

Engineering Materials (BME 15)

Material science : it deals with the study of structure, properties and application of the materials so that the properties of existing materials can be developed, and new materials can be developed to full fill our engineering needs.

- solid materials have been conveniently grouped into three basic categories, (based on chemical make up and atomic structure)
- METALS
- CERAMICS
- POLYMERS

- In addition there are **composites** , which are engineered combination of two or more different materials
- Apart from this classification we have different types of materials in present scenario, which are advance materials . (**semiconductors, bio materials, smart materials and nanoengineered materials**)

Engineering materials

Metals

polymers

ceramics

Ferrous

Steels, cast iron, stainless steel etc.

Non ferrous

Al, Cu, W, Ag etc.

Amorphous

Gels, glasses etc.

thermoplastics

Nylons, PVC, polyethylene etc.

thermosets

Epoxies, phenolics, polyimides etc.

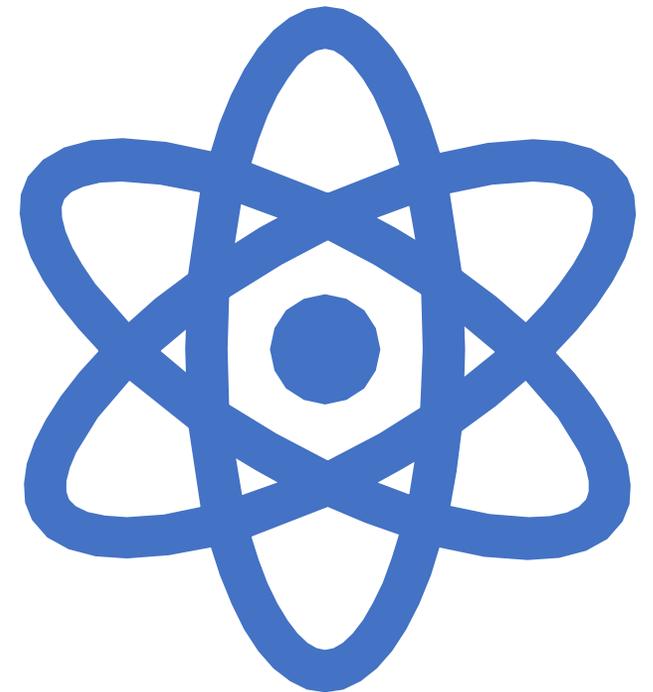
elastomers

Rubber, silicones etc.

Oxides, nitrides,
carbides, glass
ceramics, graphite,
diamond

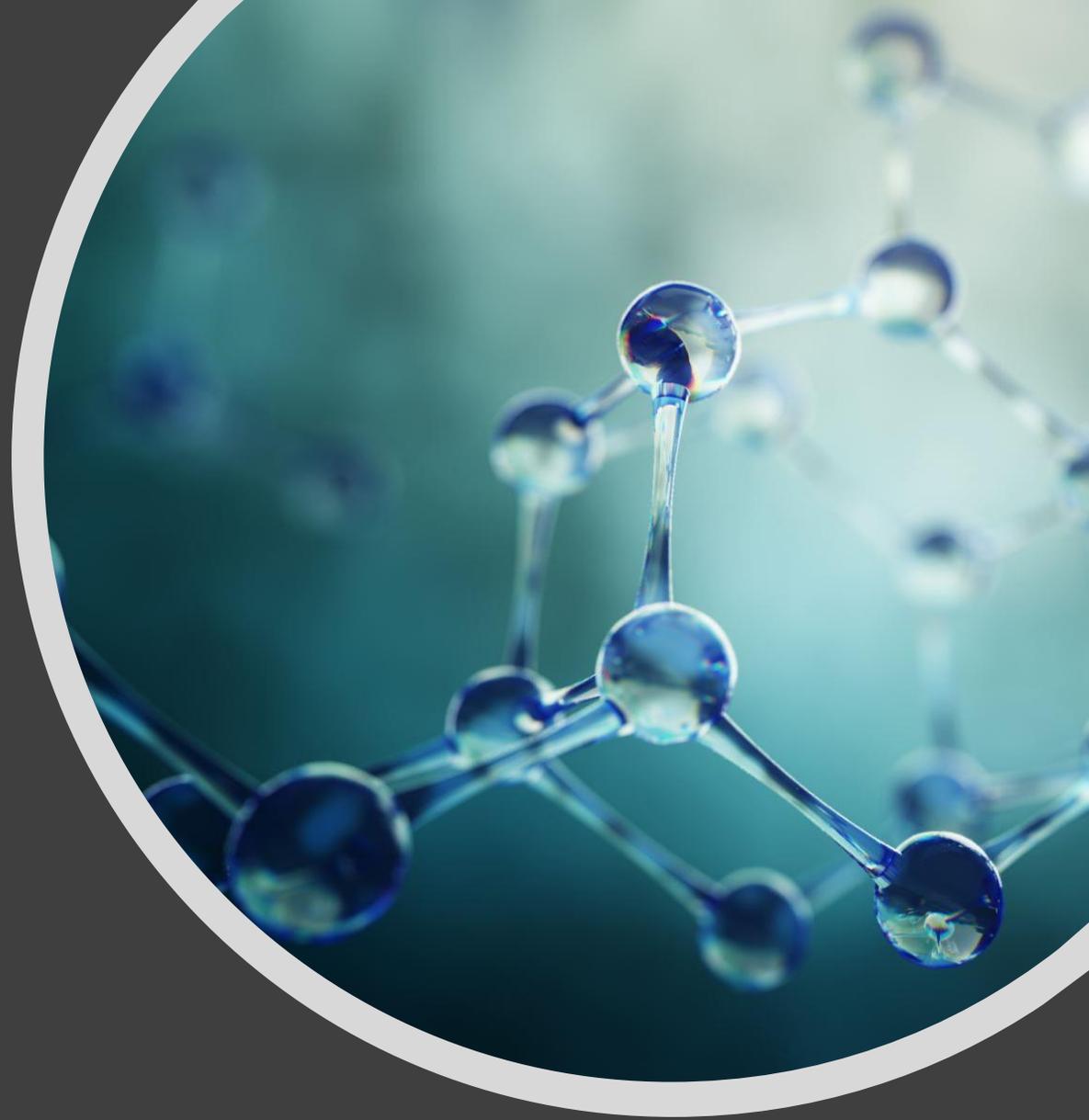
Atomic model

- During the latter part of the nineteenth century it was realized that many phenomena involving electrons in solids could not be explained in terms of classical mechanics.
- What followed was the establishment of a set of principles and laws that govern systems of atomic and subatomic entities that came to be known as **quantum mechanics**.
- An atomic model represents what the structure of an atom could look like , based on which we can predict its behavior.
- It is not necessarily a true picture of the exact structure of an atom.



Various scientists discovered the different atomic models in progression of time and keep on moving towards more accurate atomic model but none of which is the perfect atomic model to demonstrate the true picture inside the atom .

So let's study some important atomic models which are helpful to understand the concept of the structure of an atom.

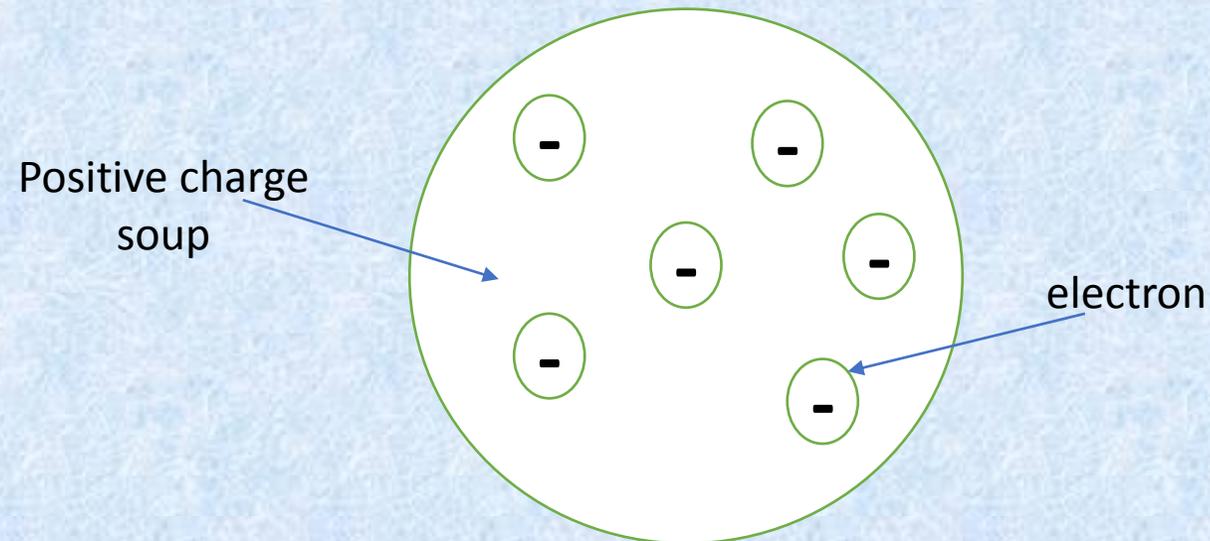


1. Dalton's model of the atom (1766-1844)

- Matters are made of very tiny particles called atoms which are **indivisible** structure.
- Atoms can neither be created nor destroyed.
- All atoms of particular elements are similar in all respects including identical mass , physical and chemical properties.
- Atoms of different elements shows different properties.
- Compound are formed when atoms of different elements combine in a fixed ratio.
- In this model electron and nucleus were **unknown**.

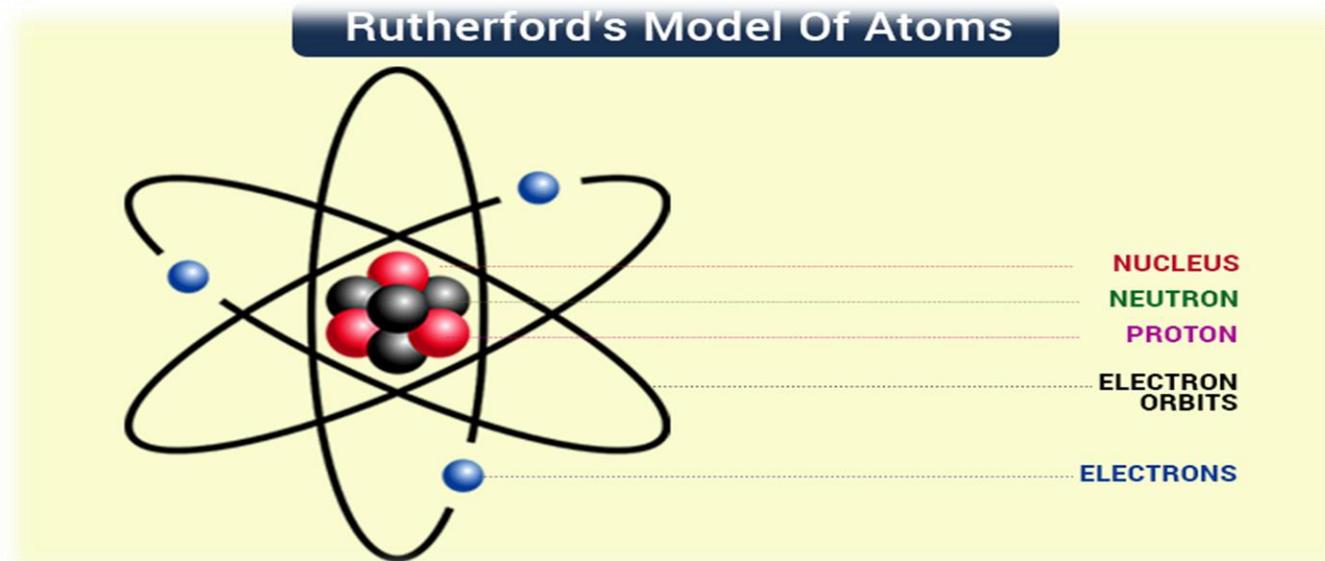
2.Thomson's atomic model (1897)

- Atoms were made up of smaller particles.
- Atoms are made up of negative electrons that float in a **soup of positive charge**.
- Also known as **plum pudding model**.



3. Rutherford's atomic model (1911)

- On the basis of alpha particles scattering experiment, Rutherford described the atom as a dense tiny positively charged core called nucleus, in which nearly all mass is concentrated, around which the lightly weighted negative elements called electron propagate at some distance similar to planets revolving around the sun.
- Also known as **planetary model** of the atom.



