Properties of Engineering Materials

The Structure of Crystalline Solids

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Fundamental Concepts

- Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another.
- 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.

Fundamental Concepts

- Some of the properties of crystalline solids depend on the **crystal structure** of the material, the manner in which atoms, ions, or molecules are spatially arranged.

- There is an extremely large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex ones.

Fundamental Concepts

- The *atomic hard-sphere model*: atoms (or ions) are thought of as being solid spheres having well-defined diameters.
  - Spheres representing nearest-neighbor atoms touch one another.
- **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).

Fundamental Concepts

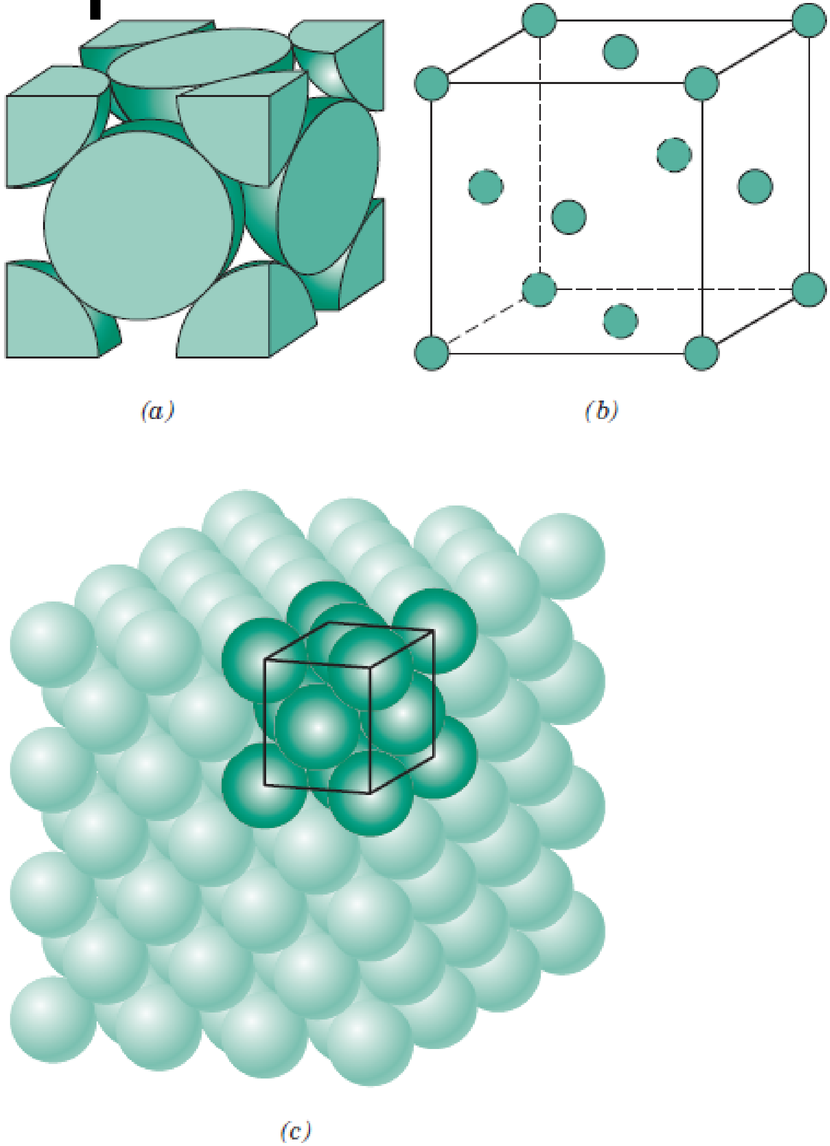


Figure 3.1 For the face-centered cubic crystal structure, (*a*) a hards-phere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms.

Unit Cells

- *Unit Cell*: small repeat entities.
- Unit cells are 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.

Metallic Crystal Structures

- Different metals: different crystal structures.
- Some metals: different crystal structures at different temperatures.

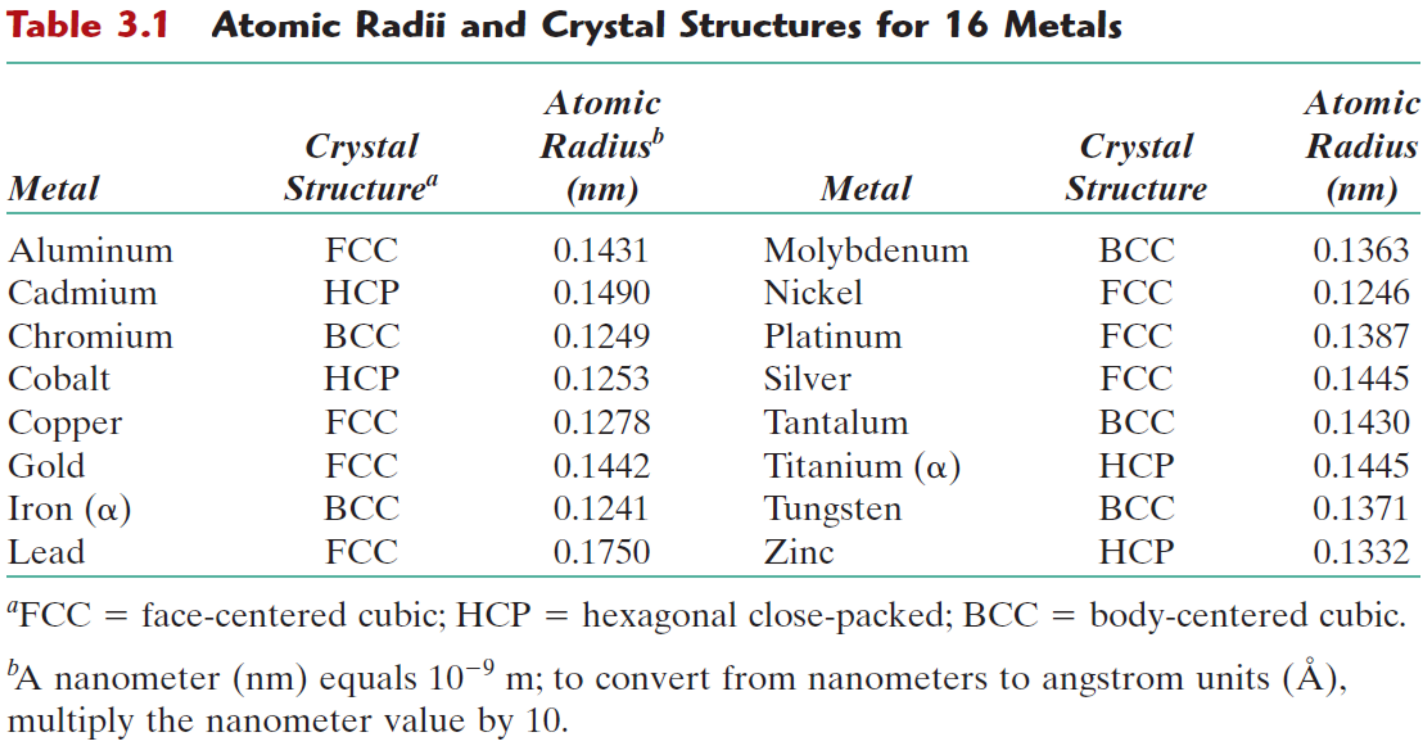


Table 3.1 **Atomic Radii and Crystal Structures for 16 Metals**

Metal	*Crystal Structure*[a]	*Atomic Radius*[b] *(nm)*	*Metal*	*Crystal Structure*	*Atomic Radius (nm)*
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a] FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

[b] A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

Metallic Crystal Structures

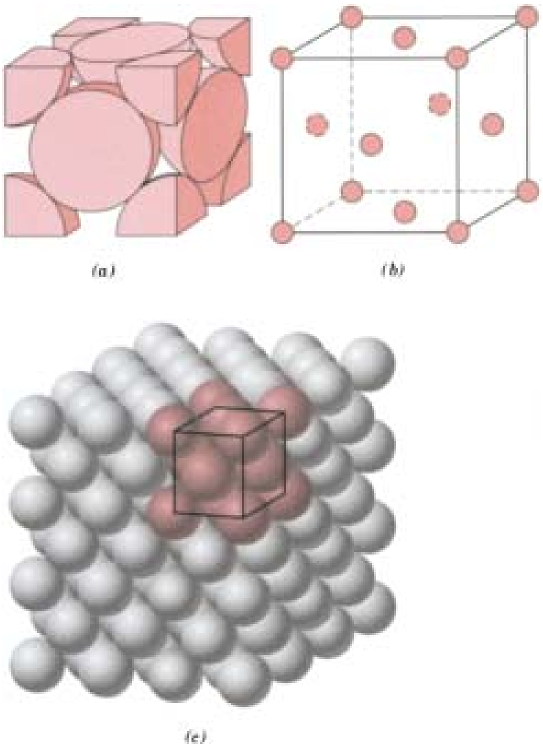
The Face-Centered Cubic Crystal Structure

FCC: a crystal structure that has a cubic unit cell with atoms located at all eight corners and six atoms at the center of each face of the cube. (total of four atoms/unit cell).

Atoms touch one another across a face diagonal.

$a = 2R\sqrt{2}$; where a is the lattice constant and R is the atomic radius.

Coordination number and atomic packing factor for FCC are 12 and 0.74, respectively.


(a) (b)

(c)

The crystal structure of γ-iron.

Metallic Crystal Structures

The Body-Centered Cubic Crystal Structure

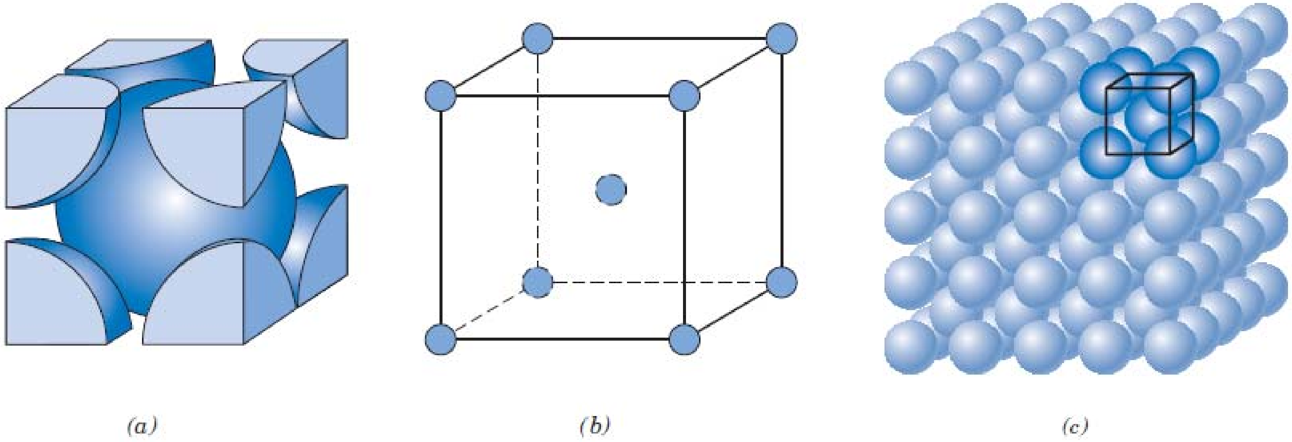

(a) (b) (c)

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.

BCC: a crystal structure that has a cubic unit cell with atoms located at all eight corners and a single atom at the cube center (total of two atoms/unit cell).

Center and corner atoms touch one another along cube diagonals.

Coordination number and atomic packing factor for BCC are 8 and 0.68, respectively.

So, what do the coordination number and atomic packing factor mean??

Metallic Crystal Structures
The Coordination Number and the Atomic Packing Factor

- Coordination number (CN): the number of nearest-neighbor atoms per atom.

- For FCC, the coordination number is 12; the front face atom has four corner nearest-neighbor atoms surrounding it, four face atoms that are in contact from behind, and four other equivalent face atoms residing in the next unit cell to the front.

- For the BCC, the coordination number is 8; each center atom has as nearest neighbors as its eight corner atoms.

Metallic Crystal Structures

The Coordination Number and the Atomic Packing Factor

- Atomic packing factor (APF): is the fraction of solid sphere volume in a unit cell, assuming the atomic hard sphere model.

- APF = Volume of atoms in a unit cell / Volume of unit cell.

