

7 Crystal Systems:

14 Bravais Lattices:

Additional Information:

See: Chapter 3
Materials Science and Engineering – An Introduction, William D. Callister, Jr. 6th Ed or 7th Ed (Wiley, 2003)

Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry	
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$		3
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$		1
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$		2
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$		1 (trigonal)
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$		4
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$		2
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$		1
				14 total

Materials Science and Engineering – An Introduction, William D. Callister, Jr. 6th Ed (Wiley, 2003)

Unit Cells of the Bravais Lattices:

One of these has a mistake. Which one?

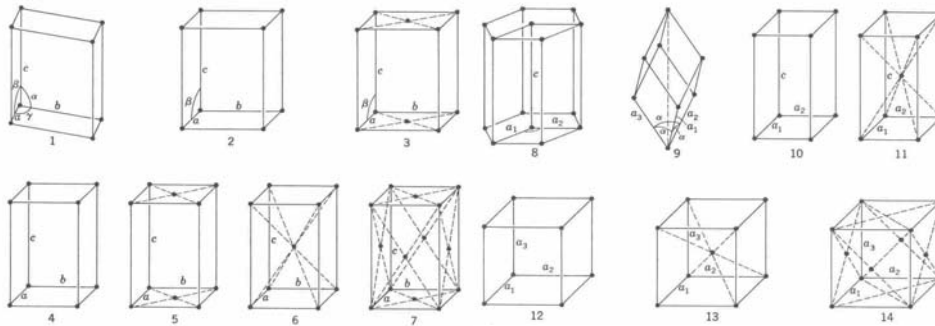


Fig. 1-3 The 14 space lattices illustrated by a unit cell of each: (1) triclinic, simple, (2) monoclinic, simple, (3) monoclinic, base-centered, (4) orthorhombic, simple, (5) orthorhombic, base-centered, (6) orthorhombic, body-centered, (7) orthorhombic, face-centered, (8) hexagonal, (9) rhombohedral, (10) tetragonal, simple, (11) tetragonal, body-centered, (12) cubic, simple, (13) cubic, body-centered, (14) cubic, face-centered.

Fundamentals of Crystallography

- ❑ Crystal Structure is described by: Bravais lattice + basis (atoms decorating lattice point)
 - ✓ Also called: Space lattice + Motif
- ❑ Examples of Crystal Structures: *Diamond Cubic Lattice & Zinc Blende*

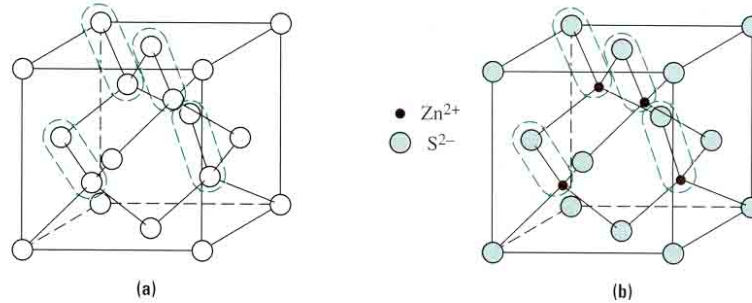


FIGURE 3.7-4 (a) The diamond cubic crystal structure is composed of an FCC lattice with two atoms per lattice point. One atom from each pair is centered on each lattice point, and the second atom is positioned at $(a_0\sqrt{3}/4)[1\ 1\ \bar{1}]$. (b) The zinc blende crystal structure is similar to the diamond cubic structure, except that the basis is composed of two different atoms.