4. Bohr's model of the atom (1913)

- Bohr modified Rutherford's atomic structure by describing that electrons have motion in fixed shells.
- Each shell has a certain energy level.
- It described electrons in atom in terms of both position (shell or orbit) and energy(quantized energy levels).

$$E_n = \frac{-13.56 z^2}{n^2} \text{ eV} \qquad R_n = \frac{0.529 n^2}{z} \text{ \AA}$$

Where

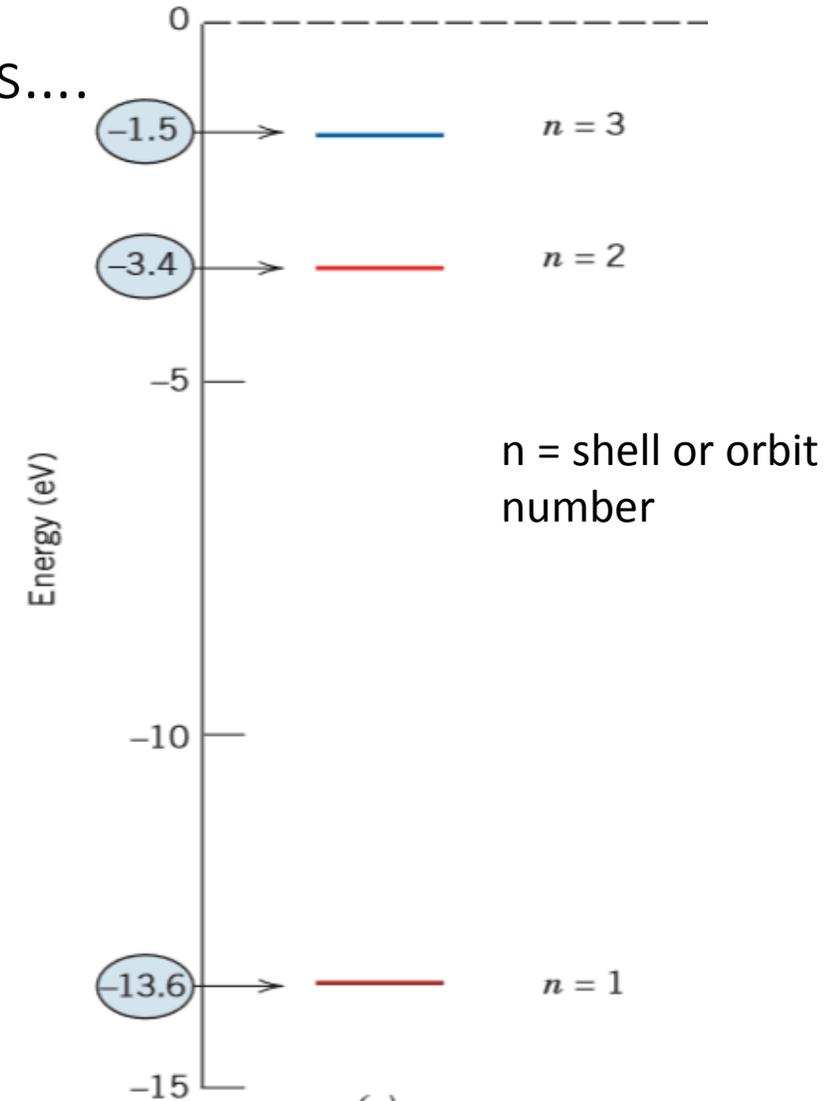
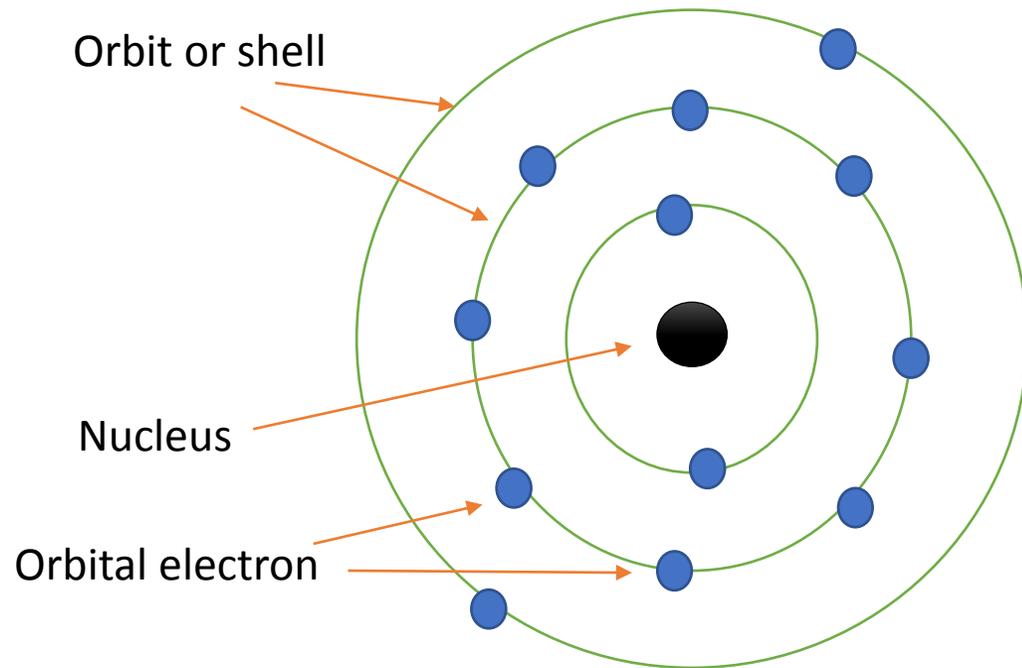
E_n = energy required for a electron to jump out of the n th orbit

R_n = radius of n th orbit

n = number of orbit

Z = atomic number of element

Bohr's model of the atom (1913) continues....

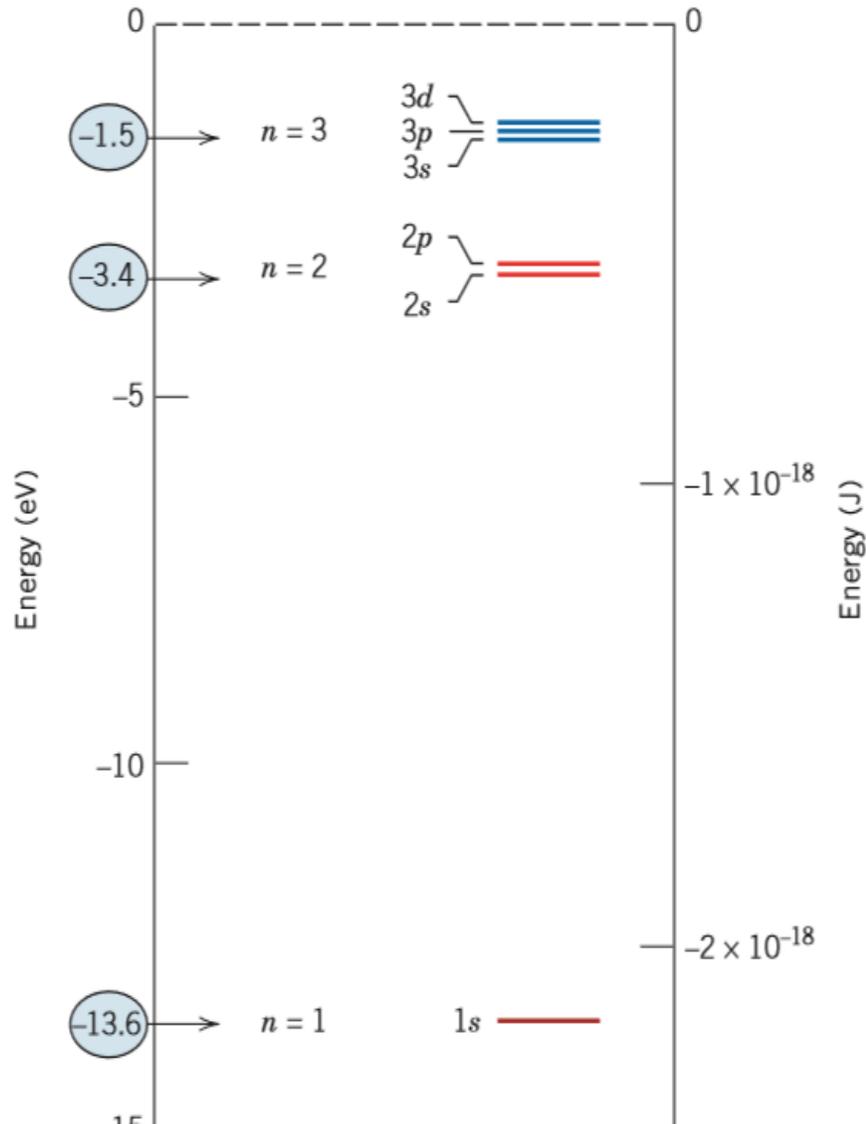


The first 3 electron energy states for the Bohr hydrogen atom.

5. Wave mechanical model / electron model (1927) by Erwin Schrodinger

- He combined the Bohr's model with De Broglie's hypothesis.
- He proposed the electron was a 3D waveform circling the nucleus in a whole number of wavelengths allowing the waveform to repeat itself as a stable standing wave representing the energy levels of the Bohr's model.
- Position of electron is considered to be probability of an electron being at various locations around the nucleus.
- Position is described by a probability distribution or electron cloud.

Electron model (1927) continues...



- Using wave mechanics every electron in the atom is characterized by 4 parameters called quantum number.

Crystal structures

- A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms.
- Sometimes the term **lattice** is used in the context of crystal structures; in this sense ***lattice*** means a three-dimensional array of points coinciding with atom positions (or sphere centers). The point of center of atom in space lattice is known as **lattice point**.
- The properties of some materials are directly related to their crystal structures.
- significant property differences exist between crystalline and non crystalline materials having the **same composition**.
- **All metals, many ceramic materials, and certain polymers** form crystalline structures under normal solidification conditions.

Unit cell

- The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called **unit cells**.
- Unit cells for most crystal structures are parallelepipeds or prisms having three sets of parallel faces.
- the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.

Coordination number and the atomic packing factor (APF).

- For metals, each atom has the same number of nearest-neighbor or touching atoms, which is the coordination number.
- The APF is the sum of the sphere volumes of all atoms within a unit cell (assuming the atomic hard-sphere model) divided by the unit cell volume.

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

Bravais lattice

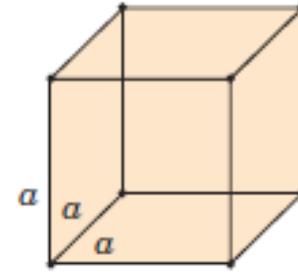
- There are only 14 independent ways of arranging points in a three dimension space on pure symmetry consideration.
- If all the atoms at the lattice points are identical , the space lattice is said to be a bravais lattice.
- These ***14 bravais lattices*** belong to ***7 crystal systems***.

| <i>Crystal System</i> | <i>Axial Relationships</i> | <i>Interaxial Angles</i> | <i>Unit Cell Geometry</i> |
|-----------------------|----------------------------|--------------------------|---------------------------|
|-----------------------|----------------------------|--------------------------|---------------------------|

Cubic

$$a = b = c$$

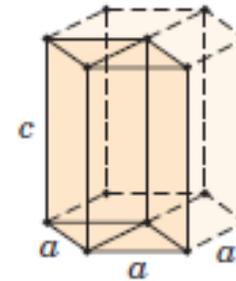
$$\alpha = \beta = \gamma = 90^\circ$$



Hexagonal

$$a = b \neq c$$

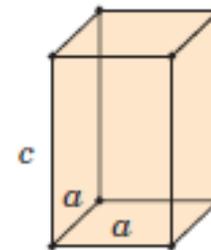
$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$



Tetragonal

$$a = b \neq c$$

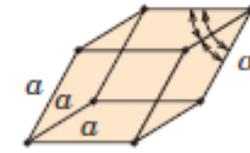
$$\alpha = \beta = \gamma = 90^\circ$$



Rhombohedral
(Trigonal)

$$a = b = c$$

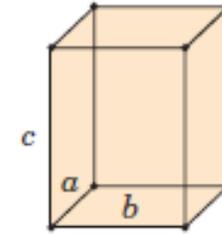
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

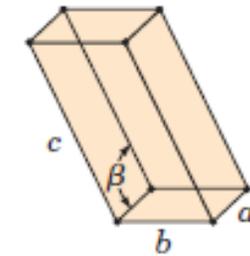
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

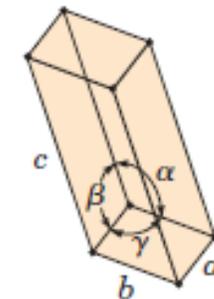
$$\alpha = \gamma = 90^\circ \neq \beta$$



Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$

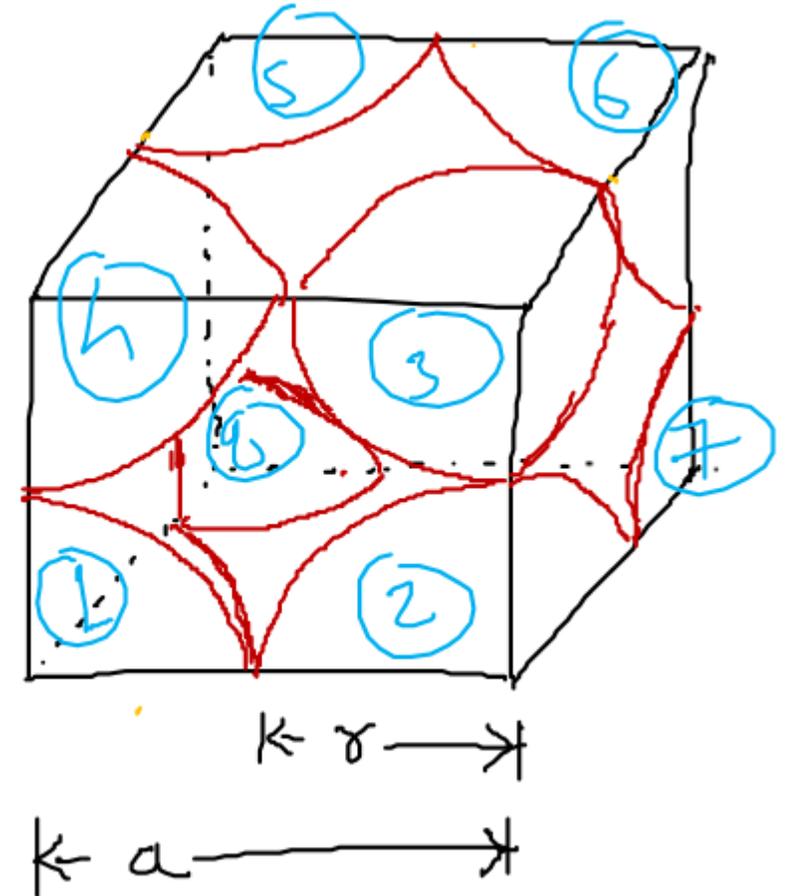


| CRYSTAL SYSTEM | Space lattice |
|--|--|
| CUBIC | <ol style="list-style-type: none"> 1. Simple 2. Body centered 3. Face centered |
| TETRAGONAL | <ol style="list-style-type: none"> 1. Simple 2. Body centered |
| ORTHORHOMBIC | <ol style="list-style-type: none"> 1. Simple 2. End centered/base centered/side centered 3. Body centered 4. Face centered |
| RHOMBOHEDRAL | <ol style="list-style-type: none"> 1. simple |
| HEXAGONAL | <ol style="list-style-type: none"> 1. simple |
| MONOCLINIC | <ol style="list-style-type: none"> 1. Simple 2. End centered |
| TRICLINIC (least symmetric among all 14) | <ol style="list-style-type: none"> 1. simple |