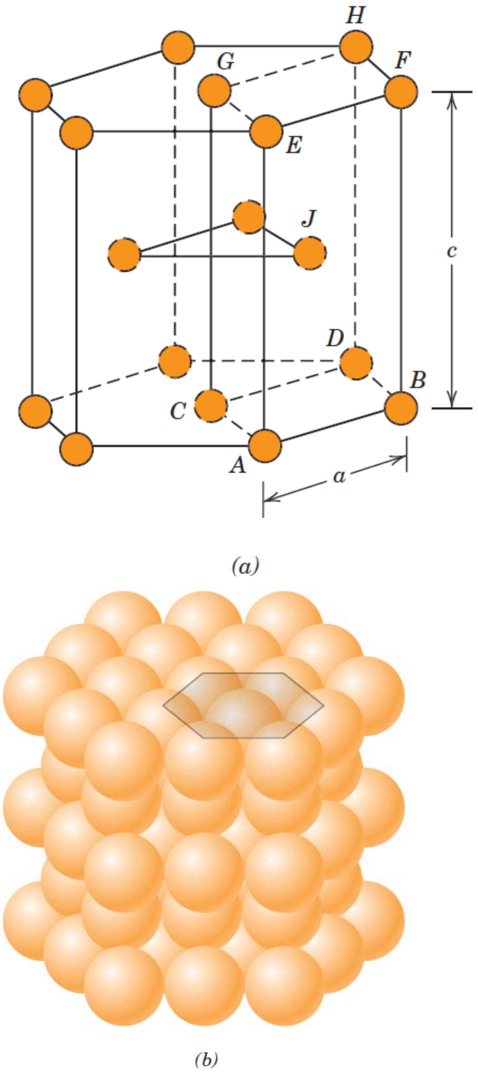
Metallic Crystal Structures

Computation of the Atomic Packing Factor for FCC

- Example 3.2: Show that the atomic packing factor for the FCC crystal structure is 0.74.

Metallic Crystal Structures

The 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.

6 atoms / unit cell, CN and APF: same as FCC.

If *a* and *c* represent, respectively, the short and long unit cell dimensions of Figure 3.3*a*, the *c*/*a* ratio should be 1.633.

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.

Density Computations

- Knowledge of crystal structures of metallic solids permits computation of its theoretical density (ρ).

$$\rho = \frac{nA}{V_C N_A}$$

where
n= the number of atoms associated with each unit cell
A = atomic weight
V_C = the unit cell volume
N_A = Avogadro’s number = 6.022×10^{23} atoms/mol

Density Computations

Theoretical Density Computation for Copper

- Example 3.3: Cu has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

Polymorphism and Allotropy

- **Polymorphism:** a phenomenon **in which** metals, as well as nonmetals, may have more than one crystal structure.
- **Allotropy:** polymorphism in elemental solids.
- The prevailing crystal structure depends on both the temperature and the external pressure.
  - One familiar example is found in carbon: graphite is the stable polymorph at ambient conditions, whereas diamond is formed at extremely high pressures.Also, pure iron has a BCC crystal structure at room temperature, which changes to FCC iron at 912 ° C.

Crystal Systems

- Many crystal systems: convenient to divide them into groups according to unit cell configurations and/or atomic arrangements.
  - Based on the unit cell geometry (the shape of the appropriate unit cell prism without regard to the atomic positions in the cell).
  - An xyz coordinate system is established with its origin at one of the unit cell corners; each of the x, y, and z axes coincides with one of the three prism edges that extend from this corner, as illustrated in Figure 3.4.

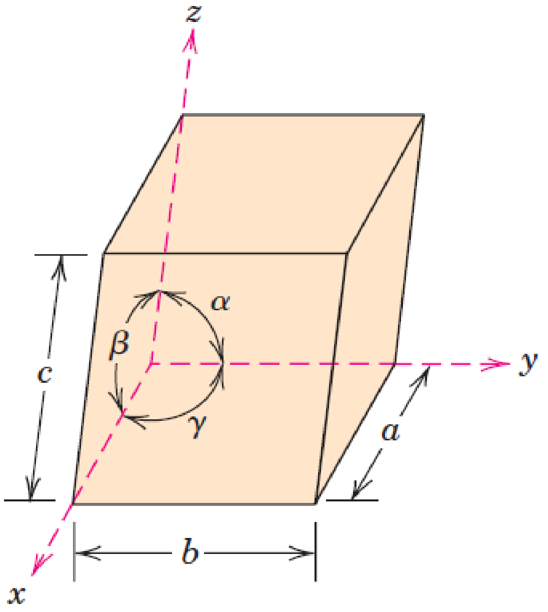


Figure 3.4 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β , and γ) “called lattice parameters”.

Crystal Systems

- We have 6 lattice parameters, so 7 different combinations (7 different crystal systems).

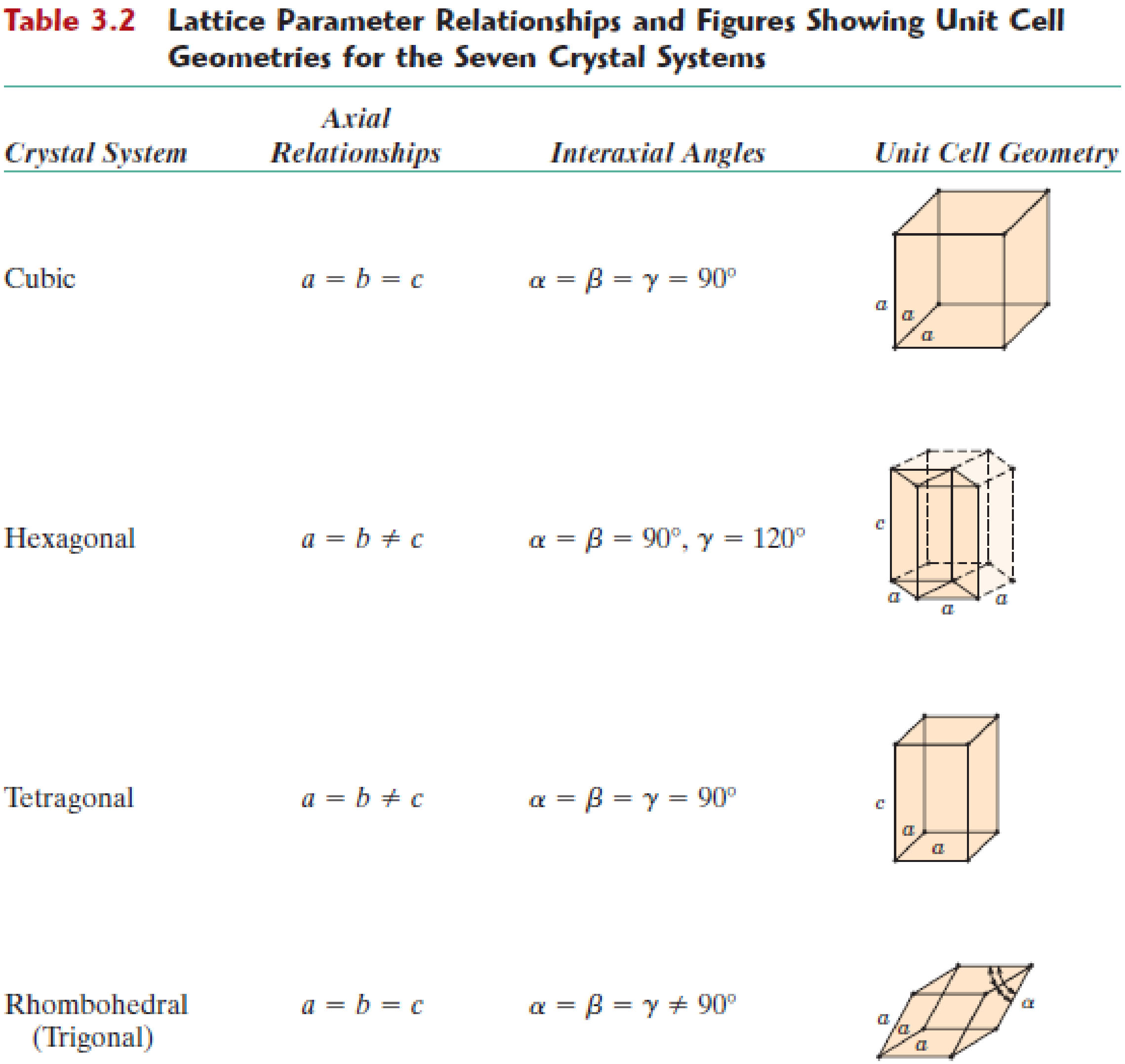
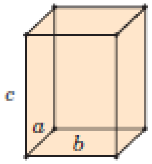
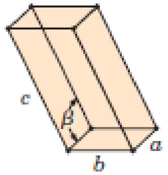
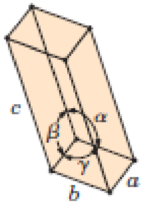


Table 3.2 **Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems**

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	

Crystal Systems

- We have 6 lattice parameters, so 7 different combinations (7 different crystal systems).

Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

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*).

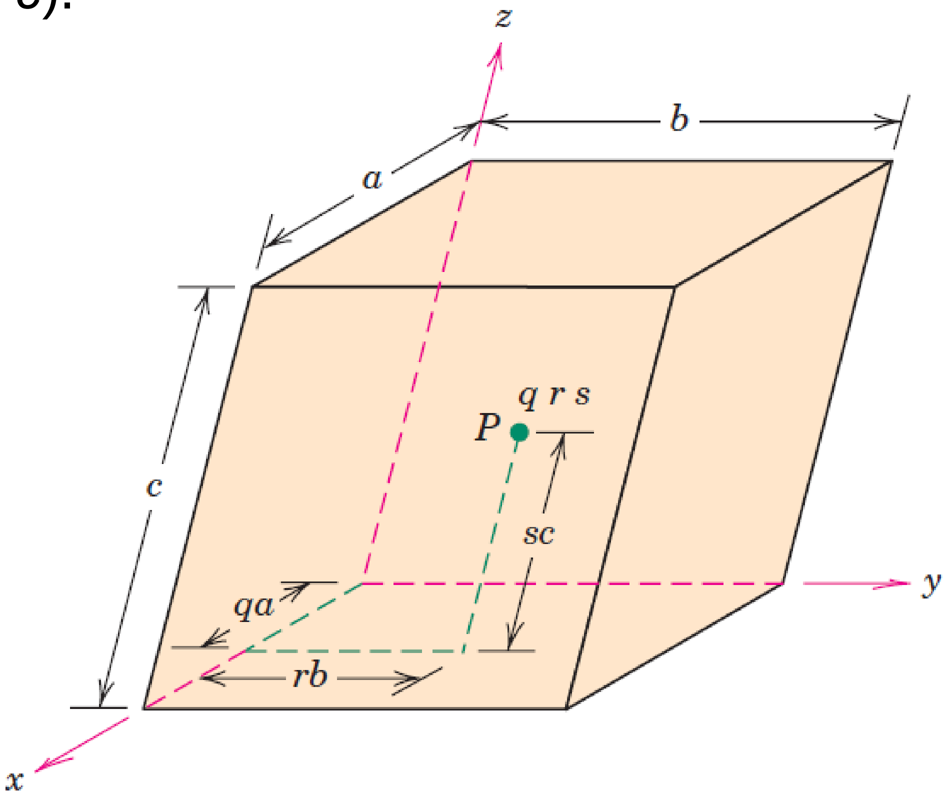
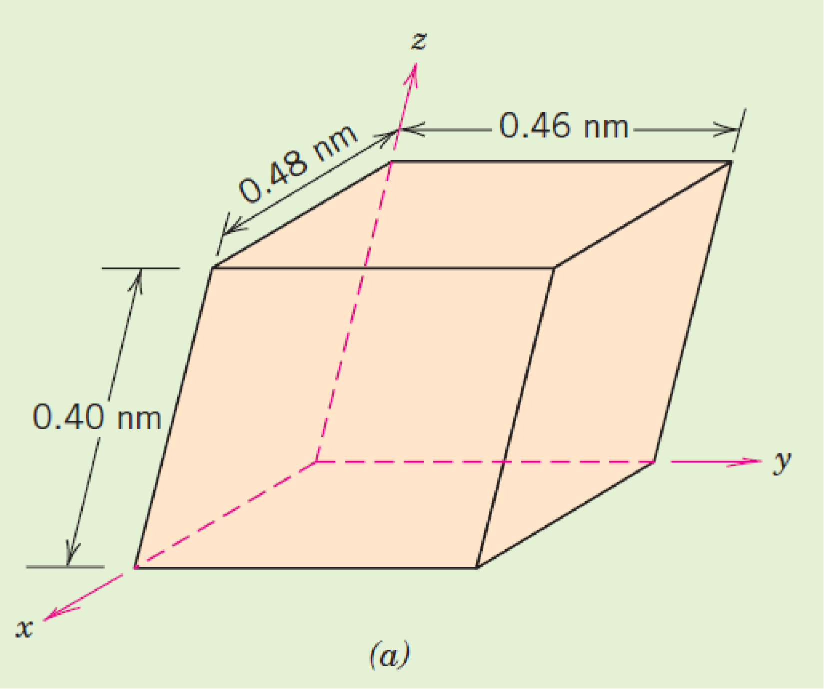


Figure 3.5 The manner in which the *q*, *r*, and *s* coordinates at point *P* within the unit cell are determined. The *q* coordinate (which is a fraction) corresponds to the distance *qa* along the *x* axis, where *a* is the unit cell edge length. The respective *r* and *s* coordinates for the *y* and *z* axes are determined similarly.