Examples of: a) Si & Ge; b) ZnS, ZnSe, GaAs

Fundamentals of Crystallography

- ❑ Unit Cells of the Bravais Lattices:
 - ✓ *Unit Cells* are an array of lattice points in a specific *Bravais lattice* that, when periodically repeated, forms the entire lattice.
 - ✓ There are two types of *unit cells*:
 - o *Conventional unit cell*
 - Most geometrically convenient
 - 1 or more *lattice points* per unit cell
 - o *Primitive unit cell*
 - Smallest unit cell possible
 - Only one *lattice point*

□ Examples of *Primitive Unit Cells*:

- ✓ FCC & BCC

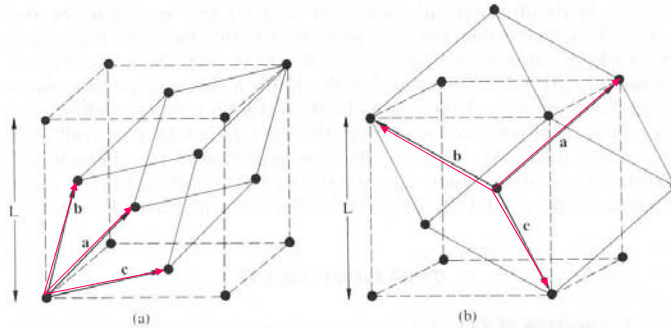


Figure 1-15 (a) The face-centered-cubic lattice, and (b) the body-centered-cubic lattice. Each part of the figure shows the conventional unit cube as dashed lines, with one possible rhombohedral form for the primitive unit cell as solid lines. If \hat{x} , \hat{y} , and \hat{z} are unit vectors along three mutually perpendicular axes, then the F.C.C. primitive cell is generated by the vectors $a = \frac{1}{2}L(\hat{x} + \hat{y})$, $b = \frac{1}{2}L(\hat{y} + \hat{z})$, $c = \frac{1}{2}L(\hat{z} + \hat{x})$. These vectors, all of length $(L/\sqrt{2})$, make 60° angles with each other. For the B.C.C. primitive cell in part (b) of the figure, the generating vectors are $a = \frac{1}{2}L(\hat{x} + \hat{y} - \hat{z})$, $b = \frac{1}{2}L(\hat{y} + \hat{z} - \hat{x})$, $c = \frac{1}{2}L(\hat{z} + \hat{x} - \hat{y})$. These vectors, all of length $(L\sqrt{3}/2)$, make 109° angles with each other.

Blakemore, Solid State Physics 2nd Ed (Cambridge, 1985)

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□ **PEROVSKITES** - Example of:

- ✓ Primitive Unit Cell
- ✓ Crystal Structure = Bravais Lattices/space lattice + Basis

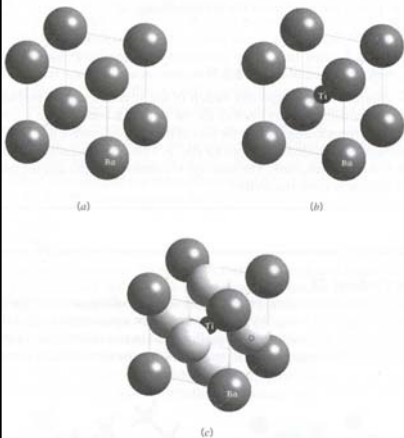


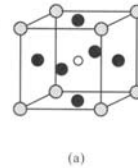
Figure EPI0 High-temperature cubic form of barium titanate, $BaTiO_3$: (a) primitive cubic cell, with Ba^{2+} ions inserted in sites $1a$; (b) Ti^{4+} ions added in site $1b$. (c) Perovskite structure is obtained after adding O^{2-} ions in sites $3c$.

Allen & Thomas, The Structure of Materials, (Wiley, 1999)

Information

Formula: $M'M''X_3$
Bravais Lattice: *simple cubic*
Basis: 5 ions ($1Ba^{2+}$, $1Ti^{4+}$, $3O^{2-}$)
Atoms per Unit Cell: 5

- Ti^{4+} : at the body center
- Ca^{2+} : at corners
- O^{2-} : at face centers



Structure: perovskite ($CaTiO_3$)-type
Bravais lattice: simple cubic
Ions/unit cell: $1Ca^{2+} + 1Ti^{4+} + 3O^{2-}$
Typical ceramics: $CaTiO_3$, $BaTiO_3$

Figure 3-14 Perovskite ($CaTiO_3$) unit cell showing (a) ion positions and (b) full-size ions. (Part (b) courtesy of Molecular Simulations, Inc.)

