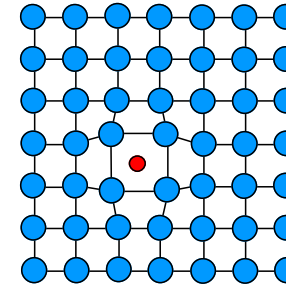
(b) A substitutional impurity in the crystal. The impurity atom is larger than the host atom.

Substitutional

Doping

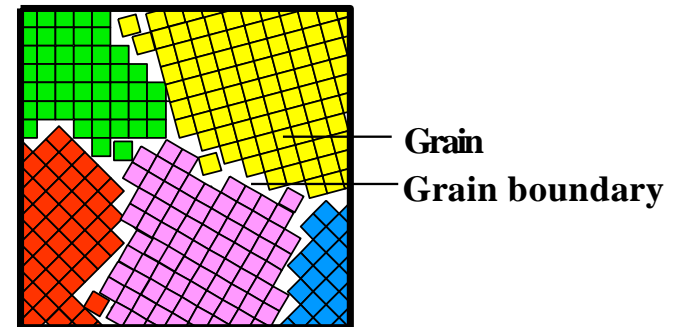
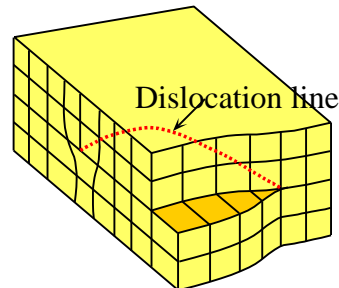
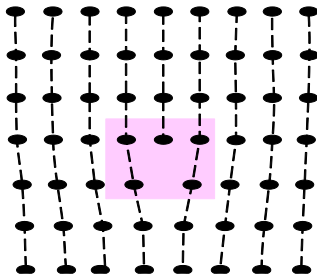


(c) A substitutional impurity in the crystal. The impurity atom is smaller than the host atom.



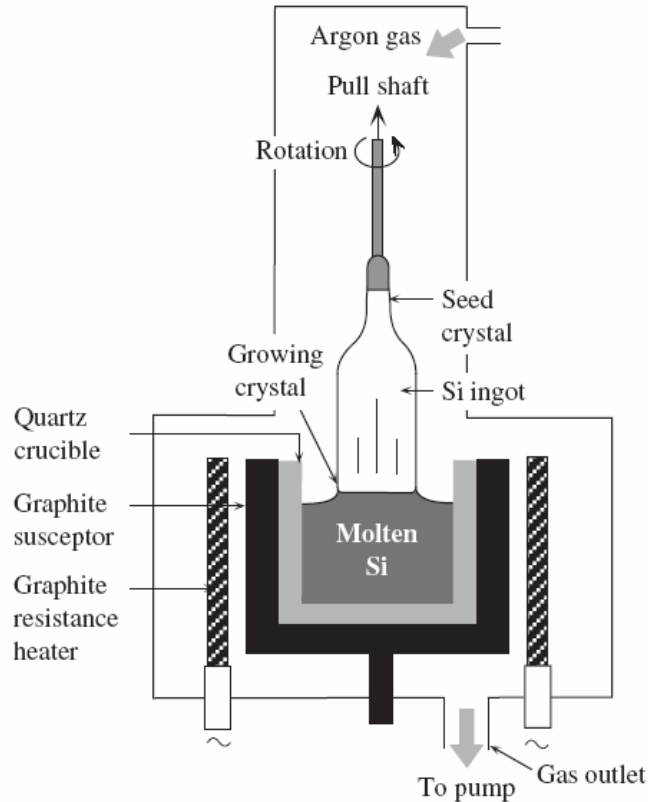
(d) An interstitial impurity in the crystal. It occupies an empty space between host atoms.

## Line defects and Planar Defects





## Growth from a Melt



### Schematic illustration of the growth of a single-crystal Si ingot by the Czochralski technique.

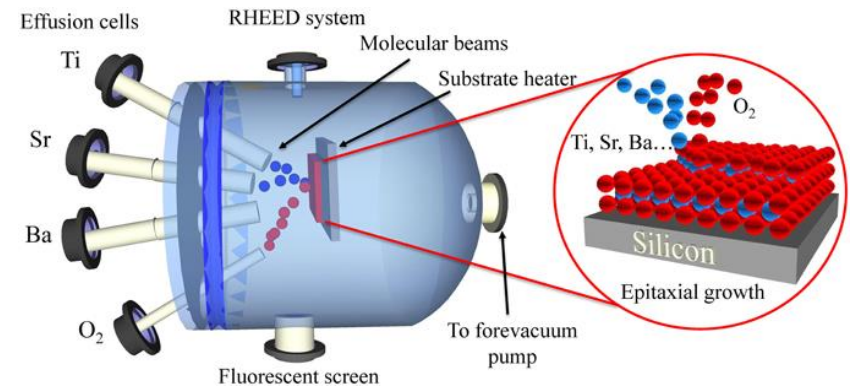
A small piece of single-crystal (seed) is brought into contact with the surface of the same material in liquid phase, and then slowly pulled from the melt. As the seed is slowly pulled, solidification occurs along the plane between the solid-liquid interface.