Point Coordinates

- Example 3.4: For the unit cell shown in the accompanying sketch (*a*), locate the point having coordinates ¼ 1 ½.



Point Coordinates

- Example 3.5: Specify point coordinates for all atom positions for a BCC unit cell.

Crystallographic Directions

- A crystallographic direction is defined as a line between two points, or a vector.
- Determined by:
  - A vector of convenient length is positioned such that it passes through the origin of the coordinate system.
  - 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*.
  - These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
  - 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.

Crystallographic Directions

- The [100], [110], and [111] directions are common ones; they are drawn in the unit cell shown in Figure 3.6.

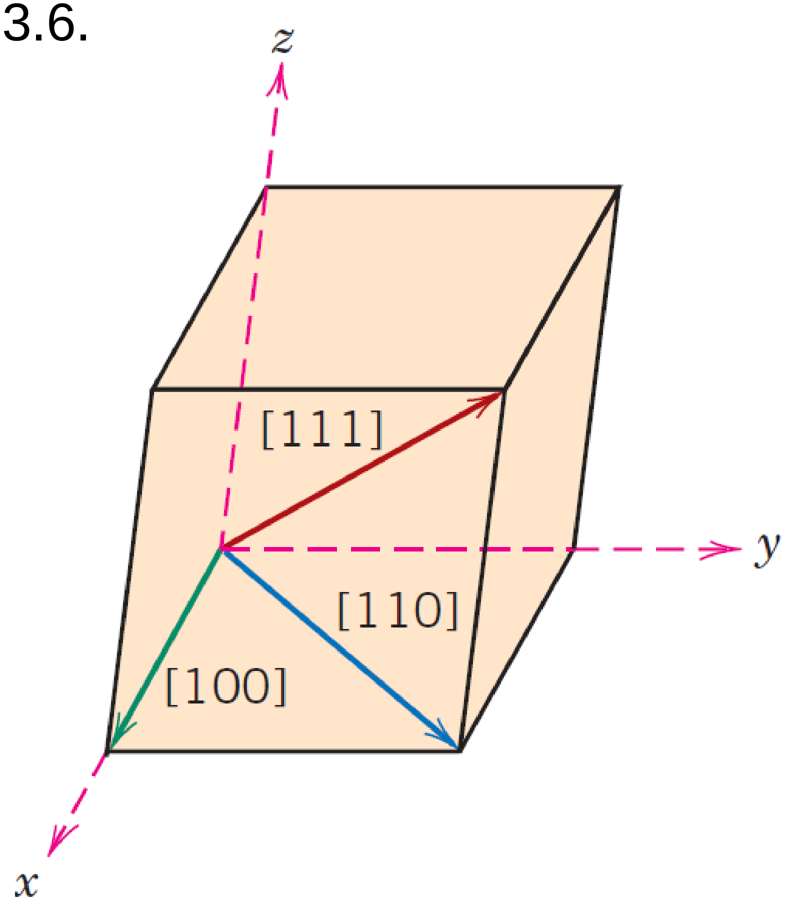
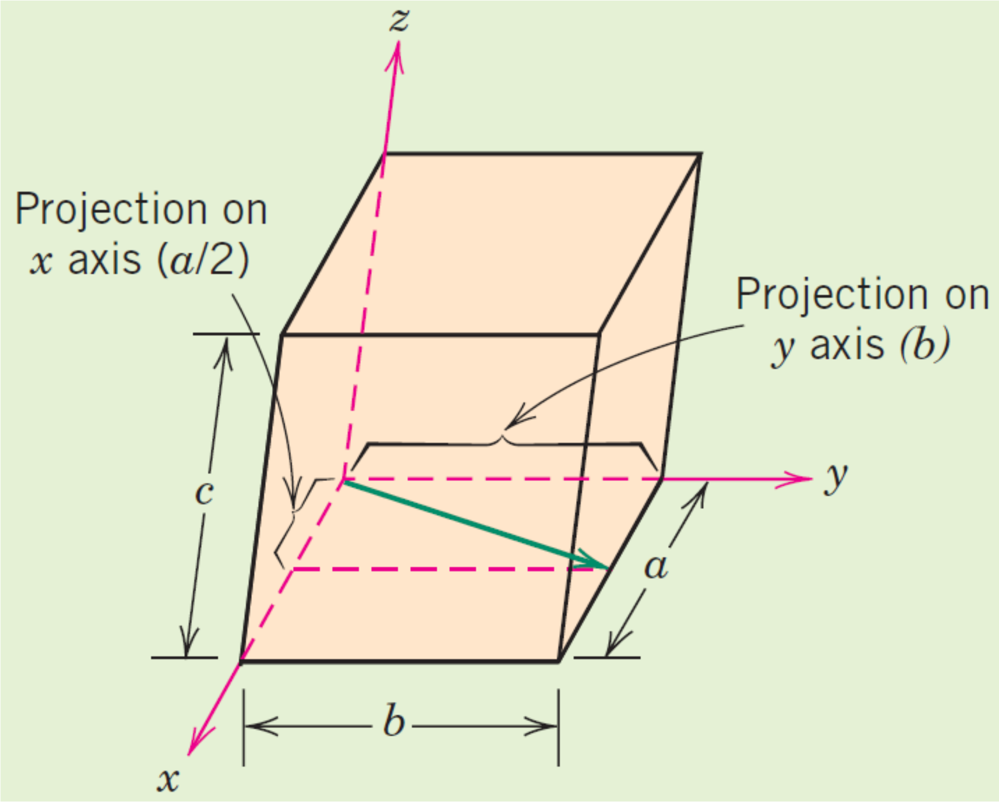


Figure 3.6 The [100], [110], and [111] directions within a unit cell.

Crystallographic Directions

- Example 3.6: Determine the indices for the direction shown in the accompanying figure.



Crystallographic Directions

- Example 3.7: Draw a [$1\bar{1}0$] direction within a cubic unit cell..

Crystallographic Directions

- A *family of directions*: a group of equivalent directions.
    - 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 $[00\bar{1}]$.
    - This family is enclosed in angle brackets, i.e. <100>.
    - 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 Directions

Hexagonal Crystals

- In hexagonal crystal, a fourth axis is needed. This is called *Miller–Bravais,* coordinate system as shown in Figure 3.7.
- a_1, a_2, and a_3 axes are all contained within a single plane (called the basal plane) and are at 120° angles to one another. The *z* axis is perpendicular to this basal plane.
- Directional indices, is denoted by four indices, as [*uvtw*].

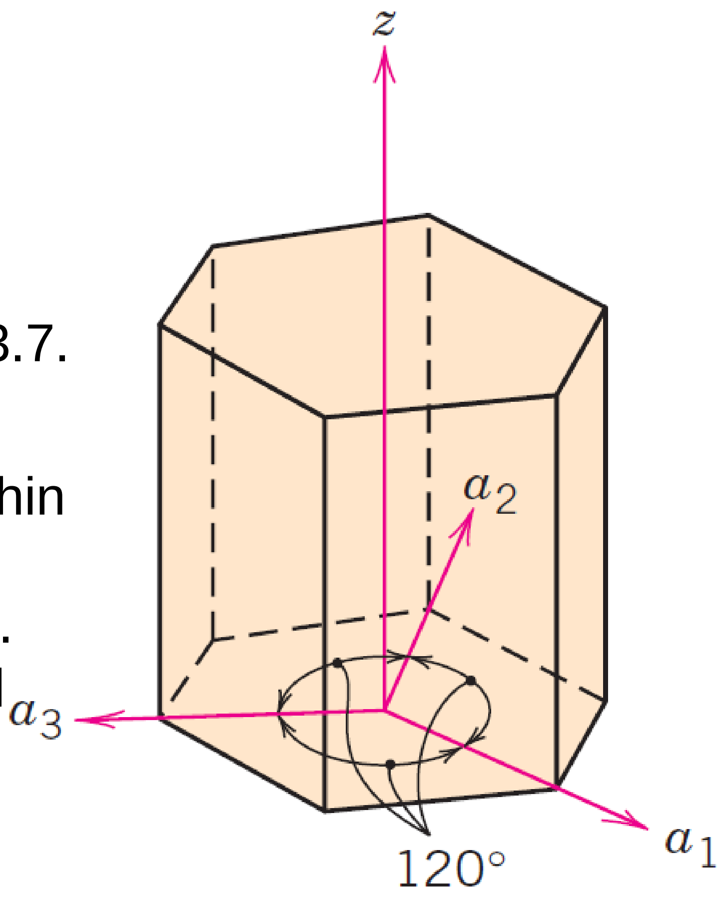


Figure 3.7 Coordinate axis system for a hexagonal unit cell (Miller–Bravais scheme).

Crystallographic Directions
Hexagonal Crystals

- Conversion from the three-index system to the four-index system:
  - $[u' \, v' \, w'] \longrightarrow [u \, v \, t \, w]$
- Accomplished by:
  - $u = 1/3\,(2u' - v')$
  - $v = 1/3\,(2v' - u')$
  - $t = -(u + v)$
  - $w = w'$

Crystallographic Directions

Hexagonal Crystals

- Example 3.8:

(a) Convert the [111] direction into the four-index system for hexagonal crystals.

(b) Draw this direction within a reduced-scale coordinate system.

(c) Now draw the [111] direction within a hexagonal unit cell that utilizes a three-axis (a_1, a_2, z) coordinate system.

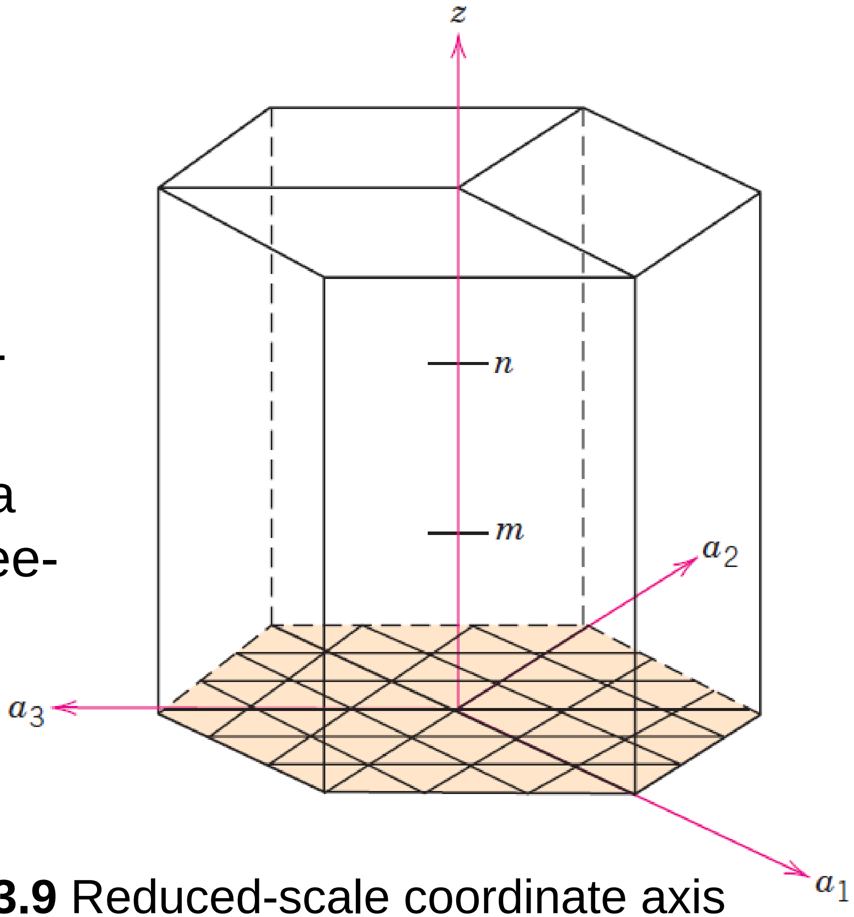


Figure 3.9 Reduced-scale coordinate axis system for hexagonal unit cells that may be used to plot crystallographic directions.