Simple cubic structure

- Atoms located at all eight corners
- Number of atom in a unit cell is $1 = \frac{1}{8} \times 8$
- Mn has SC structure.
- Coordination number = 6.

$$\begin{aligned} \text{APF} &= \frac{n \times \frac{4}{3} \pi r^3}{a^3} \\ &= \frac{1 \times \frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} \\ &= 0.52 \end{aligned}$$

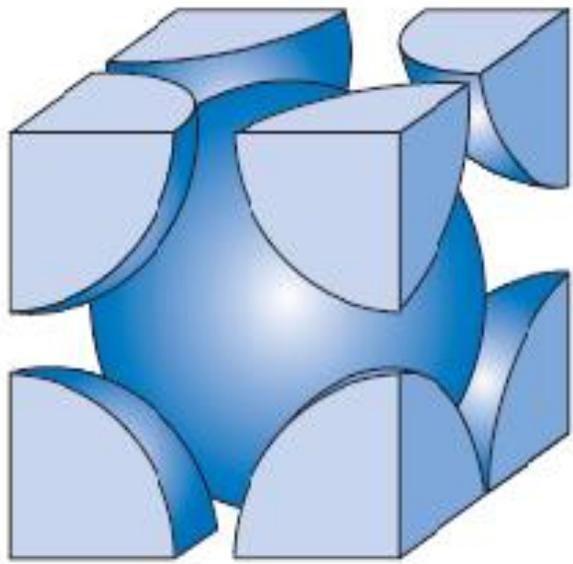


Body centered cubic structure

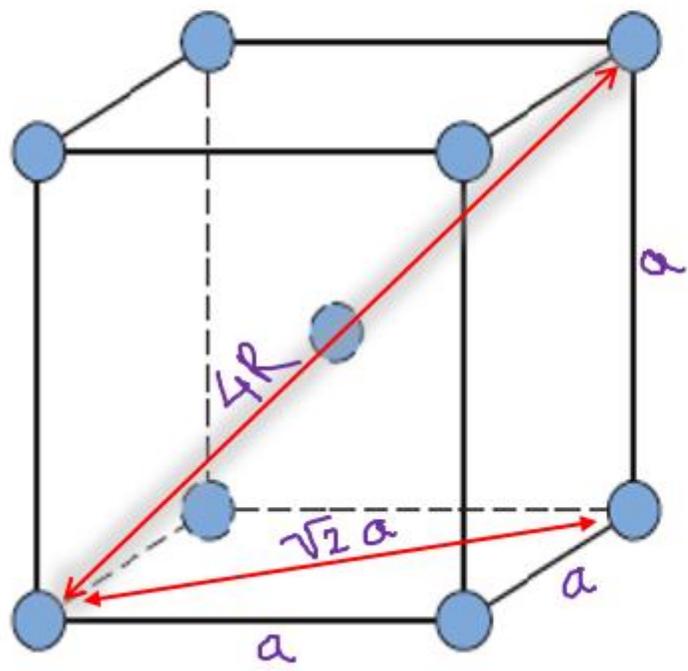
- Atoms located at all eight corners and a single atom at the cube center.
- unit cell length a and atomic radius R are related through
- Chromium, iron, tungsten exhibit a BCC structure.
- Two atoms are associated with each BCC unit cell: the equivalent of one atom from the eight corners, each of which is shared among eight unit cells, and the single center atom, which is wholly contained within its cell.
- The coordination number for the BCC crystal structure is 8.
- Atomic packing factor for BCC is 0.68.

$$a = \frac{4R}{\sqrt{3}}$$

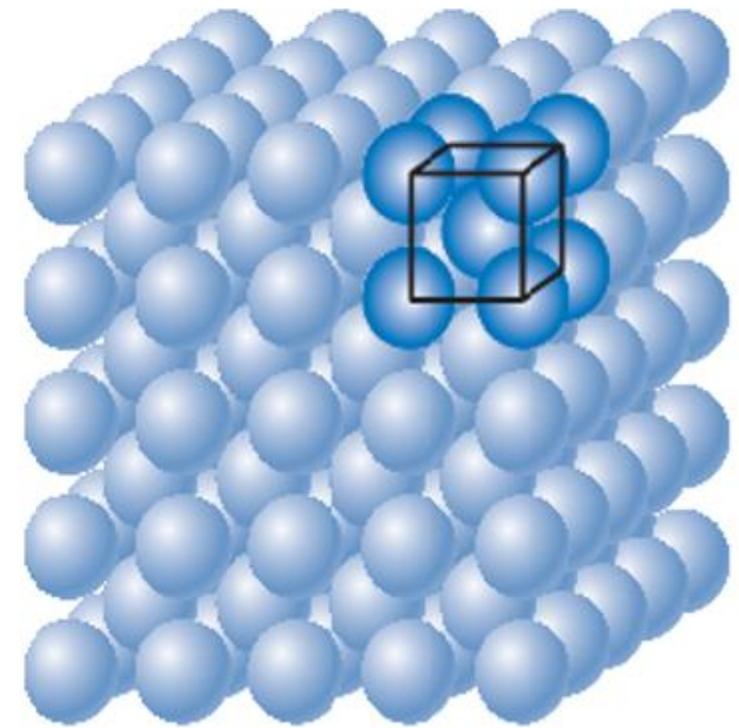
$$(4R)^2 = (\sqrt{2}a)^2 + a^2$$



(a)



(b)



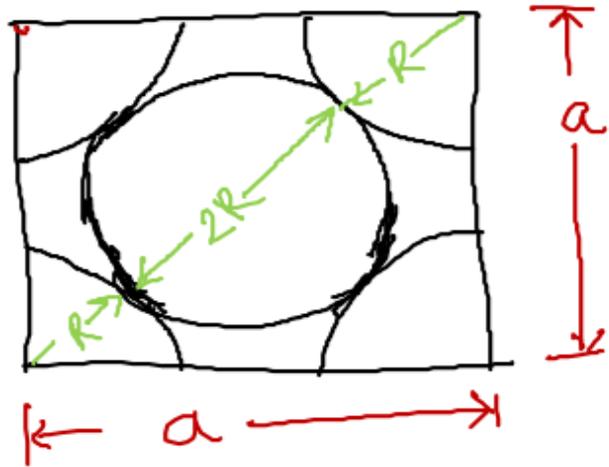
(c)

Figure 3.2 For the body-centered cubic crystal structure, (a) a hard-sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. [Figure

Face centered cubic structure (FCC)

- The crystal structure found for many metals has a unit cell of cubic geometry, with atoms located at each of the corners and the centers of all the cube faces.
- Some of the familiar metals having this crystal structure are copper, aluminum, silver, and gold.
- Coordination number = 12
- Number of atoms within unit cell = 4

- These spheres or ion cores touch one another across a face diagonal; the cube edge length a and the atomic radius R are related through



$$R + 2R + R = \sqrt{a^2 + a^2}$$

$$\Rightarrow 4R = \sqrt{2} a$$

$$\Rightarrow a = 2\sqrt{2} R$$

$$a = 2\sqrt{2} R$$

- Atomic packing factor for FCC is 0.74.

$$APF = \frac{n \times \frac{4}{3} \pi R^3}{a^3} = \frac{4 \times \frac{4}{3} \pi R^3}{(2\sqrt{2} R)^3} = 0.74$$

Hexagonal Close-Packed Crystal Structure (HCP)

- The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the center. Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes.
- The **coordination number** and the **atomic packing factor** for the HCP crystal structure are the same as for FCC: **12** and **0.74**, respectively.
- Total number of atoms within the unit cell is 6.

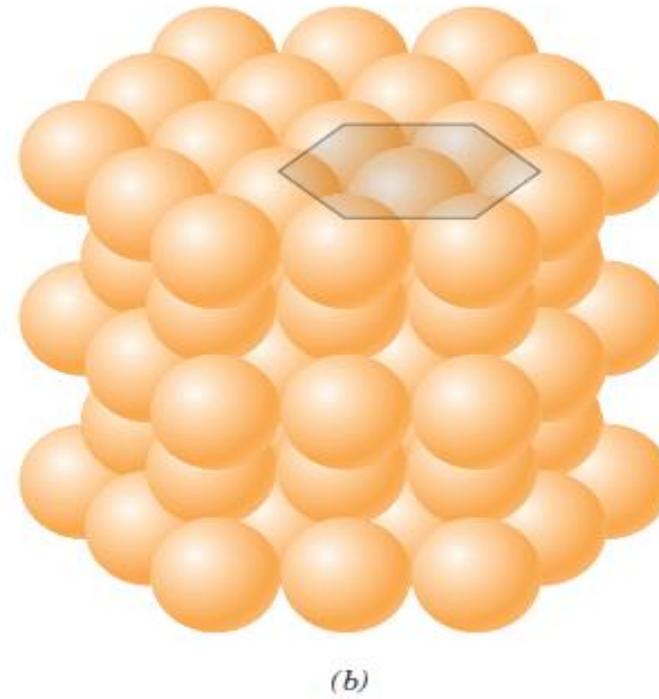
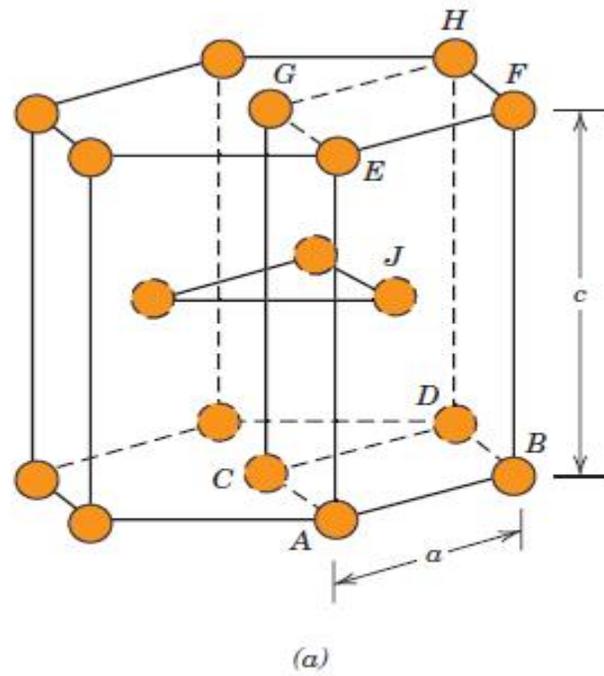
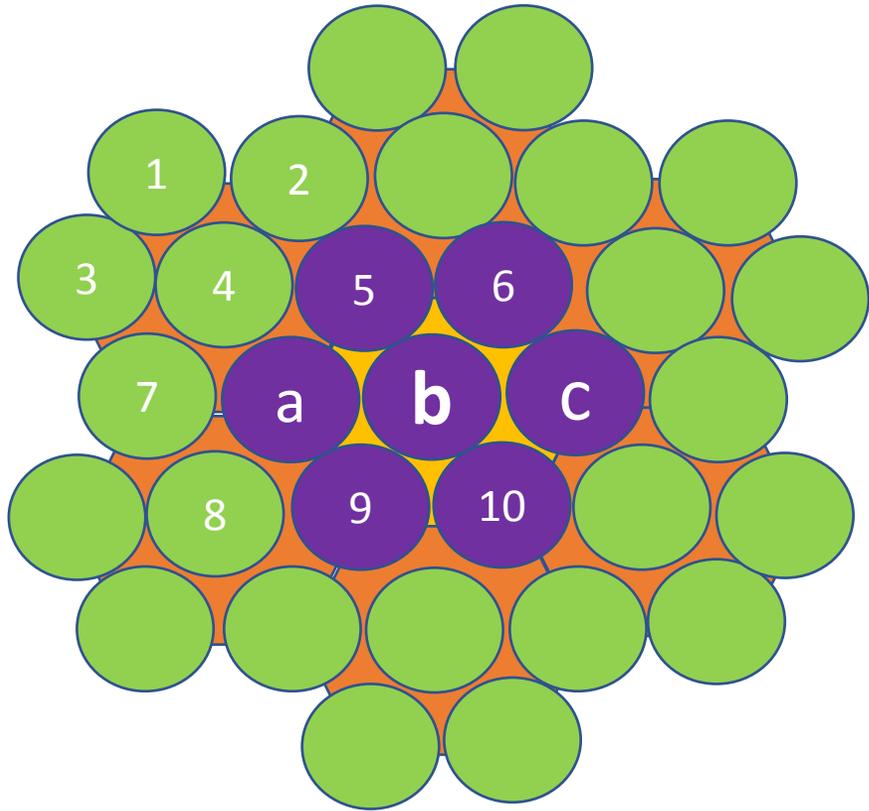