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Shackelford, Intro to Materials Science for Engineers, 5th Ed. (Prentice Hall, 2002)

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Fundamentals of Crystallography

Crystallographic Directions: a crystallographic direction is defined as a line between 2 pts, or a vector. The following steps are utilized in the determination of the 3 directional indices:

- ✓ 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.
- ✓ The length of the vector projection on each of the 3 axes is determined; *these are measured in terms of the unit cell dimensions a , b , and c .*
- ✓ These 3 numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
- ✓ The 3 indices (not separated by commas) are enclosed in square brackets:
 - o $[uvw]$ where u , v , and w integers correspond to the reduced projection along the x , y , and z axes, respectively.

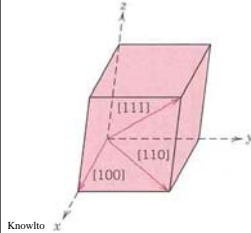


FIGURE 3.5 The $[100]$, $[110]$, and $[111]$ directions within a unit cell.

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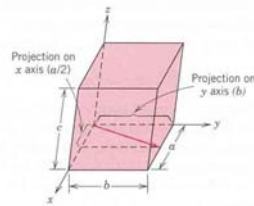
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Fundamentals of Crystallography

Crystallographic Directions: an Example

EXAMPLE PROBLEM 3.4

Determine the indices for the direction shown in the accompanying figure.



SOLUTION

The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary. Projections of this vector onto the x , y , and z axes are, respectively, $a/2$, b , and $0c$, which become $\frac{1}{2}$, 1 , and 0 in terms of the unit cell parameters (i.e., when the a , b , and c are dropped). Reduction of these numbers to the lowest set of integers is accompanied by multiplication of each by the factor 2. This yields the integers 1, 2, and 0, which are then enclosed in brackets as $[120]$.

This procedure may be summarized as follows:

	x	y	z
Projections	$a/2$	b	$0c$
Projections (in terms of a , b , and c)	$\frac{1}{2}$	1	0
Reduction	1	2	0
Enclosure	$[120]$		

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Fundamentals of Crystallography

❑ **Crystallographic Directions:** *an Example*

- ✓ What directions are the bonds in Si & Zinc Blende materials?

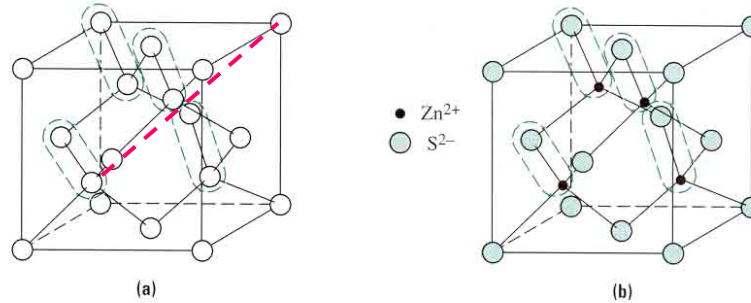


FIGURE 3.7-4 (a) The diamond cubic crystal structure is composed of an FCC lattice with two atoms per lattice point. One atom from each pair is centered on each lattice point, and the second atom is positioned at $(a_0\sqrt{3}/4)[1\ 1\ \bar{1}]$. (b) The zinc blende crystal structure is similar to the diamond cubic structure, except that the basis is composed of two different atoms.

Examples of: a) Si & Ge; b) ZnS, ZnSe, GaAs

Fundamentals of Crystallography

❑ **Crystallographic Planes:** a crystallographic planes in all but the hexagonal crystal system are specified by 3 *Miller indices*: (hkl) . Any 2 planes parallel to each other are equivalent & have identical indices. The procedure used in determination of the h , k , and l Miller index numbers is as follows:

- ✓ 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.
- ✓ At this point, the crystallographic plane either intersects or parallels each of the 3 axes; the length of the planar intercept for each axis is determined in terms of the lattice constants a , b , and c .
- ✓ The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, &, therefore, a zero index.
- ✓ If necessary, these 3 numbers are changed to the set of smallest integers by multiplication or division by a common factor.
- ✓ Finally, the integer indices (not separated by commas) are enclosed in parentheses: (hkl) .