## Epitaxial growth

- Homo-epitaxy
- Hetero-epitaxy

The term *epitaxy* comes from the [Greek](#) roots *epi* (ἐπί), meaning "above", and *taxis* (τάξις), meaning "an ordered manner". It can be translated as "arranging upon".

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



- Molecular beam epitaxy (MBE)



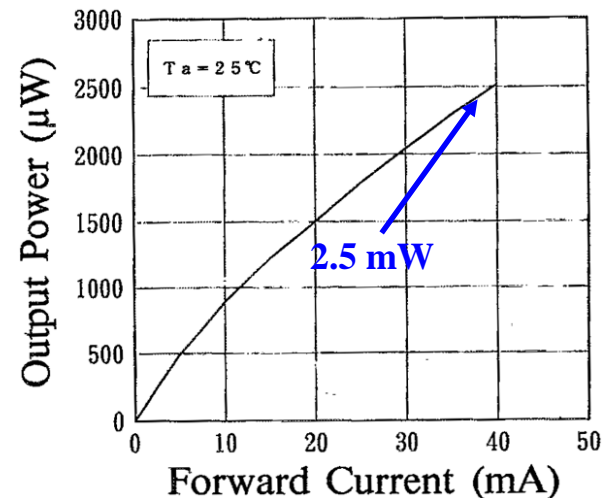
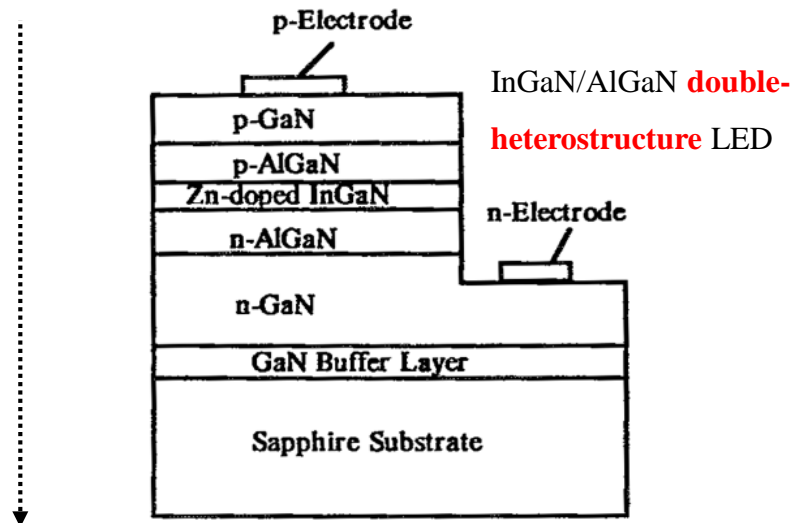
# Candela-class high-brightness InGaN/AlGaN double-heterostructure blue-light-emitting diodes

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Candela-class high-brightness InGaN/AlGaN double-heterostructure (DH) blue-light-emitting diodes (LEDs) with the luminous intensity over 1 cd were fabricated. As an active layer, a Zn-doped InGaN layer was used for the DH LEDs. The typical output power was  $1500\ \mu\text{W}$  and the external quantum efficiency was as high as 2.7% at a forward current of 20 mA at room temperature. The peak wavelength and the full width at half-maximum of the electroluminescence were 450 and 70 nm, respectively. This value of luminous intensity was the highest ever reported for blue LEDs.



## Homework #1

Size 3<sup>rd</sup> edition, P1.1, P1.3 and P1.4

1. (a) Find the maximum fraction of a conventional unit-cell volume which can be filled by identical hard spheres in a diamond lattice.  
(b) Find the number of atoms per square centimeter in silicon in (111) plane at 300 K.
  
3. For a face centered cubic, the volume of a conventional unit cell is  $a^3$ . Find the volume of a fcc primitive unit cell with three basis vectors:  $(0,0,0 \rightarrow a/2, 0, a/2)$ ,  $(0,0,0 \rightarrow a/2, a/2, 0)$ , and  $(0,0,0 \rightarrow 0, a/2, a/2)$ .
  
4. (a) Derive an expression for the bond length  $d$  in the diamond lattice in terms of the lattice constant  $a$ .  
(b) In a silicon crystal, if a plane has intercepts at 10.86 Å, 16.29 Å, and 21.72 Å along the three Cartesian coordinates, find the Miller indices of the plane.