Figure 3.3 For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell (a and c represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms. [Figure (b) from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure*

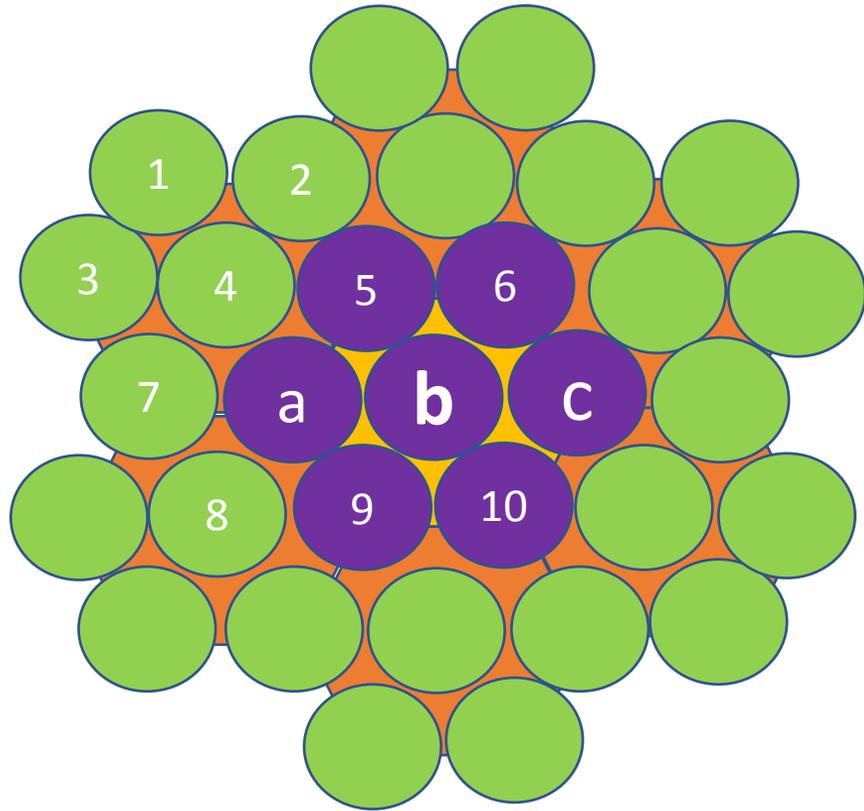


Consider atom 'a' that touches 6 atoms in the plane shown. We can see the arrangement of atoms in this plane. similar planes are also present over and below the plane shown. So think how can atoms arrange themselves to accommodate properly.



In similar way another three atoms touches atom 'a'

So total 12 atoms touches atom 'a' . It is true for any atom in the structure. That is ***coordinator number***

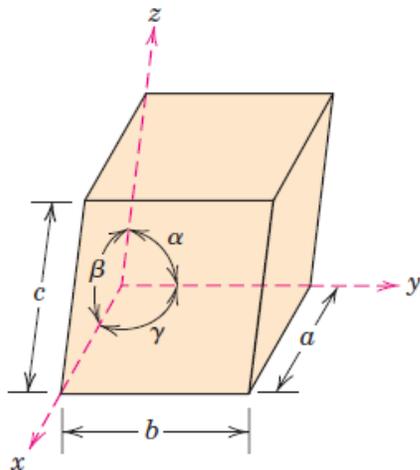


- Hexagonal consists of 3 layers of atoms (see 1st fig) and suppose the layer shown here is the top layer of hexagonal. (in middle layer, 3 atoms present that are within the hexagonal and not shared with other.)
- Consider 3 hexagonal which has centered atom named 4, b and 8.
- 'a' is common in these 3 hexagonal and above this layer there is another layer (hexagonal) ,where 'a' is shared by 3 hexagonal.
- So the corner atom is shared by 6 hexagonal.
- Center atom (b) is shared by 2 hexagonal . That is above the plane shown.

$$\text{atoms/cell} = \underbrace{12 \times \frac{1}{6}}_{\text{corner}} + \underbrace{2 \times \frac{1}{2}}_{\text{face centered}} + \underbrace{3}_{\text{middle layer}} = 6$$

Crystallographic Points, Directions, and Planes

- When dealing with crystalline materials, it often becomes necessary to specify a particular point within a unit cell, a crystallographic direction, or some crystallographic plane of atoms.
- Labeling conventions have been established in which three numbers or indices are used to designate point locations, directions, and planes.
- The basis for determining index values is the unit cell, with a right-handed coordinate system consisting of three (x , y , and z) axes situated at one of the corners and coinciding with the unit cell edges, as shown in Figure .
- For some crystal systems—namely, hexagonal, rhombohedral, monoclinic, and triclinic—the three axes are *not* mutually perpendicular, as in the familiar Cartesian coordinate scheme.



A unit cell with x , y , and z coordinate axes, showing axial lengths (a , b , and c) and interaxial angles (α , β , and γ).

LINEAR AND PLANAR DENSITIES

- Directional equivalency is related to *linear density* in the sense that, for a particular material, equivalent directions have identical linear densities. The corresponding parameter for crystallographic planes is *planar density*, and planes having the same planar density values are also equivalent.
- **Linear density (LD)** is defined as the number of atoms per unit length whose centers lie on the direction vector for a specific crystallographic direction; (1 diameter= 1 atom)
- $LD = \frac{\text{Number of atoms centered on direction vector}}{\text{length of direction vector}}$

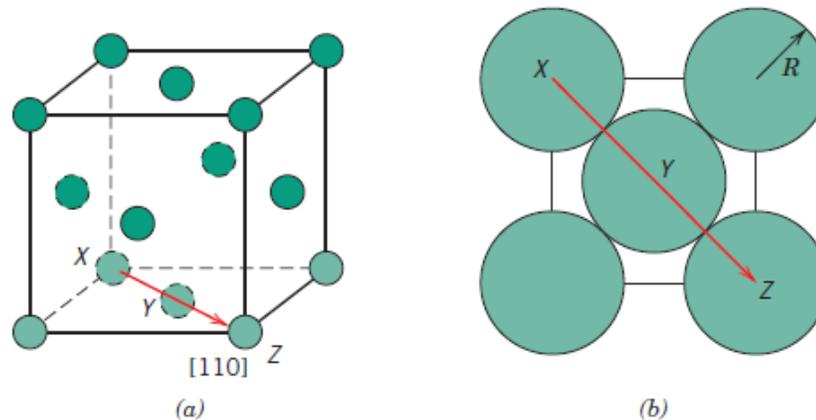


Figure 3.13 (a) Reduced-sphere FCC unit cell with the [110] direction indicated. (b) The bottom face-plane of the FCC unit cell in (a) on which is shown the atomic spacing in the [110] direction, through atoms labeled X, Y, and Z.

- For example, let us determine the linear density of the [110] direction for the FCC crystal structure. An FCC unit cell (reduced sphere) and the [110] direction therein are shown in Figure 3.13*a*. Represented in Figure 3.13*b* are the five atoms that lie on the bottom face of this unit cell; here the [110] direction vector passes from the center of atom *X*, through atom *Y*, and finally to the center of atom *Z*. With regard to the numbers of atoms, it is necessary to take into account the sharing of atoms with adjacent unit cells (as discussed in Section 3.4 relative to atomic packing factor computations). Each of the *X* and *Z* corner atoms is also shared with one other adjacent unit cell along this [110] direction (i.e., one-half of each of these atoms belongs to the unit cell being considered), while atom *Y* lies entirely within the unit cell. Thus, there is an equivalence of two atoms along the [110] direction vector in the unit cell. Now, the direction vector length is equal to $4R$ (Figure 3.13*b*); thus, from Equation 3.8, the [110] linear density for FCC is

$$\text{LD}_{110} = \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

Planar Density (PD)

- planar density (PD) is taken as the number of atoms per unit area that are centered on a particular crystallographic plane. (*1 atom = πr^2*)

$$\text{PD} = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$

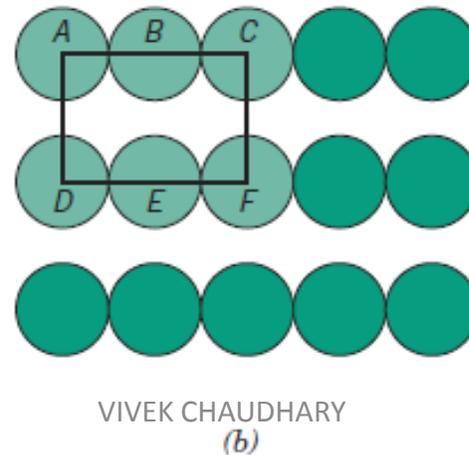
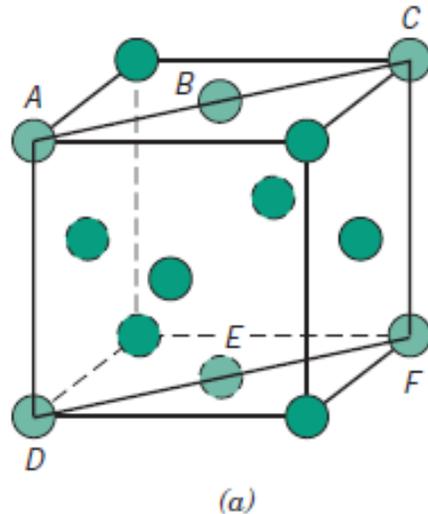


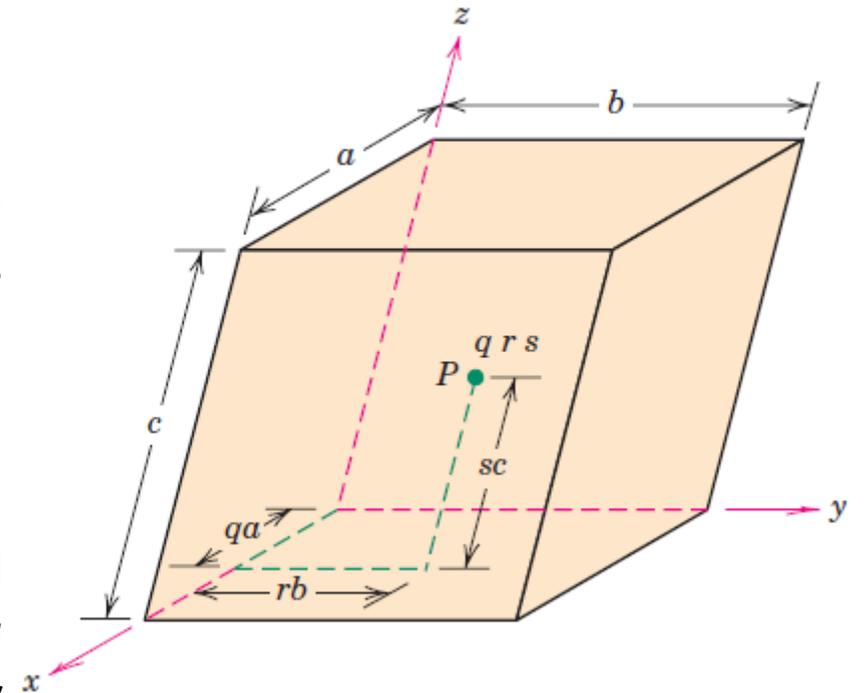
Figure 3.11 (a) Reduced-sphere FCC unit cell with the (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.