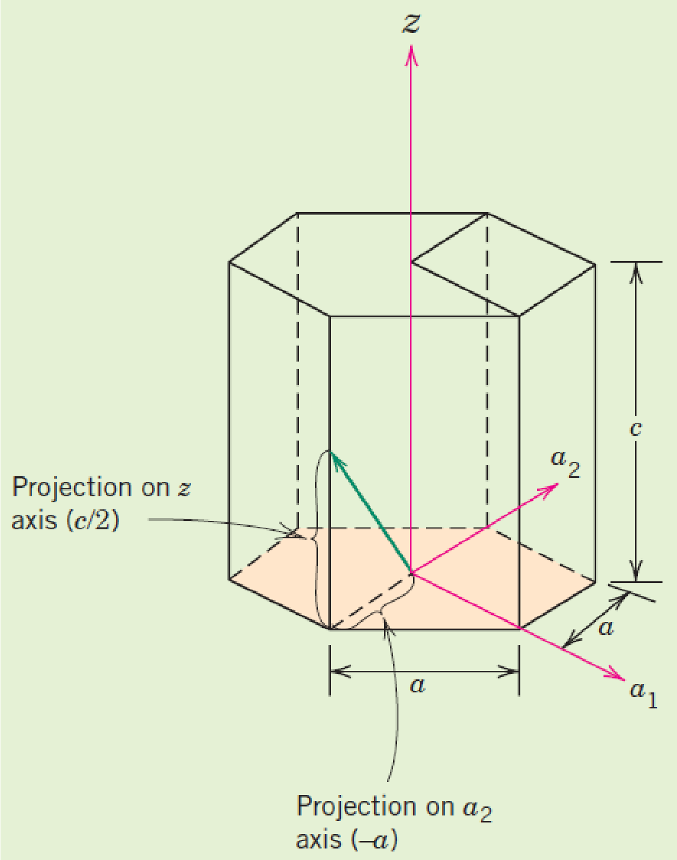
Crystallographic Directions

Hexagonal Crystals

- Example 3.8:

Crystallographic Directions
Hexagonal Crystals

- Example 3.9: Determine the directional indices (four-index system) for the direction shown in the accompanying figure.



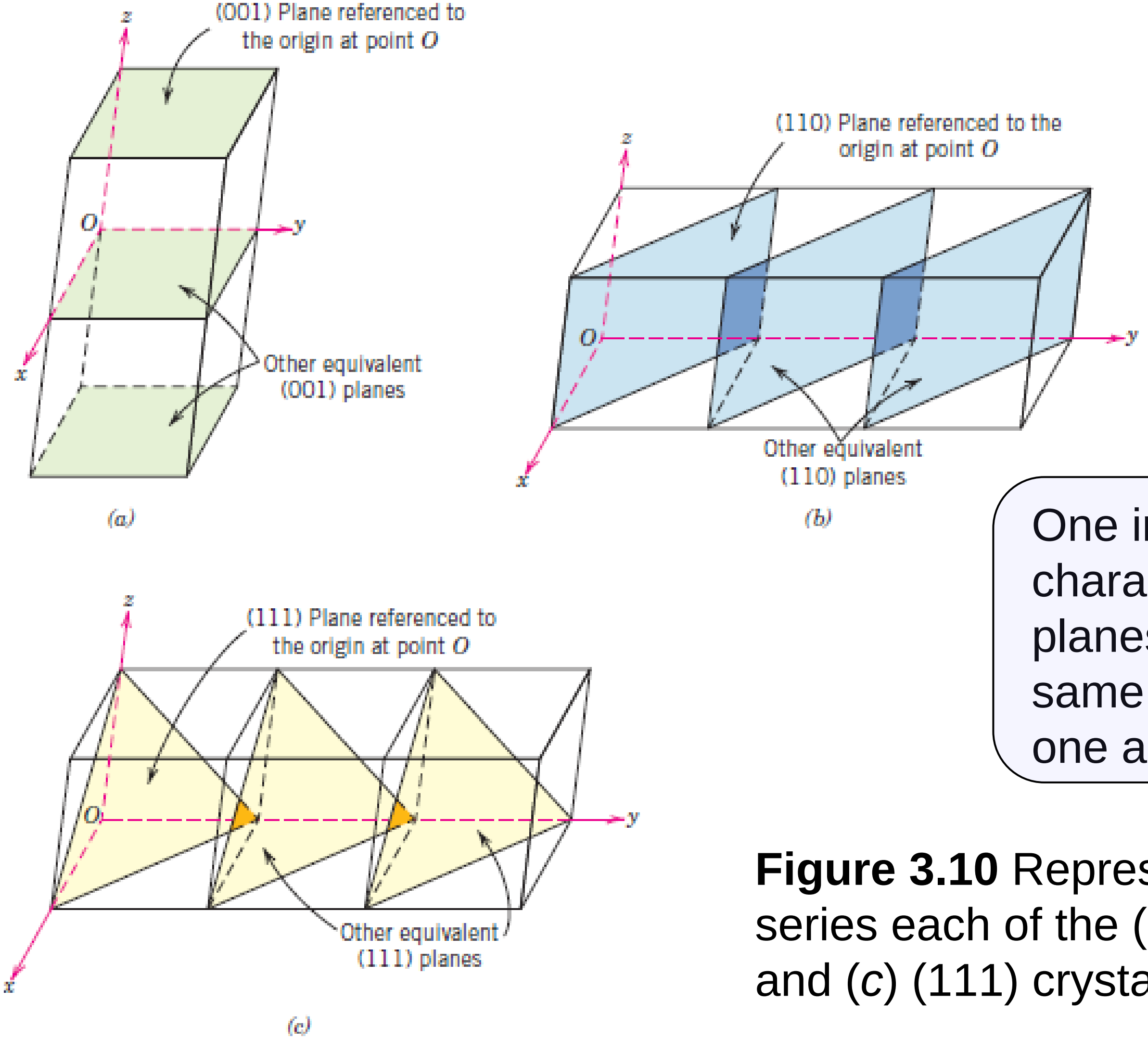
Crystallographic Planes

- In all but the hexagonal crystal system, crystallographic planes are specified by three **Miller indices** as (*hkl*).
- Any two planes parallel to each other are equivalent and have identical indices.

Crystallographic Planes

- The procedure used to determine the *h*, *k*, and *l* index numbers is:
  - 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 three axes; the length of the planar intercept for each axis is determined in terms of the lattice parameters *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, and, therefore, a zero index.
  - If necessary, these three 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 within parentheses, thus: (*hkl*).

Crystallographic Planes

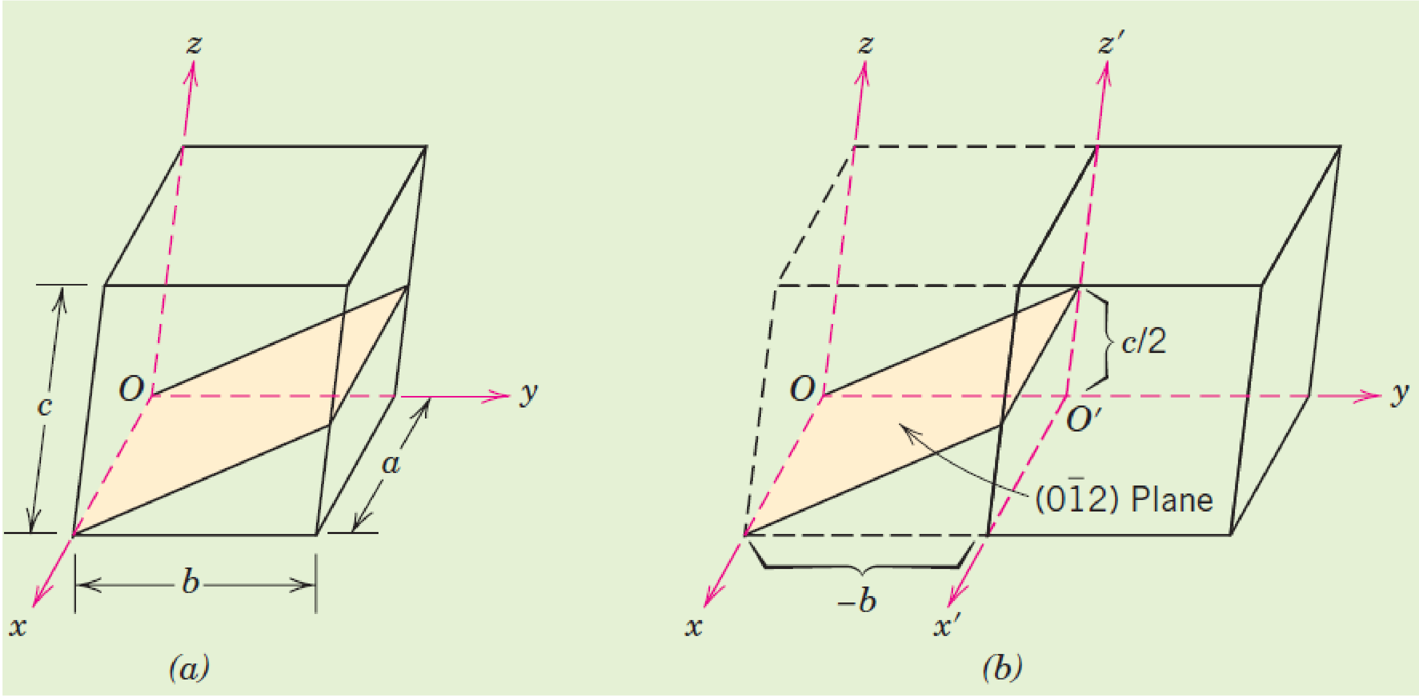


One interesting and unique characteristic of cubic crystals is that planes and directions having the same indices are perpendicular to one another

Figure 3.10 Representations of a series each of the (*a*) (001), (*b*) (110), and (*c*) (111) crystallographic planes.

Crystallographic Planes

- Example 3.10: Determine the Miller indices for the plane shown in the accompanying sketch (*a*).



Crystallographic Planes

- Example 3.10: Determine the Miller indices for the plane shown in the accompanying sketch (*a*).

Crystallographic Planes

- Example 3.11: Construct a $(0\bar{1}1)$ plane within a cubic unit cell.

Crystallographic Planes

Atomic Arrangements

- The atomic arrangement for a crystallographic plane depends on the crystal structure.

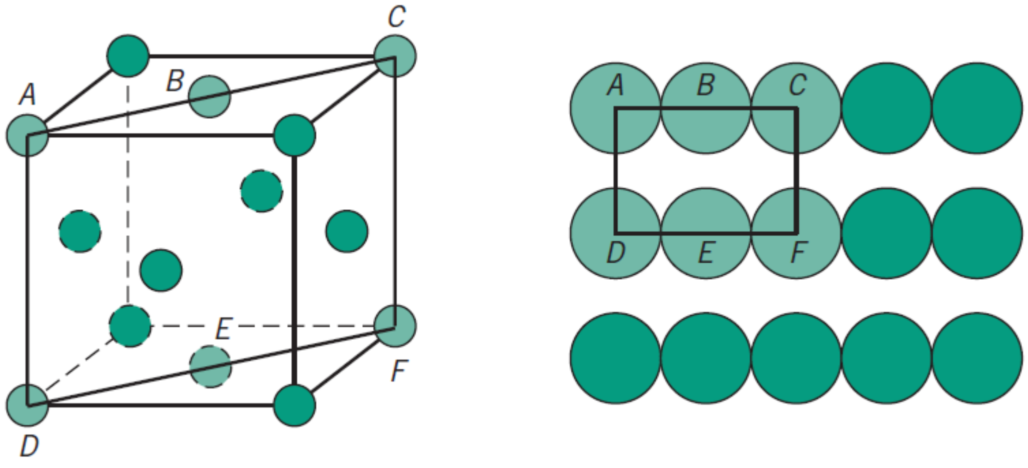
- A “family” of planes contains all planes that are crystallographically equivalent; e.g. in cubic crystals the (111), ($\bar{1}\bar{1}\bar{1}$), ($\bar{1}11$), ($1\bar{1}\bar{1}$), ($11\bar{1}$), ($\bar{1}\bar{1}1$), ($\bar{1}1\bar{1}$), and ($1\bar{1}1$) planes all belong to the {111} family.

- This is not the case for other crystal structures; e.g. the tetragonal structure.

- Also, in the cubic system only, planes having the same indices, irrespective of order and sign, are equivalent; e.g. both ($1\bar{2}3$) and ($3\bar{1}2$) belong to the {123} family.

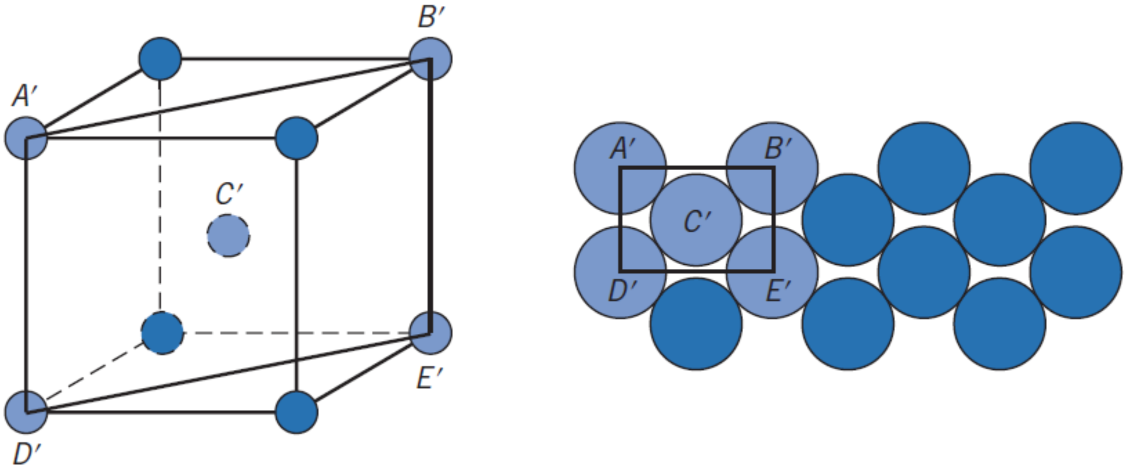
Crystallographic Planes

Atomic Arrangements



(a) (b)

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.