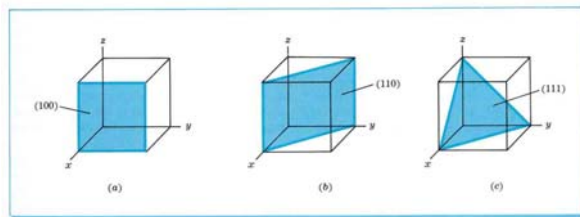
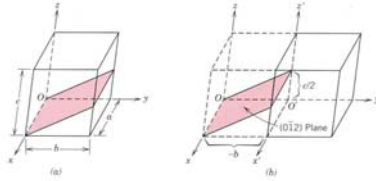


FIGURE 3.13 Miller indices of some important cubic crystal planes: (a) (100), (b) (110), and (c) (111).

Crystallographic Planes: Several Examples

EXAMPLE PROBLEM 3.6

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



SOLUTION

Since 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 ; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields $(0\bar{1}2)$.

These steps are briefly summarized below:

	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			$(0\bar{1}2)$

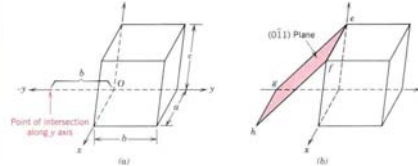
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EXAMPLE PROBLEM 3.7

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.

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Crystallographic Planes: Equivalent planes

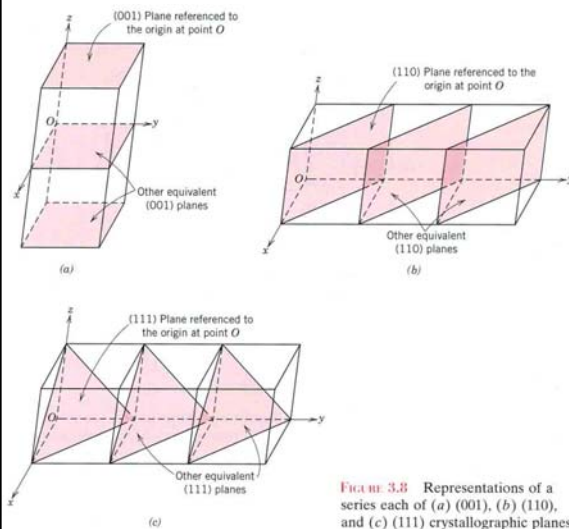


FIGURE 3.3 Representations of a series each of (a) (001), (b) (110), and (c) (111) crystallographic planes.

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Family of planes

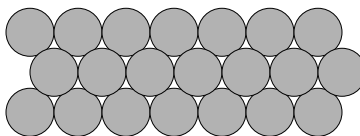
- ✓ Those planes which are equivalent in the crystal by symmetry
- ✓ Designated by { }
- ✓ $\{100\} = (100) + (010) + (001) + (-100) + (0-10) + (00-1)$

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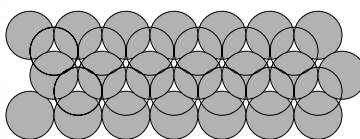
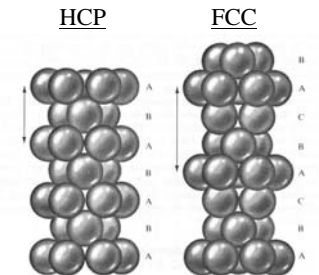
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Comparison of Packing of Atoms in the FCC & HCP Structures:

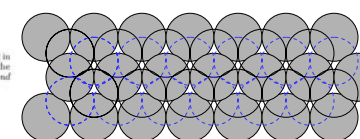
**Stacking sequence in FCC
Crystals for (111) planes:
ABCABC**



Plane A
Or
A sites



Plane B
Or
B sites



Plane C
Or
C sites

Figure 1-28 The manner in which close-packed layers of spheres can be stacked in sequence to produce (left) the hexagonal-close-packed (H.C.P.) structure and (right) the cubic-close-packed (F.C.C.) structure. After L. Pauling, *The Nature of the Chemical Bond* (Cornell, 1960).