- For example, consider the section of a (110) plane within an FCC unit cell as represented in Figures 3.11a and 3.11b. Although six atoms have centers that lie on this plane (Figure 3.11b), only one-quarter of each of atoms *A*, *C*, *D*, and *F*, and one-half of atoms *B* and *E*, for a total equivalence of just 2 atoms, are on that plane. Furthermore, the area of this rectangular section is equal to the product of its length and width. From Figure 3.11b, the length (horizontal dimension) is equal to $4R$, whereas the width (vertical dimension) is equal to $2R\sqrt{2}$, because it corresponds to the FCC unit cell edge length (Equation 3.1). Thus, the area of this planar region is $(4R)(2R\sqrt{2})=8R^2\sqrt{2}$, and the planar density is determined as follows:

$$PD_{110} = \frac{2 \text{ atoms}}{8R^2\sqrt{2}} = \frac{1}{4R^2\sqrt{2}}$$

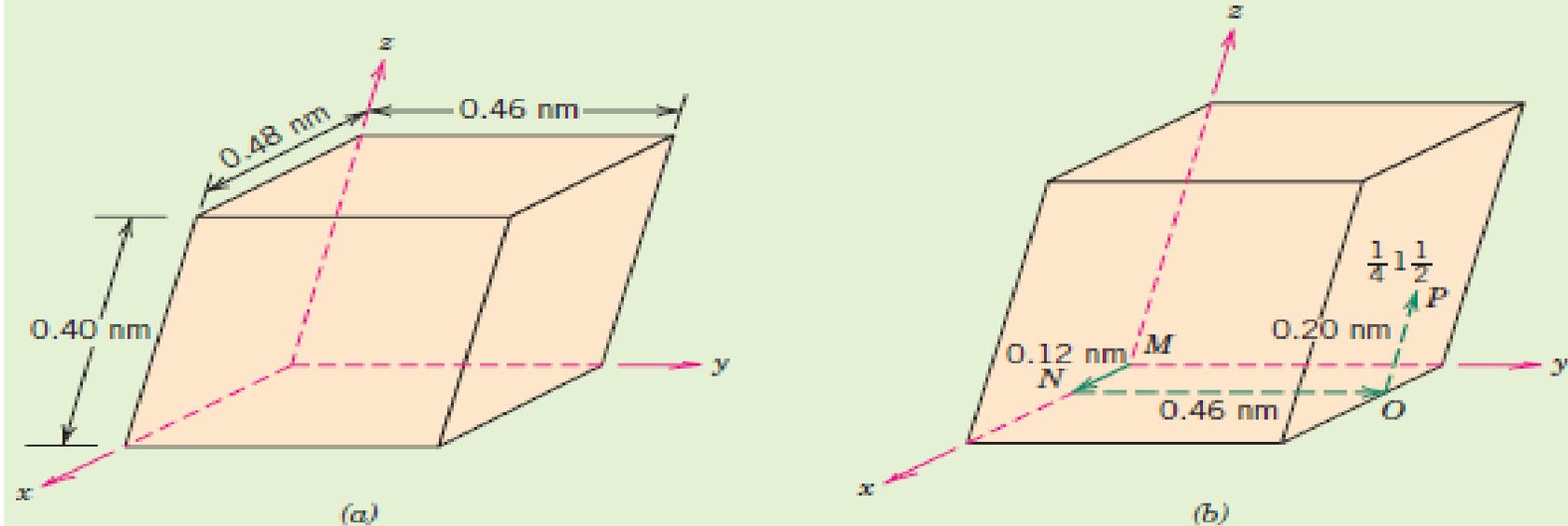
POINT COORDINATES

- The position of any point located within a unit cell may be specified in terms of its coordinates as fractional multiples of the unit cell edge lengths (i.e., in terms of a , b , and c).
- To illustrate, consider the unit cell and the point P situated therein as shown in Figure
- We specify the position of P in terms of the generalized coordinates q , r , and s where q is some fractional length of a along the x axis, r is some fractional length of b along the y axis, and similarly for s . Thus, the position of P is designated using coordinates $q r s$ with values that are less than or equal to unity.
- Furthermore, we have chosen not to separate these coordinates by commas or any other punctuation marks (which is the normal convention).



Location of Point Having Specified Coordinates

For the unit cell shown in the accompanying sketch (a), locate the point having coordinates $\frac{1}{4} 1 \frac{1}{2}$.

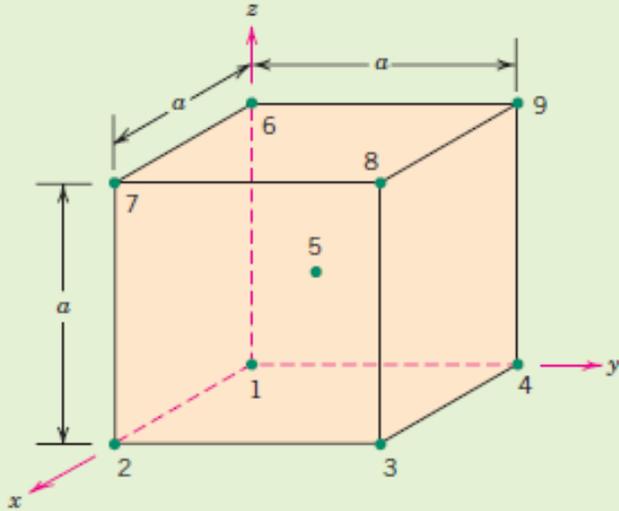


Solution

From sketch (a), edge lengths for this unit cell are as follows: $a = 0.48$ nm, $b = 0.46$ nm, and $c = 0.40$ nm. Furthermore, in light of the preceding discussion, fractional lengths are $q = \frac{1}{4}$, $r = 1$, and $s = \frac{1}{2}$. Therefore, first we move from the origin of the unit cell (point M) $qa = \frac{1}{4}(0.48 \text{ nm}) = 0.12$ nm units along the x axis (to point N), as shown in the (b) sketch. Similarly, we proceed $rb = (1)(0.46 \text{ nm}) = 0.46$ nm parallel to the y axis, from point N to point O . Finally, we move from this position, $sc = \frac{1}{2}(0.40 \text{ nm}) = 0.20$ nm units parallel to the z axis to point P as noted again in sketch (b). This point P then corresponds to the $\frac{1}{4} 1 \frac{1}{2}$ point coordinates.

Example 2

Specify point coordinates for all atom positions for a BCC unit cell.



Point coordinates for position number 1 are 0 0 0; this position is located at the origin of the coordinate system, and, therefore, the fractional unit cell edge lengths along the x , y , and z axes are, respectively, $0a$, $0a$, and $0a$. Furthermore, for position number 2, because it lies one unit cell edge length along the x axis, its fractional edge lengths are a , $0a$, and $0a$, respectively, which yield point coordinates of 1 0 0. The following table presents fractional unit cell lengths along the x , y , and z axes, and their corresponding point coordinates for each of the nine points in the preceding figure.

| Point Number | Fractional Lengths | | | Point Coordinates |
|--------------|--------------------|---------------|---------------|---|
| | x axis | y axis | z axis | |
| 1 | 0 | 0 | 0 | 0 0 0 |
| 2 | 1 | 0 | 0 | 1 0 0 |
| 3 | 1 | 1 | 0 | 1 1 0 |
| 4 | 0 | 1 | 0 | 0 1 0 |
| 5 | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ |
| 6 | 0 | 0 | 1 | 0 0 1 |
| 7 | 1 | 0 | 1 | 1 0 1 |
| 8 | 1 | 1 | 1 | 1 1 1 |
| 9 | 0 | 1 | 1 | 0 1 1 |

CRYSTALLOGRAPHIC DIRECTIONS

A crystallographic direction is defined as a line between two points, or a vector. The following steps are used to determine the three directional indices:

1. A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
2. The length of the vector projection on each of the three axes is determined; *these are measured in terms of the unit cell dimensions a , b , and c .*
3. These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
4. The three indices, not separated by commas, are enclosed in square brackets, thus: $[uvw]$. The u , v , and w integers correspond to the reduced projections along the x , y , and z axes, respectively.

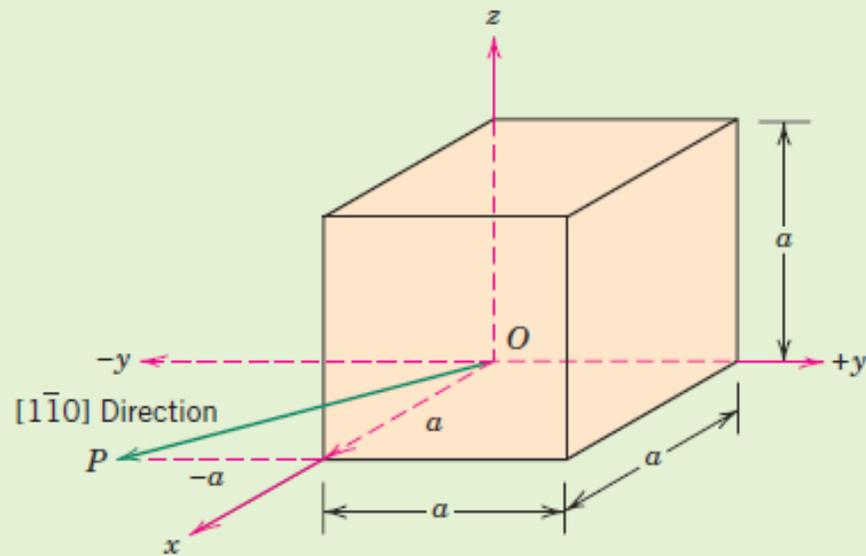
For each of the three axes, there will exist both positive and negative coordinates. Thus negative indices are also possible, which are represented by a bar over the appropriate index.

Example 3

Draw a $[1\bar{1}0]$ direction within a cubic unit cell.

Solution

First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point O , is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this $[1\bar{1}0]$ direction, the projections along the x , y , and z axes are a , $-a$, and $0a$, respectively. This direction is defined by a vector passing from the origin to point P , which is located by first moving along the x axis a units, and from this position, parallel to the y axis $-a$ units, as indicated in the figure. There is no z component to the vector, because the z projection is zero.

Family of crystallographic direction

- For some crystal structures, several nonparallel directions with different indices are crystallographically equivalent; this means that the spacing of atoms along each direction is the same. (having same linear density)
- For example, in cubic crystals, all the directions represented by the following indices are equivalent: $[100]$, $[\bar{1}00]$, $[010]$, $[0\bar{1}0]$, $[001]$, and $[00\bar{1}]$.
- As a convenience, equivalent directions are grouped together into a *family*, which are enclosed in angle brackets, thus: $\langle 100 \rangle$.
- Furthermore, directions in cubic crystals having the same indices without regard to order or sign—for example, $[123]$ and $[\bar{2}1\bar{3}]$ are equivalent.
- This is, in general, not true for other crystal systems. For example, for crystals of tetragonal symmetry, $[100]$ and $[010]$ directions are equivalent, whereas $[100]$ and $[001]$ are not.

CRYSTALLOGRAPHIC PLANES

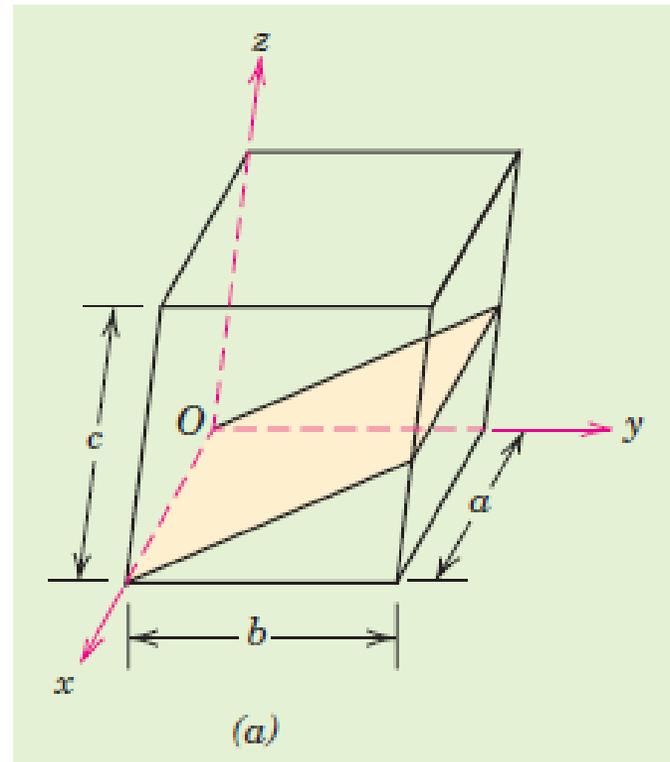
crystallographic planes are specified by three **Miller indices** as (hkl) . Any two planes parallel to each other are equivalent and have identical indices. The procedure used to determine the h , k , and l index numbers is as follows:

1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
2. At this point the crystallographic plane either intersects or parallels each of the three axes; the length of the planar intercept for each axis is determined in terms of the lattice parameters a , b , and c .
3. The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, and, therefore, a zero index.
4. If necessary, these three numbers are changed to the set of smallest integers by multiplication or division by a common factor.
5. Finally, the integer indices, not separated by commas, are enclosed within parentheses, thus: (hkl) .

An intercept on the negative side of the origin is indicated by a bar or minus sign positioned over the appropriate index. Furthermore, reversing the directions of all indices specifies another plane parallel to, on the opposite side of, and equidistant from the origin.

Example 3

- Determine the Miller indices for the plane shown in the accompanying sketch (a).

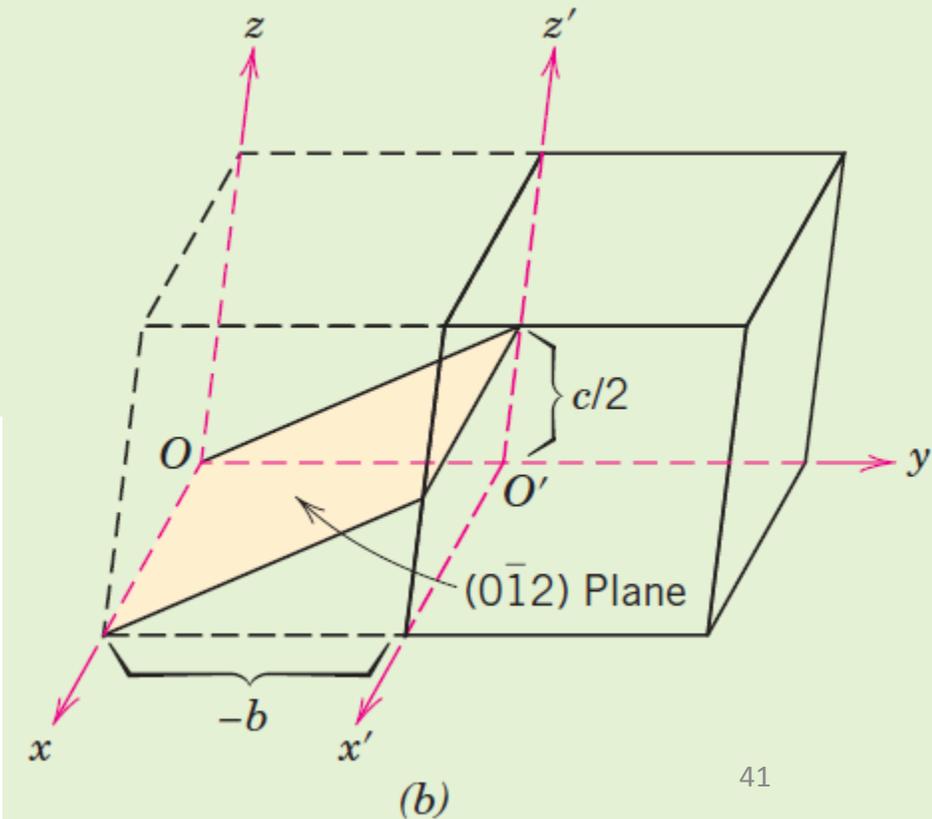


Solution

Because the plane passes through the selected origin O , a new origin must be chosen at the corner of an adjacent unit cell, taken as O' and shown in sketch (b). This plane is parallel to the x axis, and the intercept may be taken as ∞a . The y and z axes' intersections, referenced to the new origin O' , are $-b$ and $c/2$, respectively. Thus, in terms of the lattice parameters a , b , and c , these intersections are ∞ , -1 , and $\frac{1}{2}$. The reciprocals of these numbers are 0 , -1 , and 2 ; because all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields $(0\bar{1}2)$.

