

Structure and Properties of Materials

Module: M5X01185



Chapter 3: Structures of Metals & Ceramics

Lecture Aims

- What is the difference in atomic arrangement between crystalline and noncrystalline solids?
- What features of a metal's/ceramic's atomic structure determine its density?
- How do the crystal structures of ceramic materials differ from those for metals?
- Under what circumstances does a material property vary with the measurement direction?



Why study crystal structures?

- Crystal structures are directly related to a materials' properties such as brittleness or ductility
- Optical transparency occurs in non-crystalline ceramics and polymers however the same materials in crystalline form are opaque.

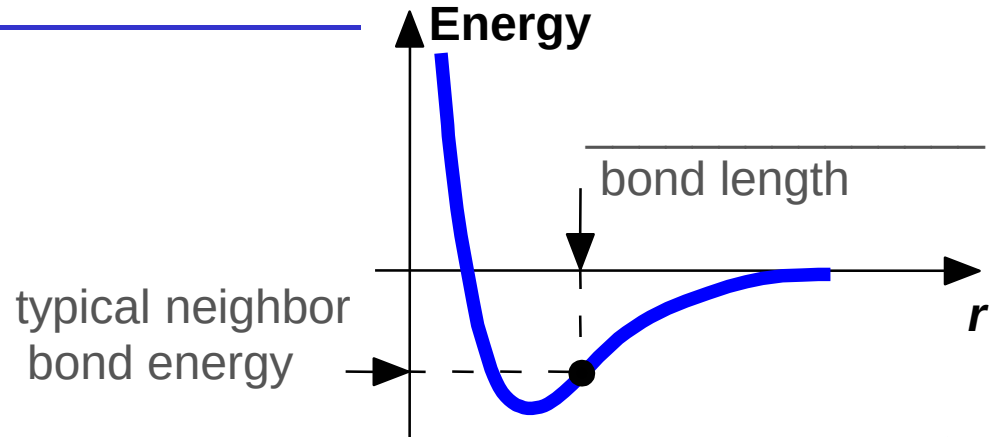
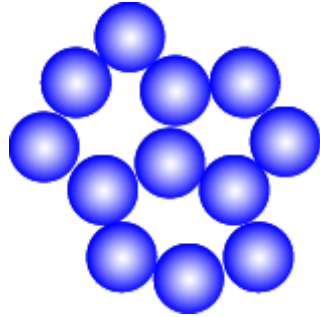
Fundamental Concepts

- A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances;
- 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.

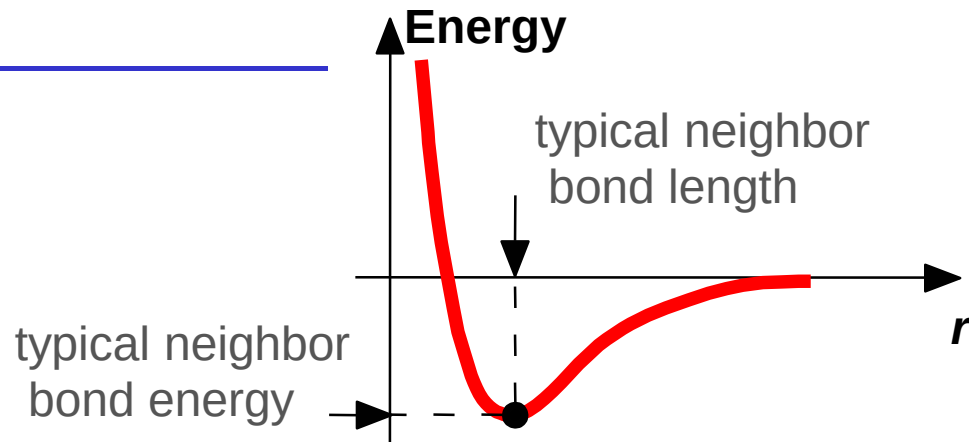
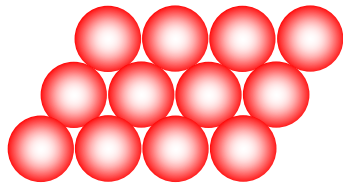


Energy and Packing

- Non dense, _____



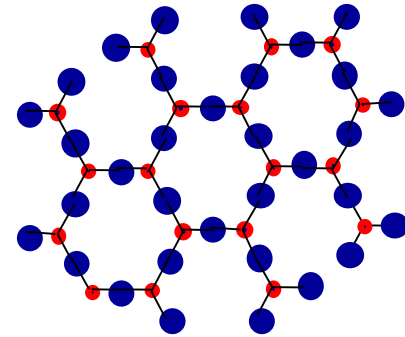
- Dense, _____



Materials and Packing

Crystalline materials...