(a) (b)

Figure 3.12 (*a*) Reduced-sphere BCC unit cell with the (110) plane. (*b*) Atomic packing of a BCC (110) plane. Corresponding atom positions from (*a*) are indicated.

Crystallographic Planes

Atomic Arrangements

- For the hexagonal structure, we have the four-index (*hkil*) scheme.
  - $i = -(h + k)$

- The three *h*, *k*, and *l* indices are identical for both indexing systems.

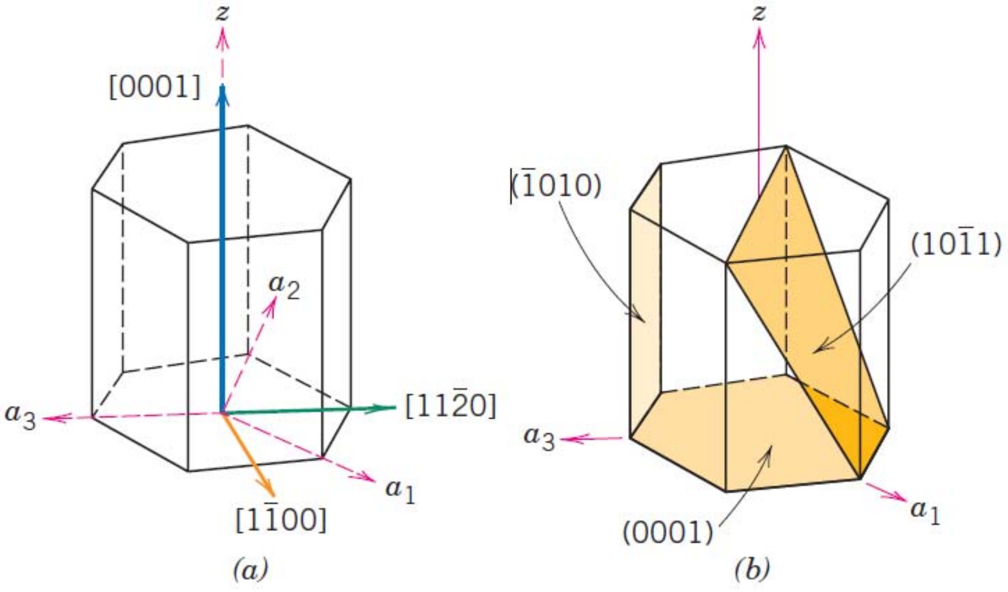
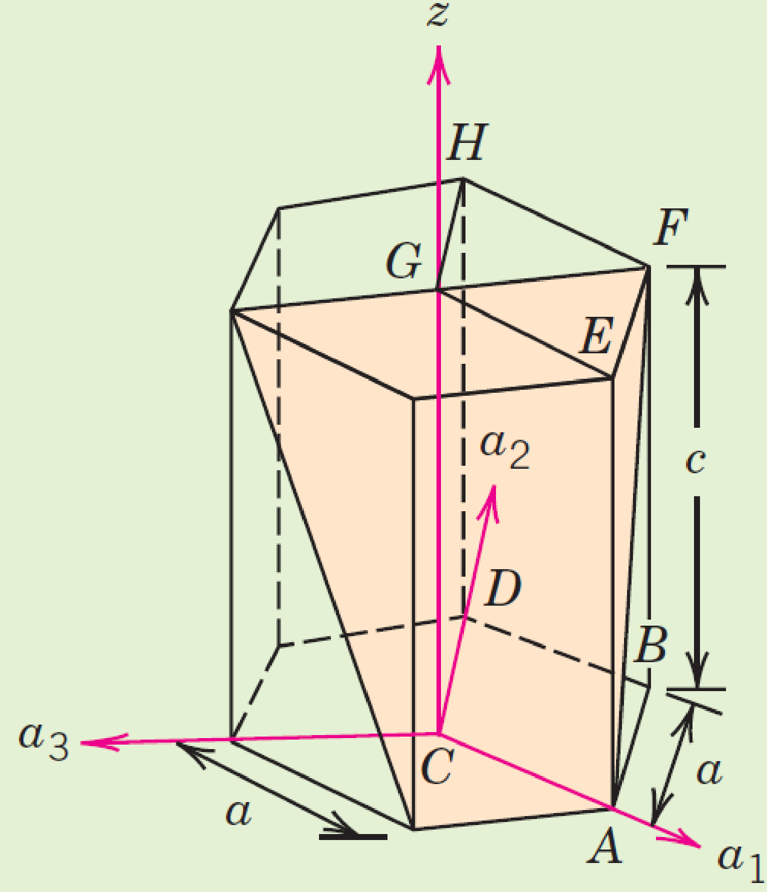


Figure 3.8 For the hexagonal crystal system, (*a*) some directions, and (*b*) some planes.

Crystallographic Planes

Atomic Arrangements

- Example 3.12: Determine the Miller–Bravais indices for the plane shown in the hexagonal unit cell.



Linear & Planner Densities

- Directional equivalency is related to *linear density*: for a particular material, equivalent directions have identical linear densities.

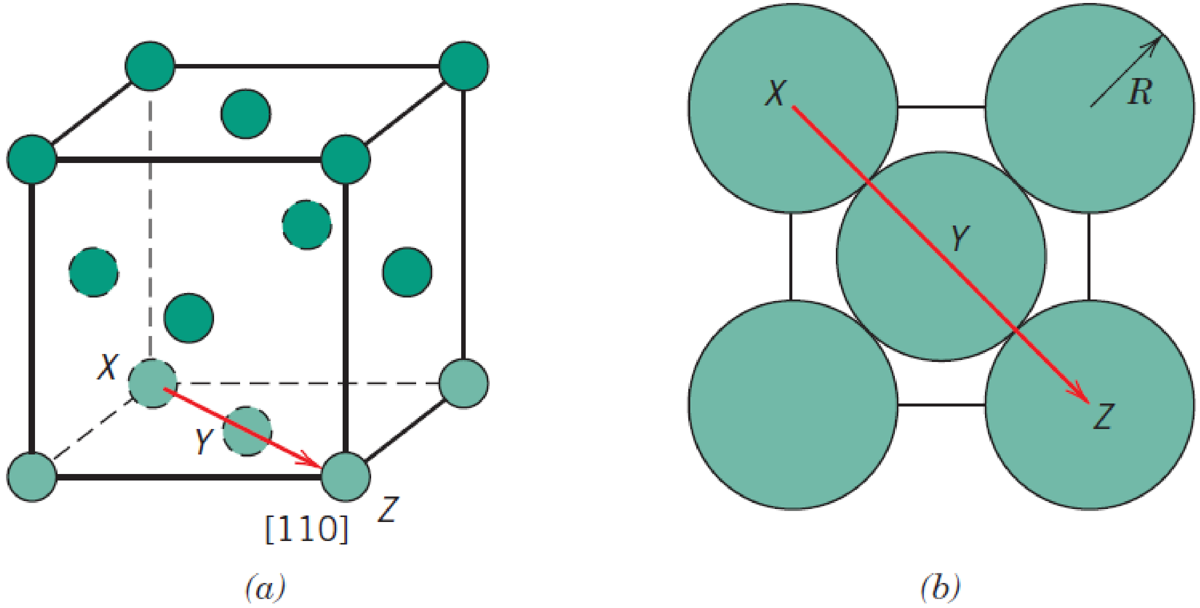
- The corresponding parameter for crystallographic planes is *planar density,* and planes having the same planar density values are also equivalent.

  - 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, in nm^{-1} or m^{-1}

$$\mathrm{LD} = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$

Linear & Planner Densities

- Example: let’s determine the LD of the [110] direction for the FCC crystal structure.



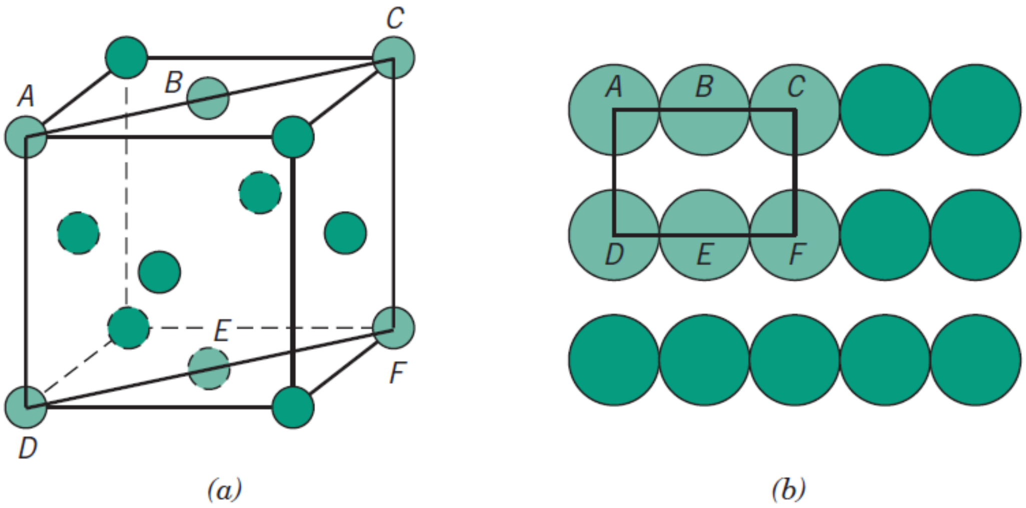
Linear & Planner Densities

- Directional equivalency is related to *linear density*: 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.
  - ☐ Planar density (PD) is taken as the number of atoms per unit area that are centered on a particular crystallographic plane, in nm^{-2} or m^{-2}

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

Linear & Planner Densities

- Example: let's determine the PD of the (110) plane for the FCC crystal structure.



Linear & Planner Densities

- Linear and planar densities are important considerations relative to the process of slip, that is:
    - The mechanism by which metals plastically deform.
- Slip occurs on the most densely packed crystallographic planes and, in those planes, along directions having the greatest atomic packing.

Close-Packed Crystal Structures

- Both face-centered cubic and hexagonal close-packed crystal structures have atomic packing factors of 0.74.
- These two crystal structures may be described in terms of close-packed planes of atoms (i.e., planes having a maximum atom or sphere-packing density).

Close-Packed Crystal Structures

- Both crystal structures may be generated by the stacking of these close-packed planes on top of one another; the difference between the two structures lies in the stacking sequence.

- The real distinction between FCC and HCP lies in where the third close-packed layer is positioned; for HCP (ABABAB…), for FCC (ABCABC…).

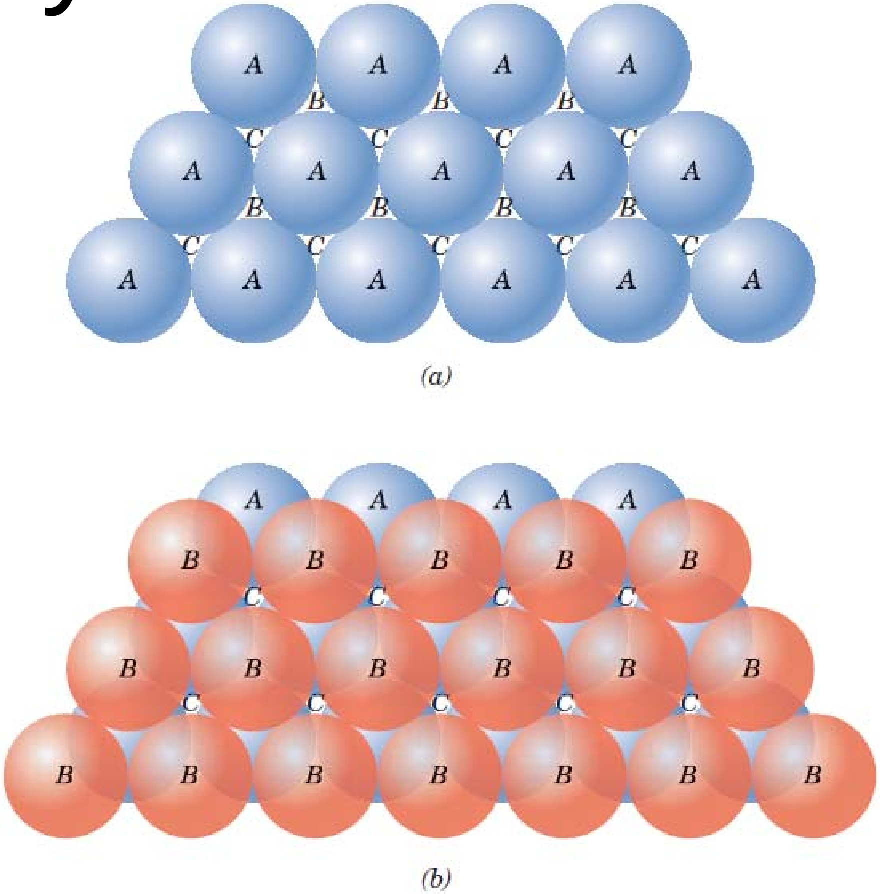


Figure 3.14 (*a*) A portion of a close-packed plane of atoms; *A*, *B*, and *C* positions are indicated. (*b*) The *AB* stacking sequence for close-packed atomic planes.