These steps are briefly summarized here:

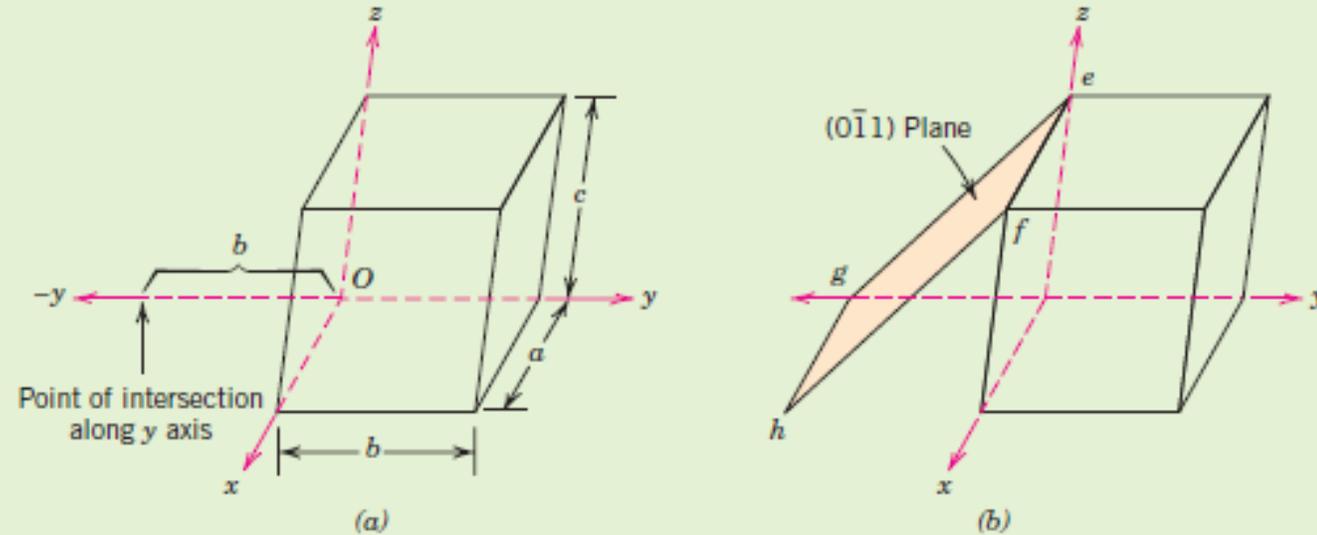
| | x | y | z |
|---|------------|------|---------------|
| Intercepts | ∞a | $-b$ | $c/2$ |
| Intercepts (in terms of lattice parameters) | ∞ | -1 | $\frac{1}{2}$ |
| Reciprocals | 0 | -1 | 2 |
| Reductions (unnecessary) | | | |
| Enclosure | | | $(0\bar{1}2)$ |



Example 4

Construction of Specified Crystallographic Plane

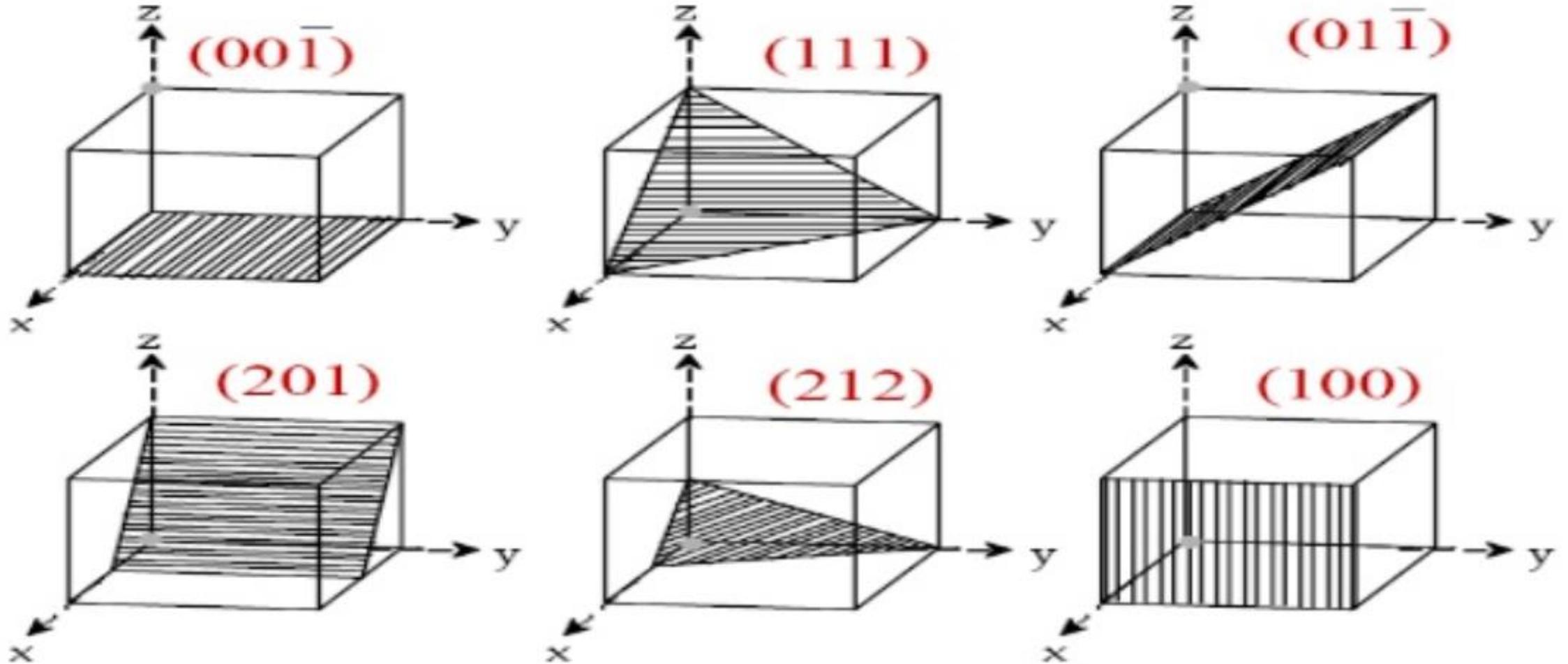
Construct a $(0\bar{1}1)$ plane within a cubic unit cell.



Solution

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin, the indices are removed from the parentheses, and reciprocals are taken, which yields ∞ , -1 , and 1 . This means that the particular plane parallels the x axis while intersecting the y and z axes at $-b$ and c , respectively, as indicated in the accompanying sketch (a). This plane has been drawn in sketch (b). A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions. For example, in this figure, line ef is the intersection between the $(0\bar{1}1)$ plane and the top face of the unit cell; also, line gh represents the intersection between this same $(0\bar{1}1)$ plane and the plane of the bottom unit cell face extended. Similarly, lines eg and fh are the intersections between $(0\bar{1}1)$ and back and front cell faces, respectively.

Some planes are shown in a cubic unit cell



Reference: <http://www.examhill.com/miller-indices/>

Imperfection in solid

- Any crystal with perfectly regular crystal structure is called ideal crystal while real crystals always have certain **defects or imperfections**.
- Many of the properties of materials are profoundly sensitive to deviations from crystalline perfection; the influence is not always adverse, and often specific characteristics are deliberately fashioned by the introduction of controlled amounts or numbers of particular defects.
- *Crystalline defect* refers to a lattice irregularity having one or more of its dimensions on the order of an atomic diameter.

| S No. | Imperfection type | Size of defect | Sub type |
|-------|--|--|--|
| 1 | Point defects | Zero dimensional defect (interatomic space) | <ol style="list-style-type: none"> 1. Vacancy 2. Substitutional impurity 3. Interstitial impurity Frenkel's defect Schottky's defect |
| 2 | Line defect | One dimensional defect | <ol style="list-style-type: none"> 1. Edge dislocation 2. Screw dislocation 3. Mixed dislocation |
| 3 | Surface imperfection (interfacial defect) | Two dimensional defect | <ol style="list-style-type: none"> 1. External surface 2. Grain boundary 3. Twinning 4. Low angle boundary 5. High angle boundary 6. Twist boundary 7. Stacking fault |
| 4 | Volume defect | Three dimensional defect | <ol style="list-style-type: none"> 1. pores 2. Foreign particle inclusion 3. Non compatibility region 4. Dissimilar natured regions |

Vacancy defect

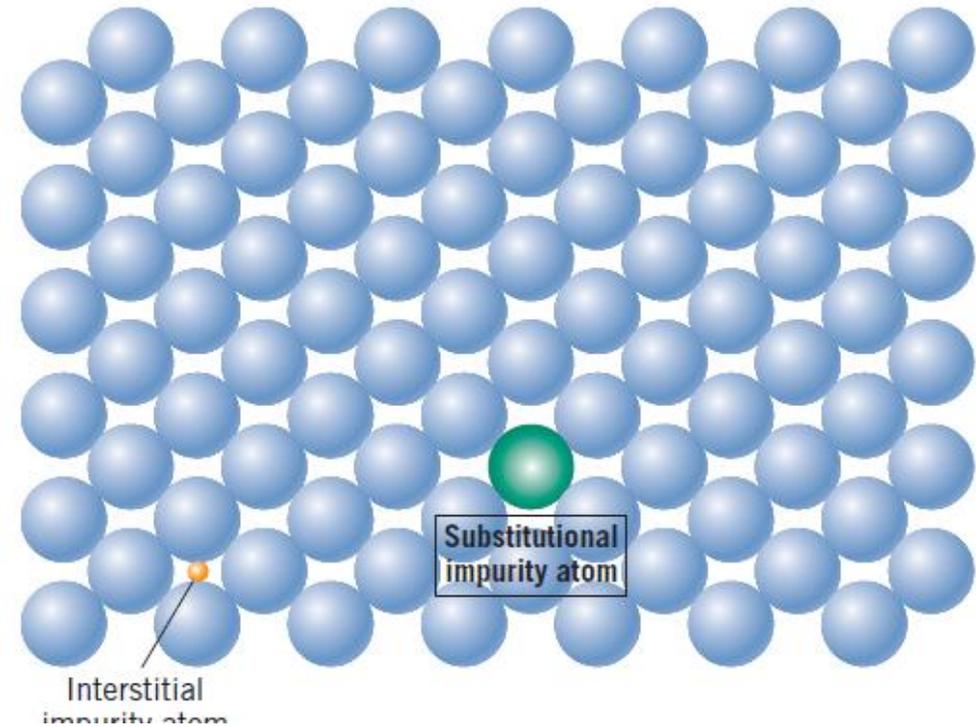
- In crystallography , a vacancy is a point defect in a crystal where a atom is missing from one of the lattice site.
- Vacancy defects are lattice sites which would be occupied in a perfect crystal, but are vacant. If a neighboring atom moves to occupy the vacant site, the vacancy moves in the opposite direction to the site which used to be occupied by the moving atom.
- The stability of the surrounding crystal structure guarantees that the neighboring atoms will not simply collapse around the vacancy. In some materials, neighboring atoms actually move away from a vacancy, because they experience attraction from atoms in the surroundings. A vacancy (or pair of vacancies in an ionic solid) is sometimes called a [Schottky defect](#).

Interstitial defect

- Interstitial defect are atoms that occupy a site in the crystal structure at which there is usually not an atom.
- They are generally high energy configurations. Small atoms (mostly impurities) in some crystals can occupy interstices without high energy, such as hydrogen in palladium.
- The interstitial atom has more chances to be lodge with in a crystal structure has low atomic packing factor.
- It produces atomic distortion.
- A nearby pair of a vacancy and an interstitial is often called a [Frenkel defect](#) or Frenkel pair. This is caused when an ion moves into an interstitial site and creates a vacancy.