Blakemore, Solid State Physics 2nd Ed (Cambridge, 1985)

Extra for those of you that are interested

Fundamentals of Crystallography

Crystallographic Directions:

✓ Example of the Hexagonal system:

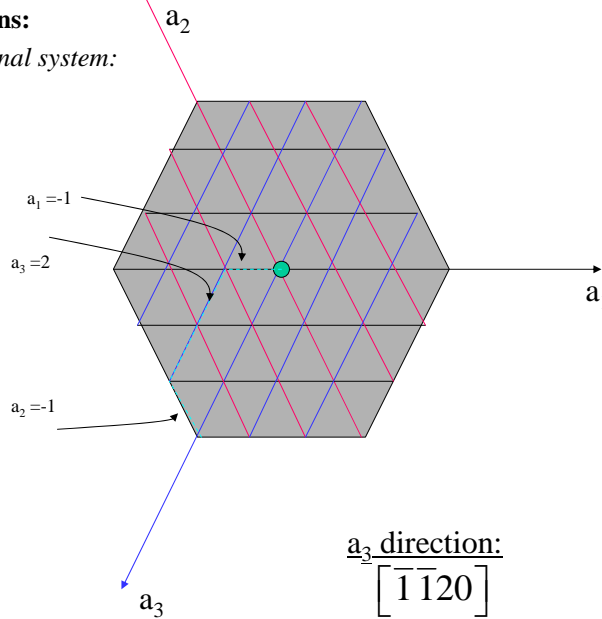
$$\vec{r} = u\vec{a}_1 + v\vec{a}_2 + t\vec{a}_3 + w\vec{c}$$

where the direction
is written:

$$[uvw]$$

and the following
condition imposed:

$$u + v + t = 0$$



a_3 direction:
$$\begin{bmatrix} 1 & \bar{1} & 2 \end{bmatrix}$$

Fundamentals of Crystallography

Crystallographic Directions:

✓ Several Examples of the Hexagonal system:

Barrett & Massalski, Structure of Metals 3rd Ed
(Pergamon, 1980)

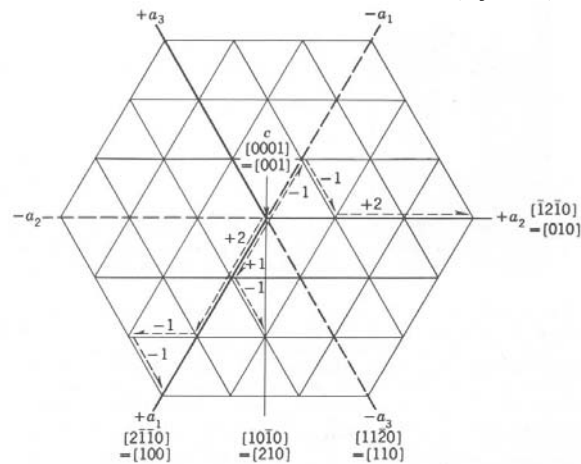
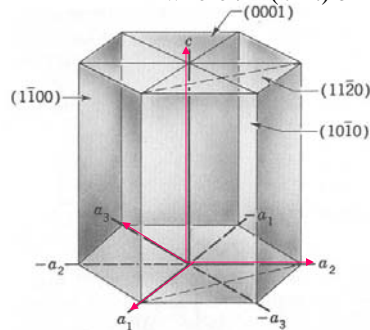


Fig. 1-8 Indices of directions in the hexagonal system with both three- and four-digit indices. The "primary" axis is c (normal to the plane of the drawing); a_1 , a_2 , and a_3 are "secondary" axes and in c.p.h. crystals are the close-packed rows of atoms.