Close-Packed Crystal Structures

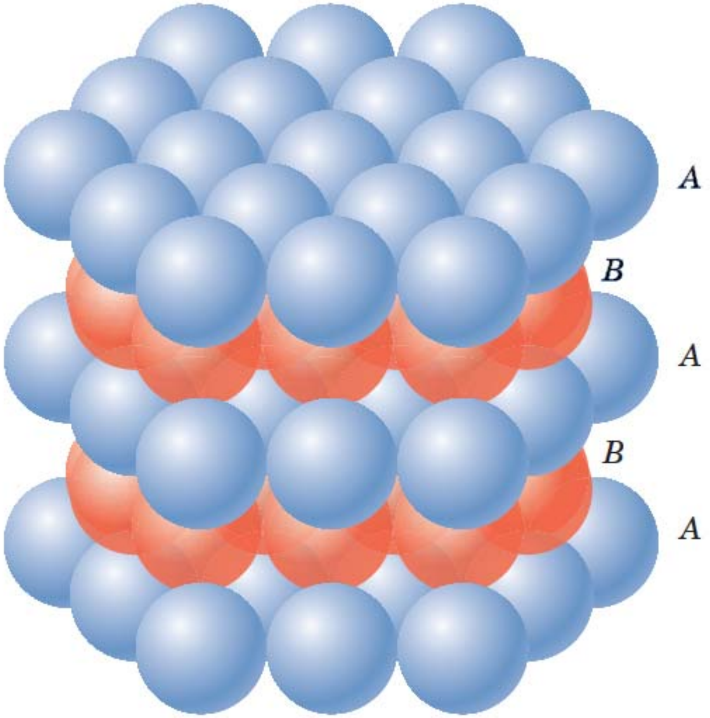


Figure 3.15 Close-packed plane stacking sequence for hexagonal close-packed.

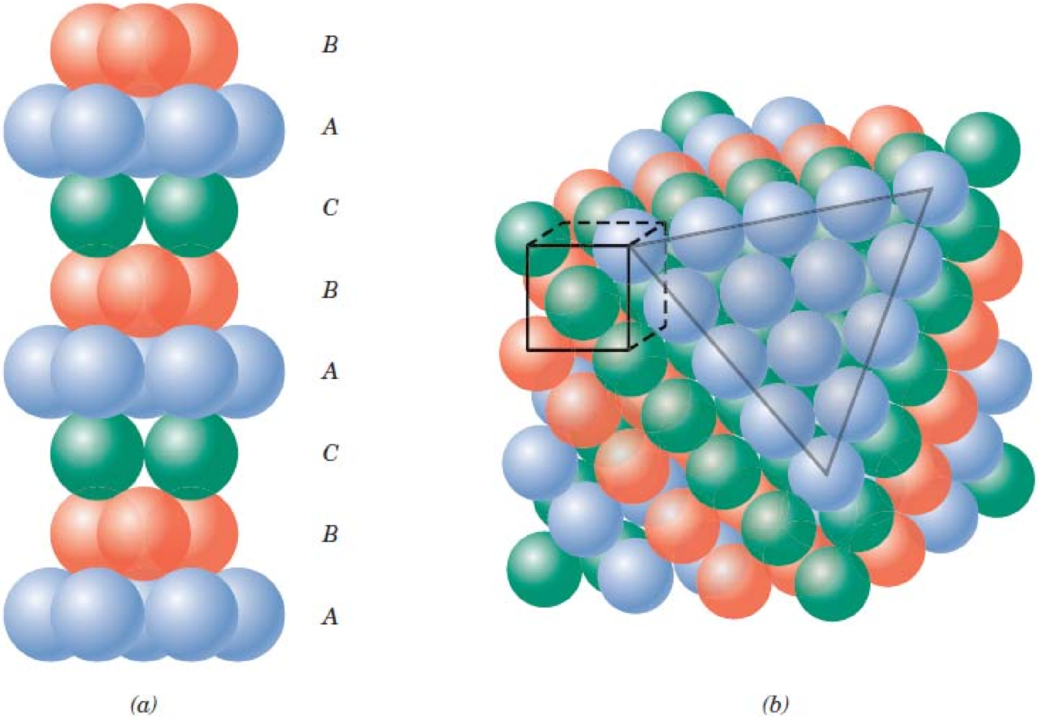


Figure 3.16 (*a*) Close-packed stacking sequence for face-centered cubic. (*b*) A corner has been removed to show the relation between the stacking of close- packed planes of atoms and the FCC crystal structure; the heavy triangle outlines a (111) plane.

Crystalline and Noncrystalline Materials
Single Crystals

- A **single crystal:** the result when the periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen without interruption.
  - Single crystals exist in nature, but they may also be produced artificially.
- The crystal assumes a regular geometric shape having flat faces, as with some of the gemstones; the shape is indicative of the crystal structure.
- Recently, single crystals have become extremely important in many of our modern technologies, in particular electronic microcircuits, which employ single crystals of silicon and other semiconductors.

Crystalline and Noncrystalline Materials

Single Crystals

Figure 3.17 Photograph of a garnet single crystal that was found in Tongbei, Fujian Province, China.

Crystalline and Noncrystalline Materials

Polycrystalline Materials

- **Polycrystalline Materials:** those materials which are composed of a collection of many small crystals or **grains.**


(a)

(b)

Figure 3.18 Schematic diagrams of the various stages in the solidification of a polycrystalline material; the square grids depict unit cells. (*a*) Small crystallite nuclei. (*b*) Growth of the crystallites; the obstruction of some grains that are adjacent to one another is also shown. (*c*) Upon completion of solidification, grains having irregular shapes have formed. (*d*) The grain structure as it would appear under the microscope; dark lines are the grain boundaries.

Crystalline and Noncrystalline Materials
Anisotropy

- **Anisotropy:** directionality of properties, i.e. single crystal materials have different properties in different directions.
    - For example, the elastic modulus, may have different values in the [100] and [111] directions.
- Anisotropy is associated with the variance of atomic or ionic spacing with crystallographic direction.
- The degree of anisotropy increases with decreasing structural symmetry—triclinic structures normally are highly anisotropic.
- Substances in which measured properties are independent of the direction of measurement are **isotropic.**

Crystalline and Noncrystalline Materials

Anisotropy

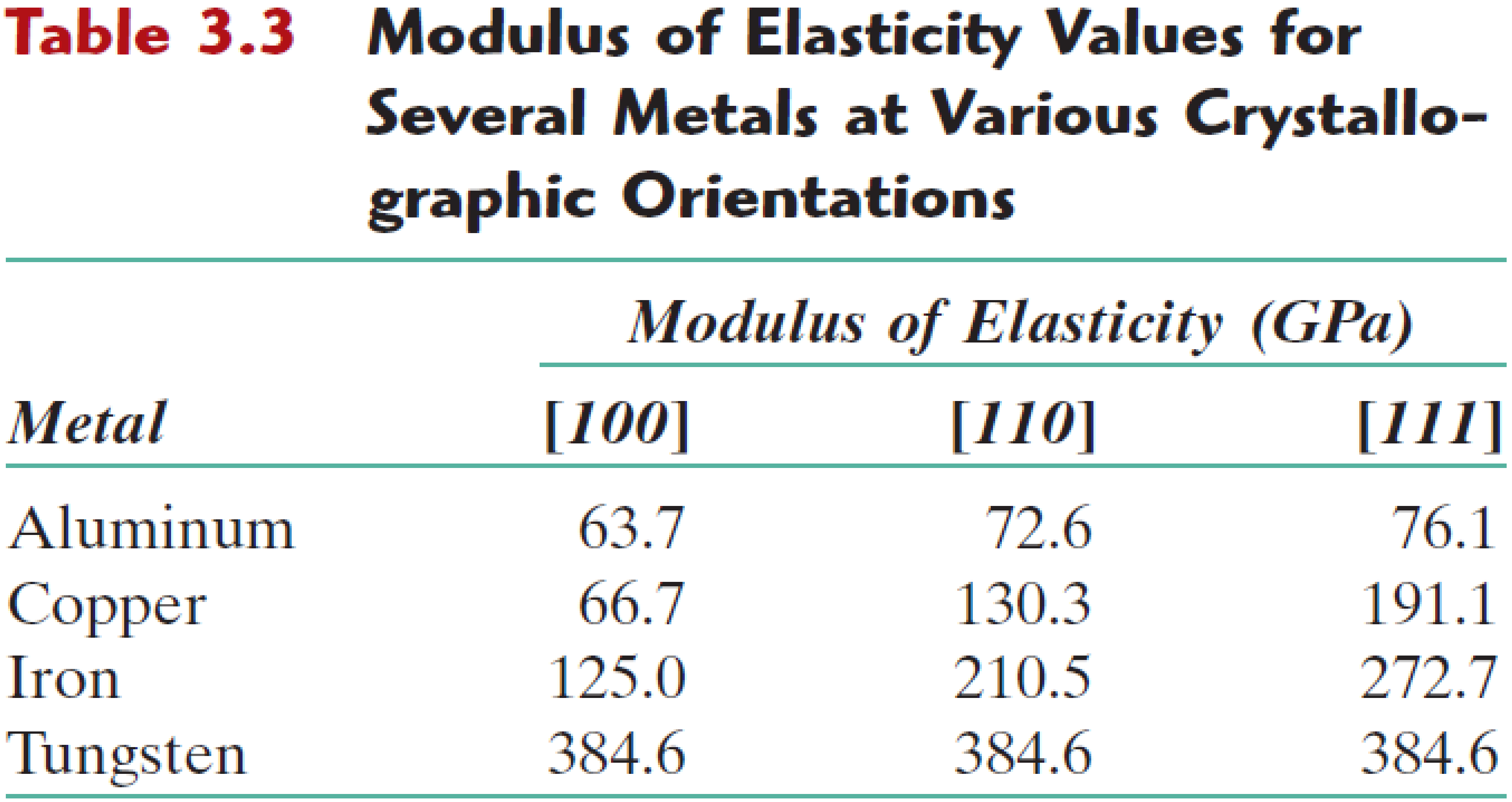


Table 3.3 **Modulus of Elasticity Values for Several Metals at Various Crystallographic Orientations**

	Modulus of Elasticity (GPa)		
Metal	*[100]*	*[110]*	*[111]*
Aluminum	63.7	72.6	76.1
Copper	66.7	130.3	191.1
Iron	125.0	210.5	272.7
Tungsten	384.6	384.6	384.6

Crystalline and Noncrystalline Materials
Anisotropy

- For many polycrystalline materials, the crystallographic orientations of the individual grains are totally random.
    - Under these circumstances, even though each grain may be anisotropic, a specimen composed of the grain aggregate behaves isotropically.
- Also, the magnitude of a measured property represents some average of the directional values.
- Sometimes the grains in polycrystalline materials have a preferential crystallographic orientation, in which case the material is said to have a “texture.”