Substitutional defects

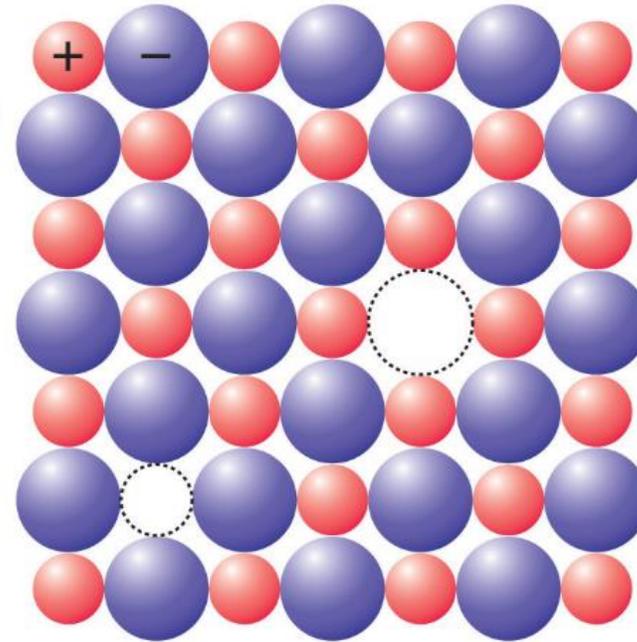
- When a foreign atom replaces the parent atom at the lattice site in the crystal
- Foreign atom is called solute and parent atoms are solvent.



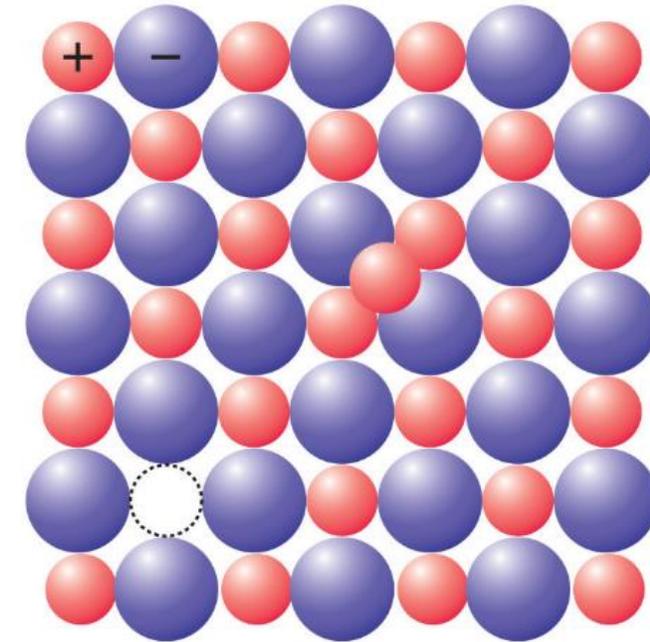
Schottky Defect vs Frenkel Defect

Schottky Defect

1. Equal number of cations and anions are missing from the lattice sites.
2. Found in highly ionic compounds with high coordination numbers and where the cations and anions are of similar size.
3. Density of the solid decreases



(a) Schottky defect



(b) Frenkel defect

Reference: <https://www.majordifferences.com/2013/02/difference-between-schottky-defect-and.html#.Xxhc8FUzblU>

Frenkel Defect

1. A cation leaves the normal lattice site and occupies an interstitial site.
2. Found in ionic compounds with low coordination numbers and where the anions are much larger in size than cations.
3. Density of the solid remains the same.

EDGE DISLOCATION

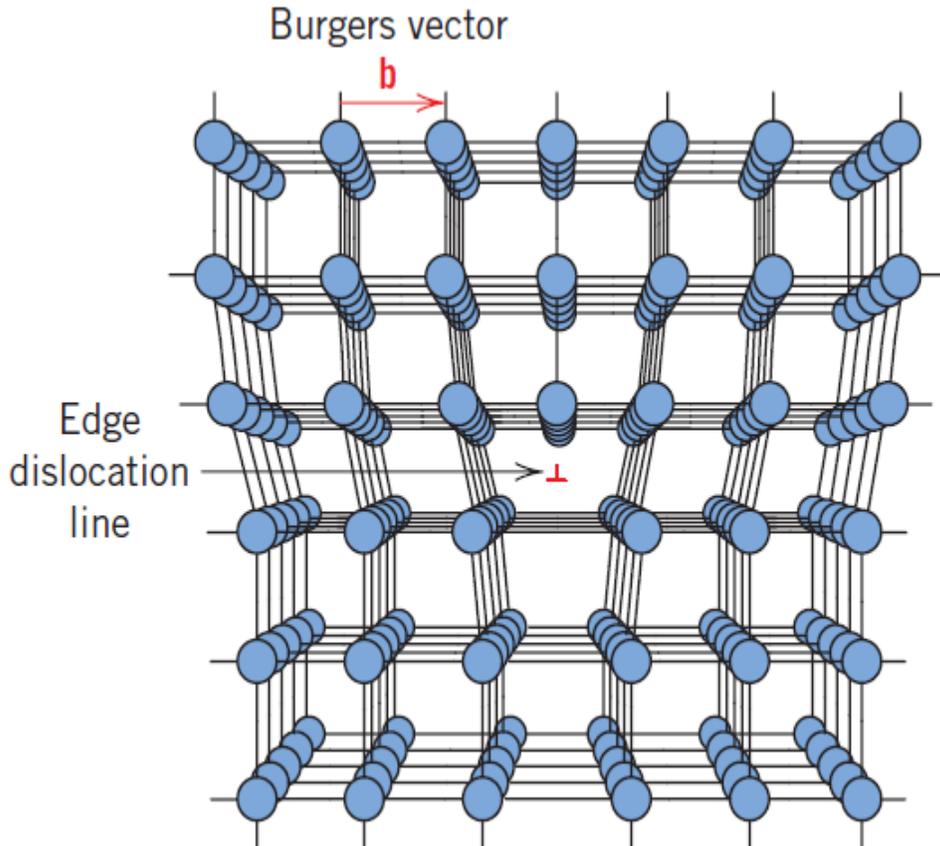
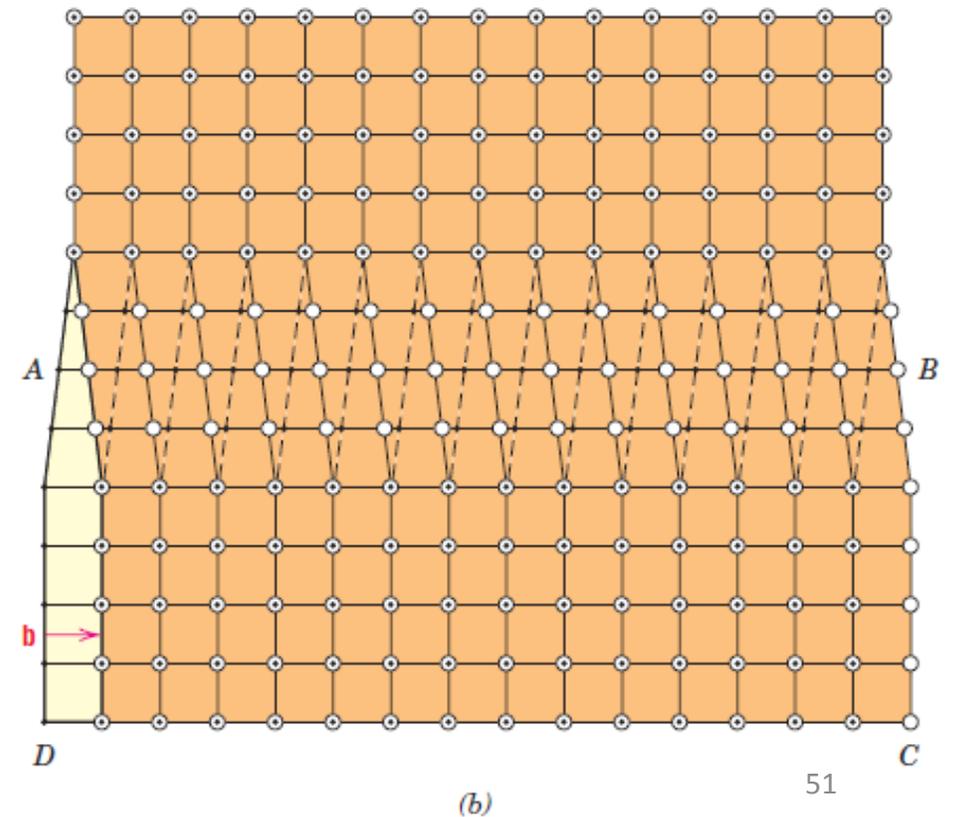
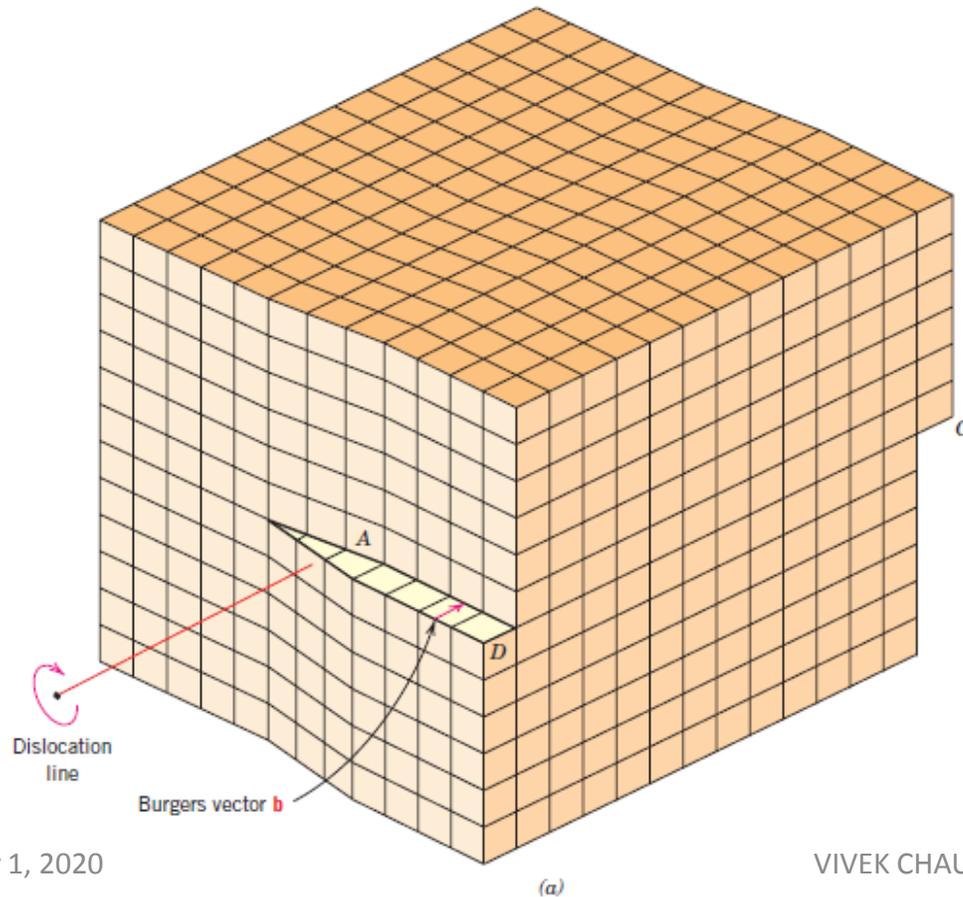


FIGURE 4.3

- It is a linear defect that centers on the line that is defined along the end of the extra half-plane of atoms. This is sometimes termed the **dislocation line**, which, for the edge dislocation in Figure 4.3 is perpendicular to the plane of the page.
- Within the region around the dislocation line there is some localized lattice distortion. The atoms above the dislocation line are squeezed together, and those below are pulled apart.
- This is reflected in the slight curvature for the vertical planes of atoms as they bend around this extra half-plane. The magnitude of this distortion decreases with distance away from the dislocation line; at positions far removed, the crystal lattice is virtually perfect.
- Symbol of edge dislocation line is shown in figure 4.3.

SCREW DISLOCATION

Figure 4.4 (a) A screw dislocation within a crystal. (b) The screw dislocation in (a) as viewed from above. The dislocation line extends along line AB . Atom positions above the slip plane are designated by open circles, those below by solid circles. [Figure (b) from W. T. Read, Jr., *Dislocations in Crystals*, McGraw-Hill Book Company, New York, 1953.]