Hexagonal Indices for Planes:

- ✓ To determine the indices for planes in the hexagonal crystal system, the 3 axes system used in the other crystal systems are not usually used because equivalent planes do not have similar indices.
- ✓ For this reason, it is preferable to use the four axes:
 - o a_1, a_2, a_3, c
- ✓ The Miller indices are: (hki)

where $i = -(h+k)$ or $h+k+i=0$



Example:

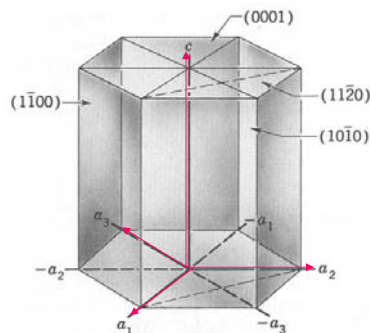
Axis:	a_1	a_2	a_3	c
Intersection:	1	1	$-1/2$	∞
Reciprocal:	1	1	-2	0
Reduce:	1	1	-2	0
Miller Indices:	1	1	-2	0

$(1\bar{1}20)$ or (110)

Fig. 1-7 Indices of some planes in a hexagonal crystal.

Determining Hexagonal Indices for Planes:

- ✓ 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.
- ✓ At this point, the crystallographic plane either intersects or parallels each of the 4 axes; the length of the planar intercept for each axis is determined in terms of the lattice constants a_1, a_2, a_3, c .
- ✓ The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, &, therefore, a zero index.
- ✓ If necessary, these 3 numbers are changed to the set of smallest integers by multiplication or division by a common factor.



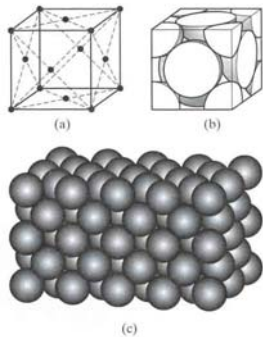
Example:

Axis:	a_1	a_2	a_3	c
Intersection:	1	1	$-1/2$	∞
Reciprocal:	1	1	-2	0
Reduce:	1	1	-2	0
Miller Indices:	1	1	-2	0

$(1\bar{1}20)$ or (110)

Fig. 1-7 Indices of some planes in a hexagonal crystal.

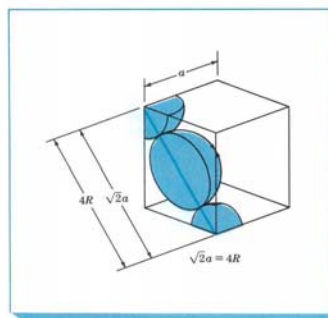
□ Packing of Atoms in the FCC Structure:



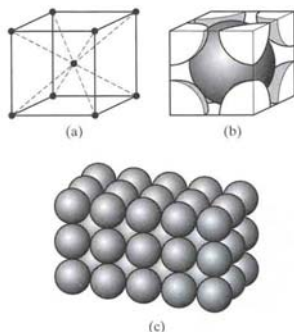
Structure: face-centered cubic (fcc)
Bravais lattice: fcc
Atoms/unit cell: $6 \times \frac{1}{2} + 8 \times \frac{1}{8} = 4$
Typical metals: γ -Fe, Al, Ni, Cu, Ag, Pt, and Au

Figure 3-5 Face-centered cubic (fcc) structure for metals showing (a) the arrangement of lattice points for a unit cell; (b) the actual packing of atoms within the unit cell; and (c) the repeating fcc structure, equivalent to many adjacent unit cells (Part (c) courtesy of Molecular Simulations, Inc.).

FIGURE 3.7 FCC unit cell showing relationship between the lattice constant a and atomic radius R . Since the atoms touch across the face diagonals $\sqrt{2}a = 4R$.



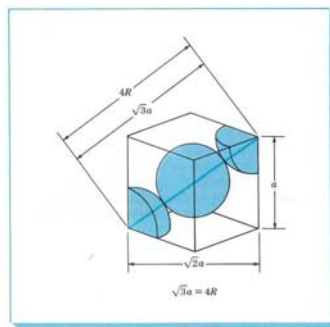
□ Packing of Atoms in the BCC Structure:



Structure: body-centered cubic (bcc)
Bravais lattice: bcc
Atoms/unit cell: $1 + 8 \times \frac{1}{8} = 2$
Typical metals: α -Fe, V, Cr, Mo, and W

Figure 3-4 Body-centered cubic (bcc) structure for metals showing (a) the arrangement of lattice points for a unit cell; (b) the actual packing of atoms (represented as hard spheres) within the unit cell; and (c) the repeating bcc structure, equivalent to many adjacent unit cells (Part (c) courtesy of Molecular Simulations, Inc.).