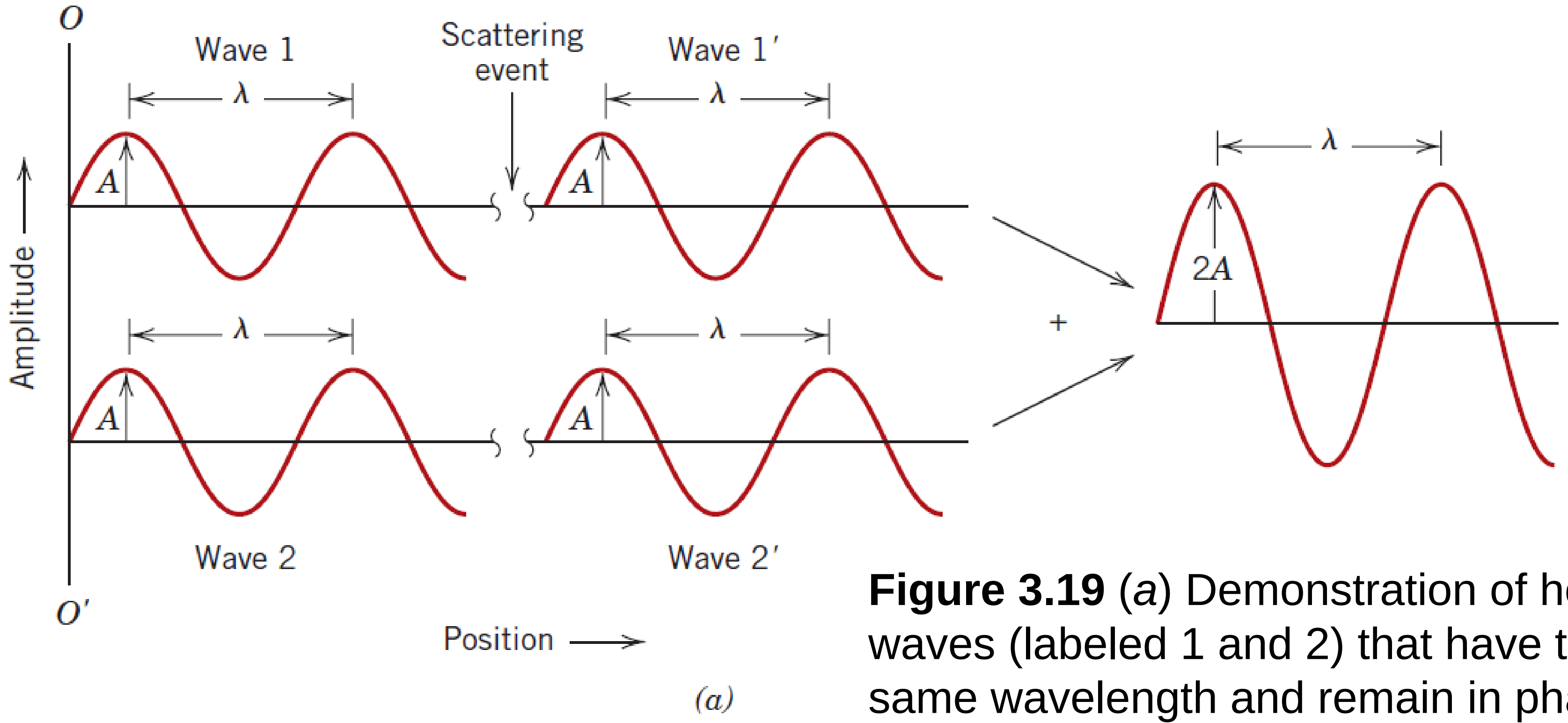
X-Ray Diffraction: Determination of Crystal Structures

The Diffraction Phenomenon

- Diffraction occurs when a wave encounters a series of regularly spaced obstacles that:
  - (1) are capable of scattering the wave, and
  - (2) have spacings that are comparable in magnitude to the wavelength.
- Furthermore, diffraction is a consequence of specific phase relationships established between two or more waves that have been scattered by the obstacles.

X-Ray Diffraction: Determination of Crystal Structures

The Diffraction Phenomenon

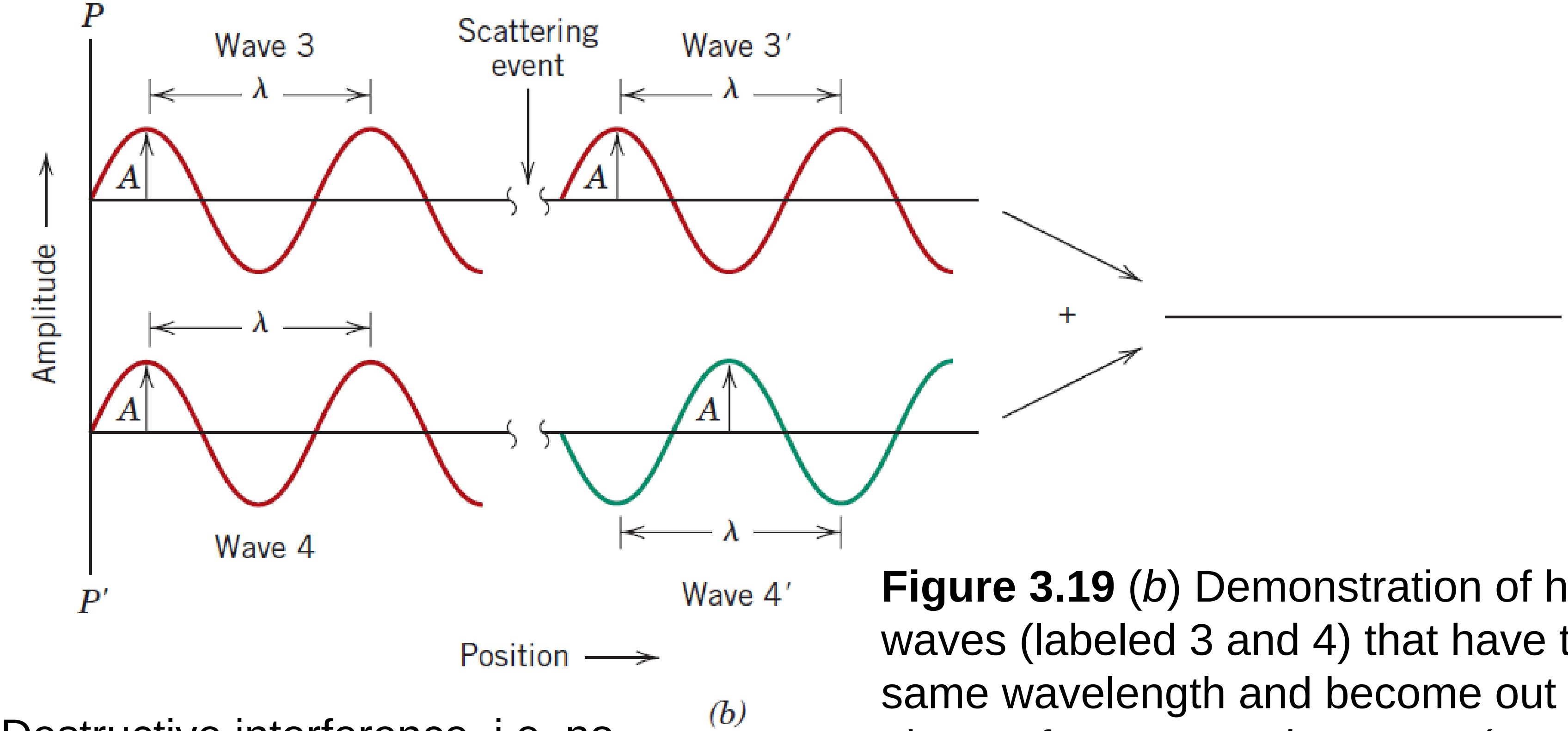


This is a manifestation of **diffraction,** and we refer to a diffracted beam as one composed of a large number of scattered waves that mutually reinforce one another.

Figure 3.19 (*a*) Demonstration of how two waves (labeled 1 and 2) that have the same wavelength and remain in phase after a scattering event (waves 1’ and 2’) constructively interfere with one another. The amplitudes of the scattered waves add together in the resultant wave.

X-Ray Diffraction: Determination of Crystal Structures

The Diffraction Phenomenon



Destructive interference, i.e. no diffraction.

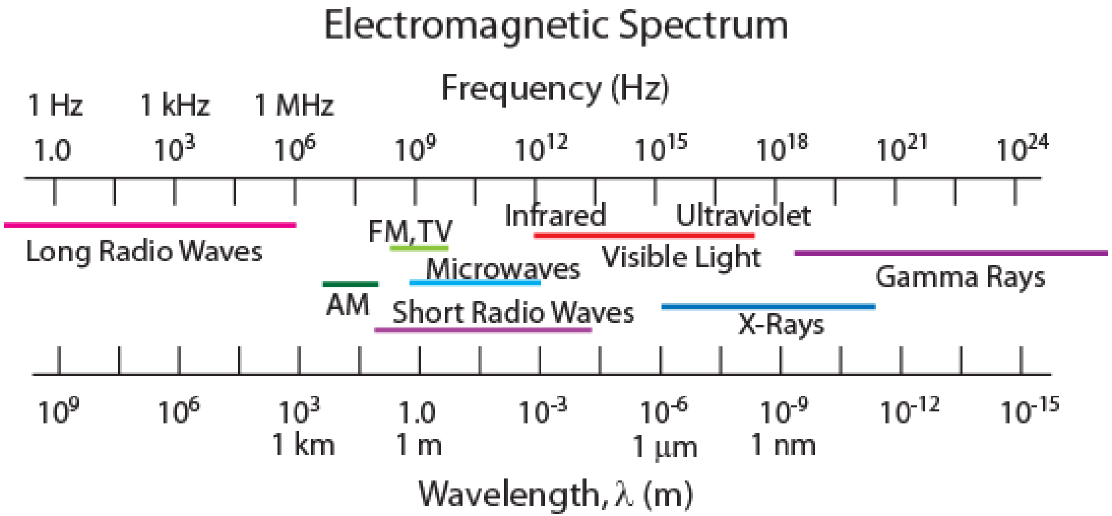
Figure 3.19 (*b*) Demonstration of how two waves (labeled 3 and 4) that have the same wavelength and become out of phase after a scattering event (waves 3’ and 4’) destructively interfere with one another. The amplitudes of the two scattered waves cancel one another.

X-Ray Diffraction: Determination of Crystal Structures

X-Ray Diffraction and Bragg's Law

- X-rays are a form of electromagnetic radiation that have high energies and short wavelengths (on the order of the atomic spacings for solids).

- When a beam of x-rays impinges on a solid material, a portion of this beam will be scattered in all directions by the electrons associated with each atom or ion that lies within the beam's path.



X-Ray Diffraction: Determination of Crystal Structures

X-Ray Diffraction and Bragg’s Law

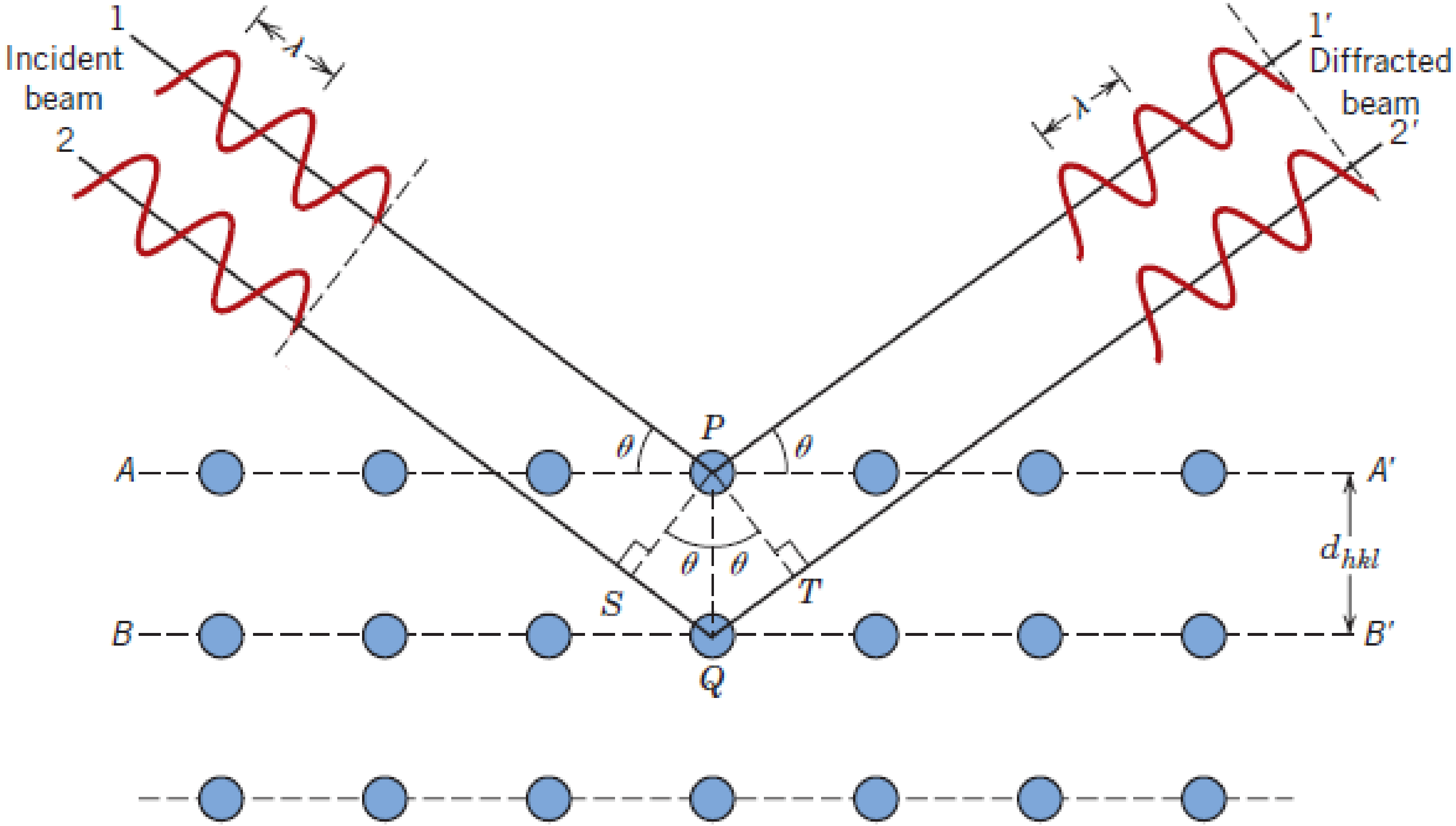


Figure 3.20 Diffraction of x-rays by planes of atoms.