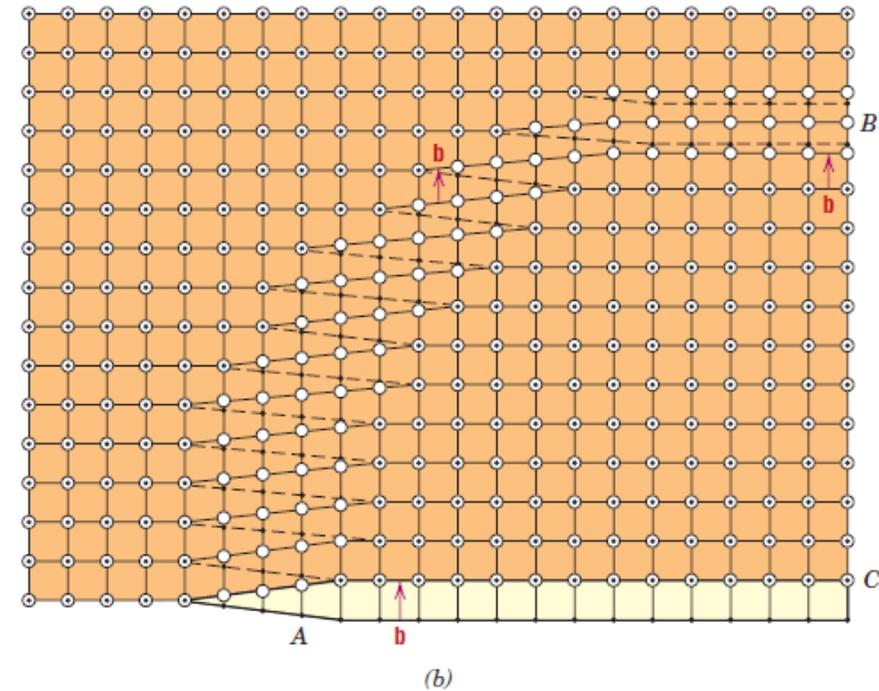
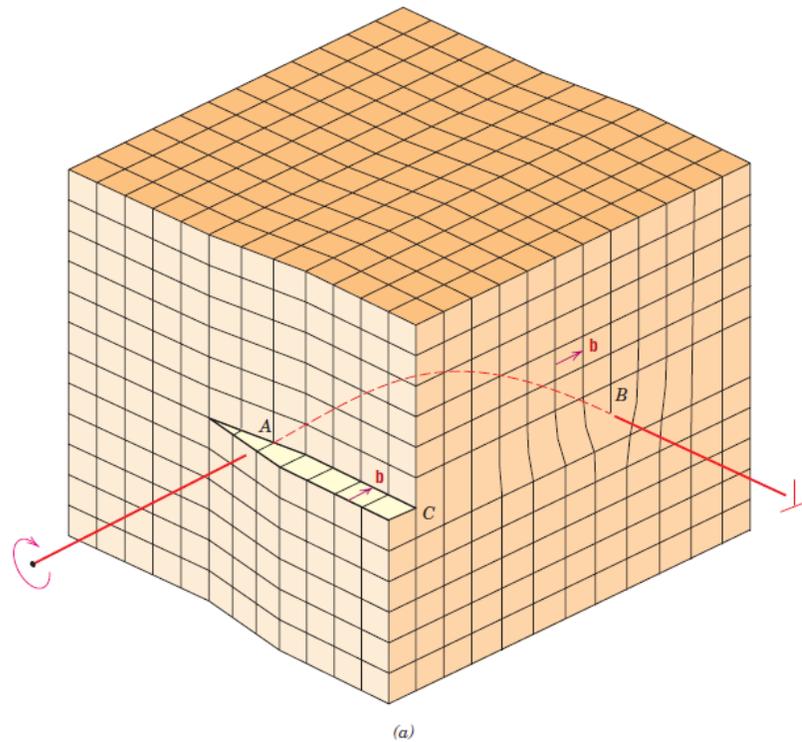




- Another type of dislocation, called a **screw dislocation**, may be thought of as being formed by a shear stress that is applied to produce the distortion shown in Figure 4.4*a*: the upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion. The atomic distortion associated with a screw dislocation is also linear and along a dislocation line, line *AB* in Figure 4.4*b*.
- The screw dislocation derives its name from the spiral or helical path or ramp that is traced around the dislocation line by the atomic planes of atoms. Sometimes the symbol \curvearrowright is used to designate a screw dislocation.

MIXED DISLOCATION

Figure 4.5 (a) Schematic representation of a dislocation that has edge, screw, and mixed character. (b) Top view, where open circles denote atom positions above the slip plane, and solid circles, atom positions below. At point *A*, the dislocation is pure screw, while at point *B*, it is pure edge. For regions in between where there is curvature in the dislocation line, the character is mixed edge and screw. [Figure (b) from W. T. Read, Jr., *Dislocations in Crystals*, McGraw-Hill Book Company, New York, 1953.]



MIXED DISLOCATION

- Most dislocations found in crystalline materials are probably neither pure edge nor pure screw, but exhibit components of both types; these are termed **mixed dislocations**.
- All three dislocation types are represented schematically in Figure 4.5; the lattice distortion that is produced away from the two faces is mixed, having varying degrees of screw and edge character.

*The magnitude and direction of the lattice distortion associated with a dislocation is expressed in terms of a **Burgers vector**, denoted by a ***b***. Burgers vectors are indicated in Figures 4.3 and 4.4 for edge and screw dislocations, respectively.*



INTERFACIAL DEFECTS

- Interfacial defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations. These imperfections include external surfaces, grain boundaries, phase boundaries, twin boundaries, and stacking faults.

External Surfaces

- One of the most obvious boundaries is the external surface, along which the crystal structure terminates.
- Surface atoms are not bonded to the maximum number of nearest neighbors, and are therefore in a higher energy state than the atoms at interior positions.
- To reduce this energy, materials tend to minimize, if at all possible, the total surface area. For example, liquids assume a shape having a minimum area—the droplets become spherical.

Grain Boundaries

- Another interfacial defect, the grain boundary is the boundary *separating* two small grains or crystals having *different crystallographic orientations* in polycrystalline materials.
- When this orientation mismatch is slight, on the order of a few degrees, then the term *small- (or low-) angle grain boundary* is used. (figure 4.7 in next slide)
- One simple small-angle grain boundary is formed when edge dislocations are aligned in the manner of Figure 4.8(in next slide). This type is called a *tilt boundary*; the angle of misorientation, is also indicated in the figure.
- There is an interfacial or grain boundary energy like the surface energy.
- The magnitude of this energy is a function of the degree of misorientation, being larger for high-angle boundaries.
- Grain boundaries are more chemically reactive than the grains themselves as a consequence of this boundary energy.
- Impurity atoms often preferentially segregate along these boundaries because of their higher energy state

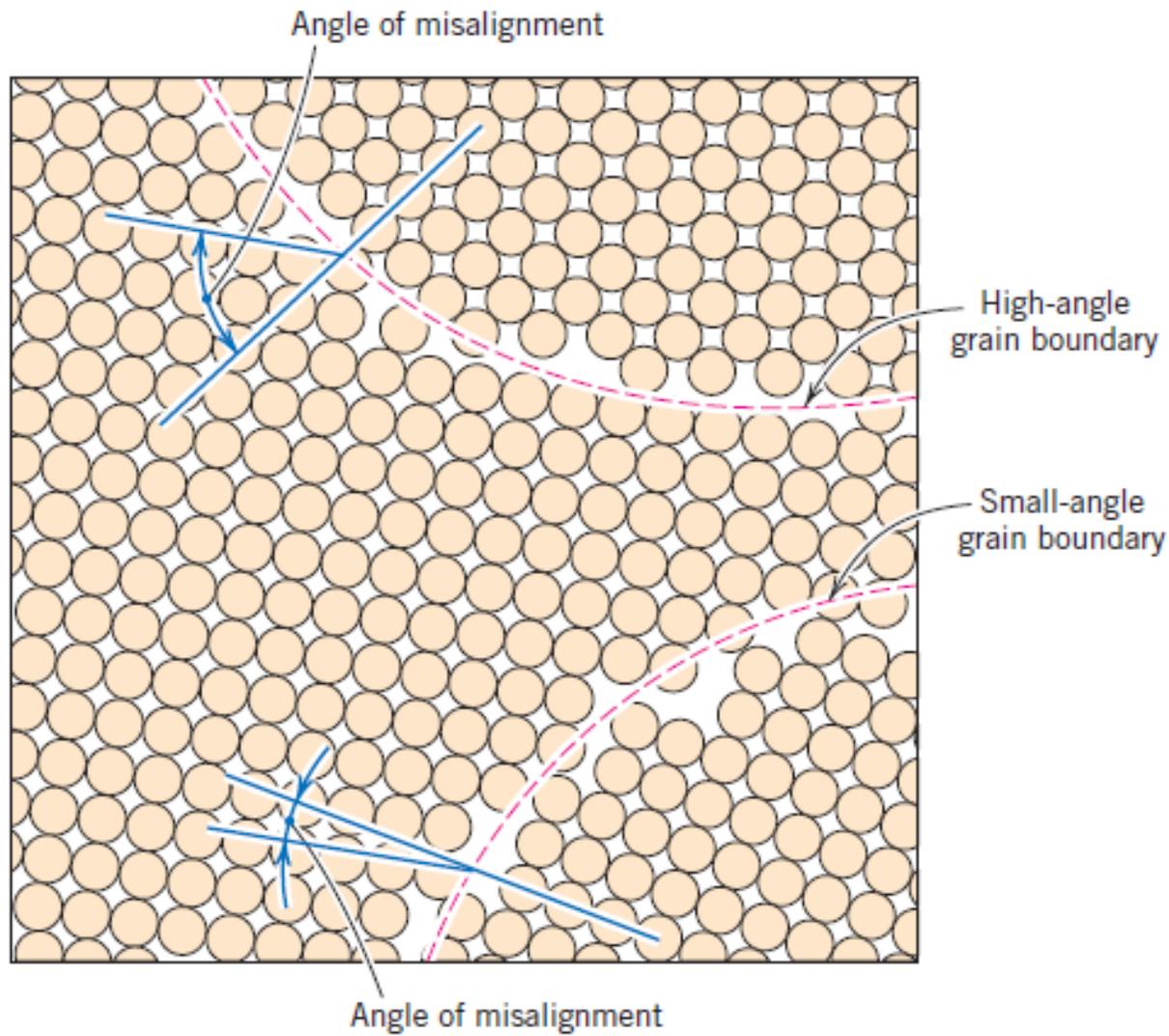


Figure 4.7

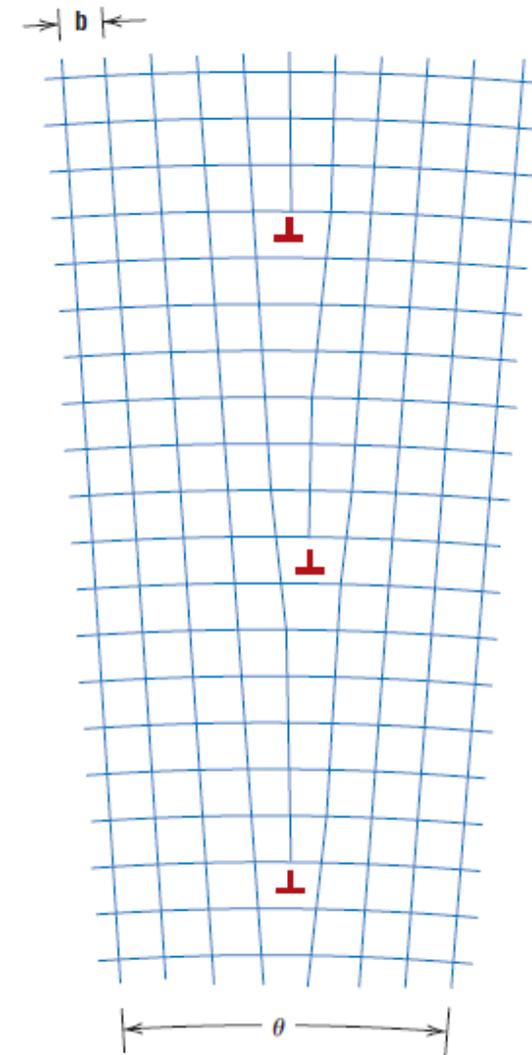
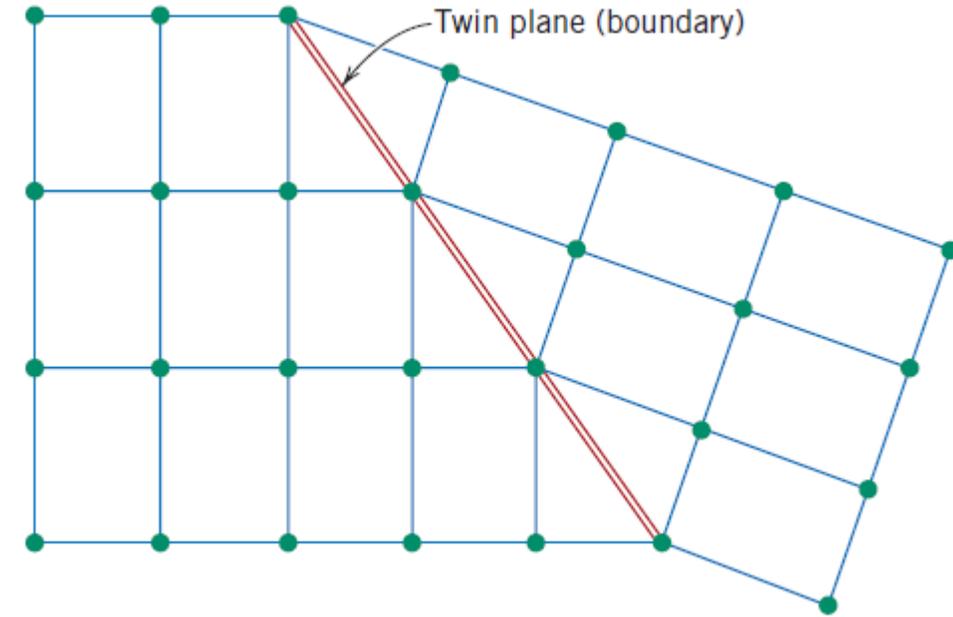


Figure 4.8

Twin Boundaries

- A *twin boundary* is a special type of grain boundary across which there is a specific mirror lattice symmetry; that is, atoms on one side of the boundary are located in *mirror-image positions* of the atoms on the other side.
- Twins result from atomic displacements that are produced from applied mechanical shear forces (mechanical twins), and also during annealing heat treatments following deformation (annealing twins).
- Annealing twins are typically found in metals that have the FCC crystal structure, whereas mechanical twins are observed in BCC and HCP metals.



Thank you