FIGURE 3.5 BCC unit cell showing relationship between the lattice constant a and the atomic radius R .



Comparison of Packing of Atoms in the FCC & HCP Structures:

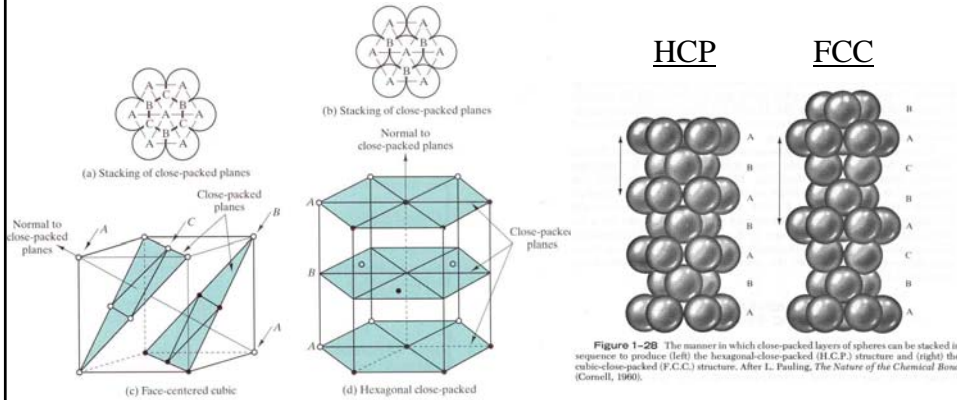


Figure 3-7 Comparison of the fcc and hcp structures. They are each efficient stackings of close-packed planes. The difference between the two structures is the different stacking sequences. (After B. D. Cullity, Elements of X-Ray Diffraction, 2nd ed., Addison-Wesley Publishing Co., Inc., Reading, Mass., 1978.)

Figure 1-20 The manner in which close-packed layers of spheres can be stacked in sequence to produce (left) the hexagonal-close-packed (H.C.P.) structure and (right) the cubic-close-packed (F.C.C.) structure. After L. Pauling, The Nature of the Chemical Bond (Cornell, 1960).

Blakemore, Solid State Physics 2nd Ed (Cambridge, 1985)

Packing of Atoms in the HCP Structure:

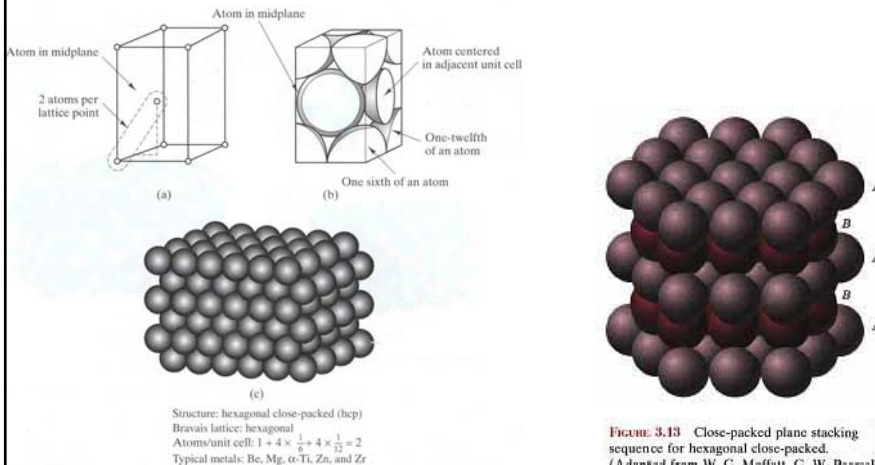


Figure 3-6 Hexagonal close packed (hcp) structure for metals showing (a) the arrangement of atom centers relative to lattice points for a unit cell. There are two atoms per lattice point (note the outlined example). (b) The actual packing of atoms within the unit cell. Note that the atom in the midplane extends beyond the unit cell boundaries. (c) The repeating hcp structure, equivalent to many adjacent unit cells (Part (c) courtesy of Molecular Simulations, Inc.).