X-Ray Diffraction: Determination of Crystal Structures

X-Ray Diffraction and Bragg’s Law

- If the path length difference between 1—*P*—1’ and 2—*Q*—2’ (i.e., $\overline{SQ} + \overline{QT}$) is equal to a whole number, *n*, of wavelengths. That is, the condition for diffraction is:

$$n\lambda = \overline{SQ} + \overline{QT}$$

or

$$n\lambda = d_{hkl}\sin\theta + d_{hkl}\sin\theta$$

$$n\lambda = 2d_{hkl}\sin\theta$$

→ Bragg’s law

n is the order of reflection, which may be any integer (1, 2, 3, . . .)

If Bragg’s law is not satisfied, then the interference will be nonconstructive in nature so as to yield a very low-intensity diffracted beam.

X-Ray Diffraction: Determination of Crystal Structures

X-Ray Diffraction and Bragg’s Law

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

→ For cubic

d_{hkl}: The magnitude of the distance between two adjacent and parallel planes of atoms (the interplanar spacing).

a: lattice parameter.

For the BCC crystal structure, $h + k + l$ must be even if diffraction is to occur, whereas for FCC, h, k, and l must all be either odd or even.

X-Ray Diffraction: Determination of Crystal Structures

Diffraction Techniques

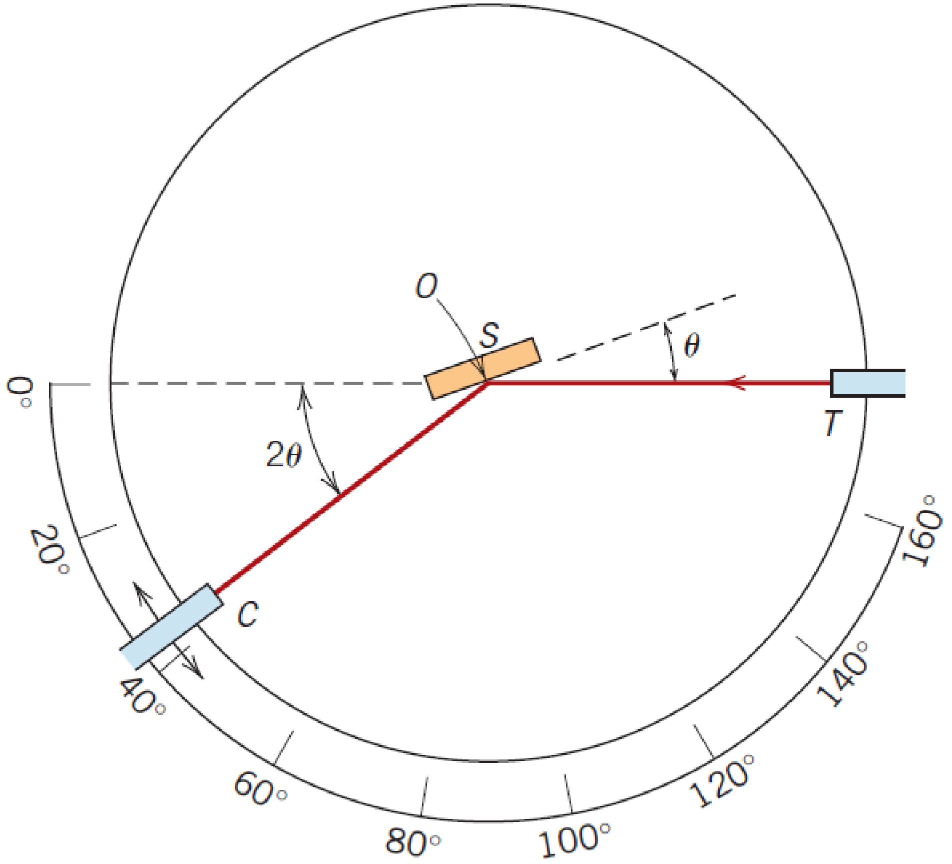


Figure 3.21 Schematic diagram of an x-ray diffractometer; *T:* x-ray source, *S:* specimen, *C:* detector, *O:* the axis around which the specimen and detector rotate, and 2 *θ* : the diffraction angle.

One of the primary uses of x-ray diffractometry is for the determination of crystal structure. The unit cell size and geometry may be resolved from the angular positions of the diffraction peaks, whereas arrangement of atoms within the unit cell is associated with the relative intensities of these peaks.

X-Ray Diffraction: Determination of Crystal Structures

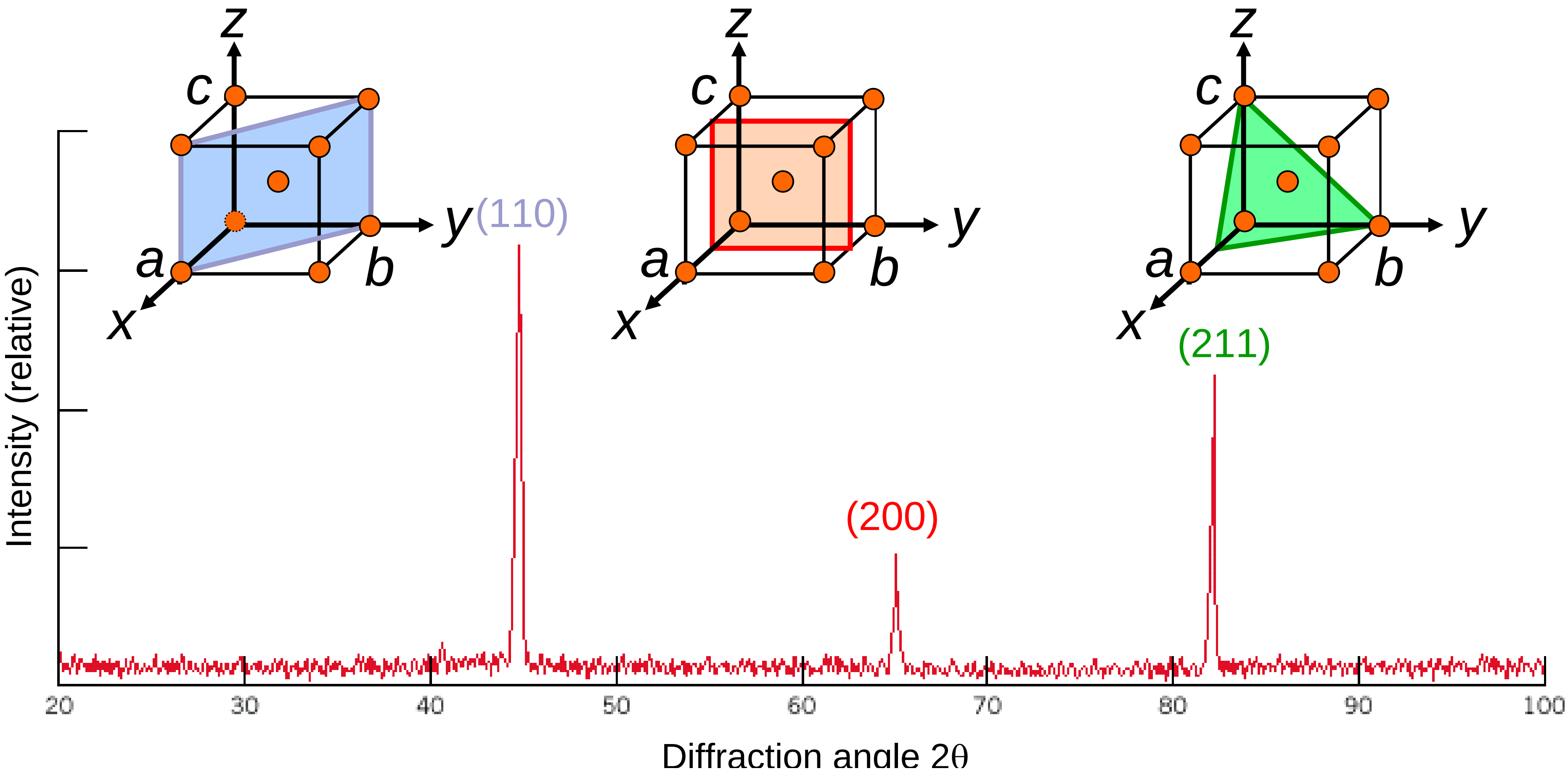


Figure 3.22 Diffraction pattern for polycrystalline α-iron (BCC)

X-Ray Diffraction: Determination of Crystal Structures

X-Ray Diffraction and Bragg’s Law

- Example 3.13: For BCC iron, compute (a) the interplanar spacing and (b) the diffraction angle for the (220) set of planes. The lattice parameter for Fe is 0.2866 nm. Also, assume that monochromatic radiation having a wavelength of 0.1790 nm is used, and the order of reflection is 1.

Noncrystalline Solids

- **Noncrystalline (amorphous)** solids: lack a systematic and regular arrangement of atoms over relatively large atomic distances.

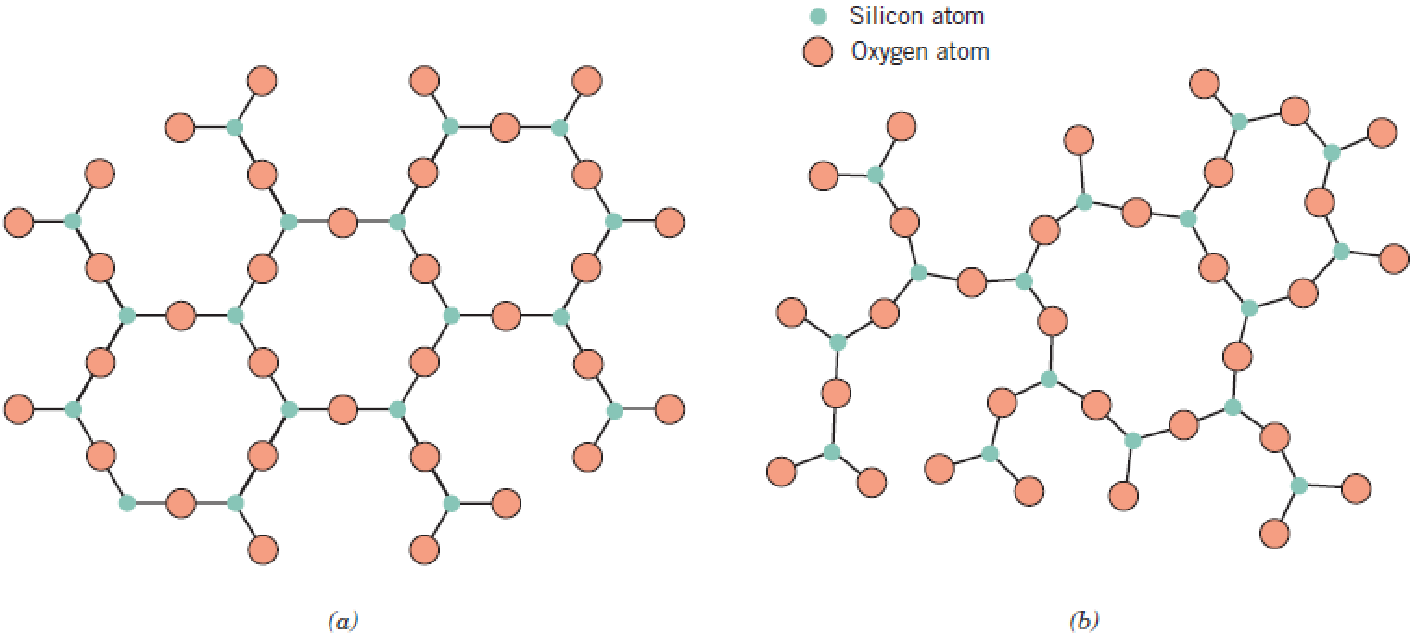


Figure 3.23 Two-dimensional schemes of the structure of (*a*) crystalline silicon dioxide and (*b*) noncrystalline silicon dioxide.

Noncrystalline Solids

- Whether a crystalline or amorphous solid forms depends on
  - The ease with which a random atomic structure in the liquid can transform to an ordered state during solidification.
- Amorphous materials, therefore, are characterized by atomic or molecular structures that are relatively complex and become ordered only with some difficulty.
  - Furthermore, rapidly cooling through the freezing temperature favors the formation of a noncrystalline solid, because little time is allowed for the ordering process.

Noncrystalline Solids

- Metals normally form crystalline solids.
- Some ceramic materials are crystalline, whereas others, the inorganic glasses, are amorphous.
- Polymers may be completely noncrystalline and semi-crystalline consisting of varying degrees of crystallinity.