Figure 3.13 Close-packed plane stacking sequence for hexagonal close-packed. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, The Structure and Properties of Materials, Vol. 1, Structure, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

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Crystalline and Noncrystalline Materials:

- ✓ **Question:** How would you calculate the density of a material given the:
 - o Lattice constant or Radius of Atom
 - o Crystal structure
 - o Atomic weight

where density is given by: *mass/volume*?

- ✓ **Use Following Information:** Cu, FCC, $r_{Cu} = 0.128$ nm, Atomic Mass=63.5g/mole.

Crystalline and Noncrystalline Materials:

- ✓ **Isotropic Materials:**
 - o If the properties of the material are *independent* of the direction in which they are measured, the material is categorized as **isotropic**.

- ✓ **Anisotropy Materials:**
 - o If the properties of the material are *dependent* of the direction in which they are measured, the material is categorized as **anisotropic**.
 - o Examples of these properties include:
 - Periodicity of atoms in a crystal structure.
 - Density of a material of crystalline solids.
 - Carrier velocity.
 - Phonon velocity.

□ Crystalline and Noncrystalline Materials:

- ✓ Allotropy:
 - o Elements that can exhibit more than one crystal structure are *allotropic*.
- ✓ Polymorphism:
 - o Compounds that behave in the same manner as allotropic materials are referred to as *polymorphic*.

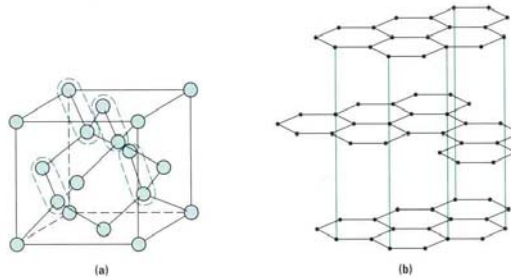


FIGURE 3.10-1 A comparison of the polymorphs of carbon: (a) diamond and (b) graphite.

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Shackelford, Intro to Materials Science for Engineers, 5th Ed. (Prentice Hall, 2002)

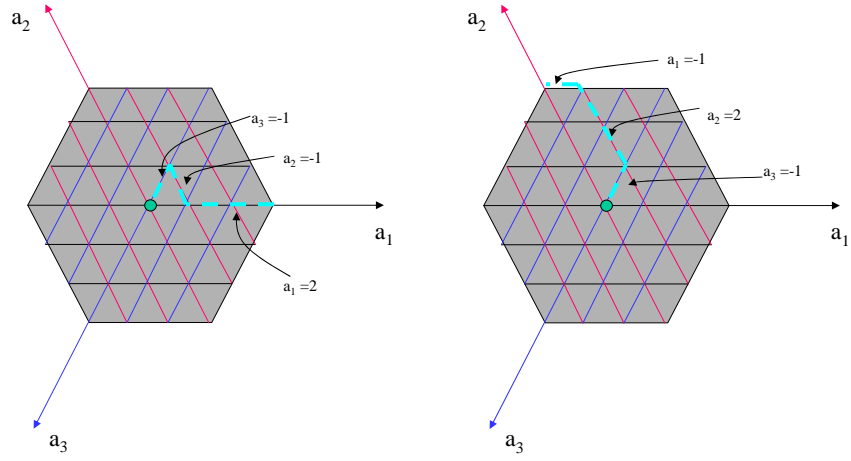
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□ Crystalline and Noncrystalline Materials:

- ✓ Single Crystal:
 - o A continuous periodic crystal structure only interrupted by the boundaries of the solid
- ✓ Amorphous:
 - o Although short range periodicity may be present, long range periodicity is absent. Hence, amorphous material is not crystalline.
- ✓ Polycrystalline:
 - o A material composed of from two to many single crystal grains.

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$$[\bar{1}\bar{1}20]$$