- atoms pack periodically in 3D arrays



crystalline SiO₂

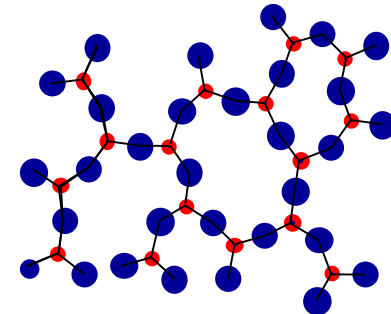
Adapted from Fig. 3.41(a),
Callister & Rethwisch 4e.

Noncrystalline materials...

- atoms have no periodic packing

"Amorphous" AKA Noncrystalline

• Si • Oxygen



noncrystalline SiO₂

Adapted from Fig. 3.41(b),
Callister & Rethwisch 4e.

Metallic Crystal Structures

- Atomic bonding is non-directional (due to metallic bonding, i.e. positive ion core attracted to a sea of electrons)
- Large numbers of nearest neighbours
- Dense atomic packing for most metallic structures
- Most common structures are face centred cubic (fcc), body centred cubic (bcc) and hexagonal close packed (hcp)

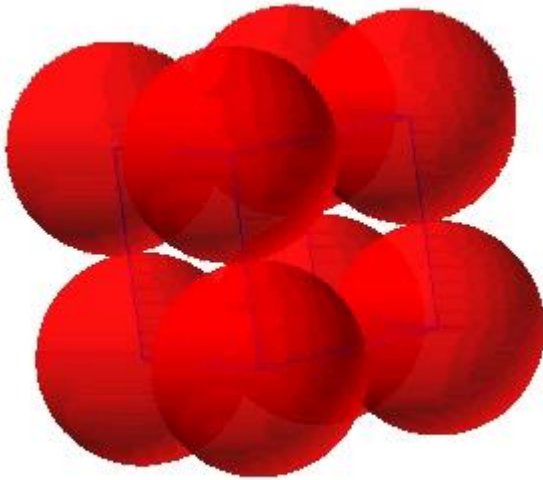


Simple Cubic Structure (SC)

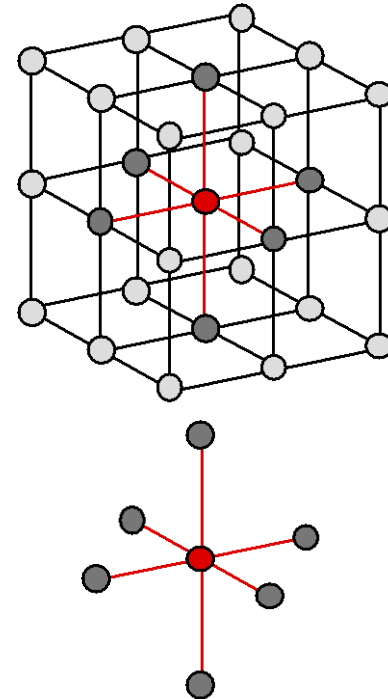
- Rare due to low packing density (only Po has this structure)

$a = 2R$, where a = cube length and R is the atomic radius

- **Coordination #** = 6
(# nearest neighbors)



Click once on image to start animation
(Courtesy P.M. Anderson)



Atomic Packing Factor (APF) (SC)

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

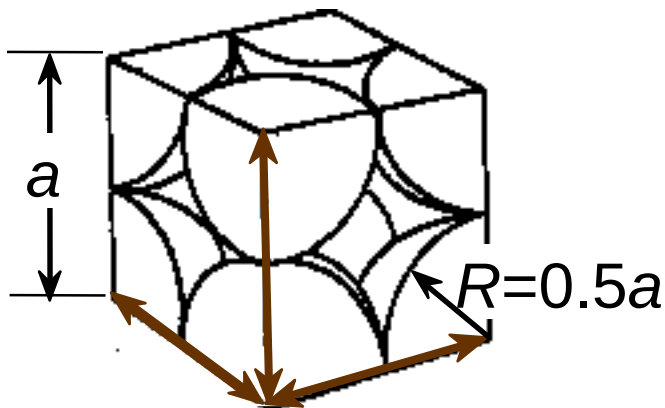
To find the APF

1. find the number of atoms in the unit cell
2. Multiply that number by the volume of a sphere with the radius (R) is given in terms of cube length (a)
3. Divide by the volume of a cube

NB when calculating R in terms of a, use pythagoras with a triangle drawn along the line where the ion cores touch.

i.e. fcc – ion cores touch along a face diagonal

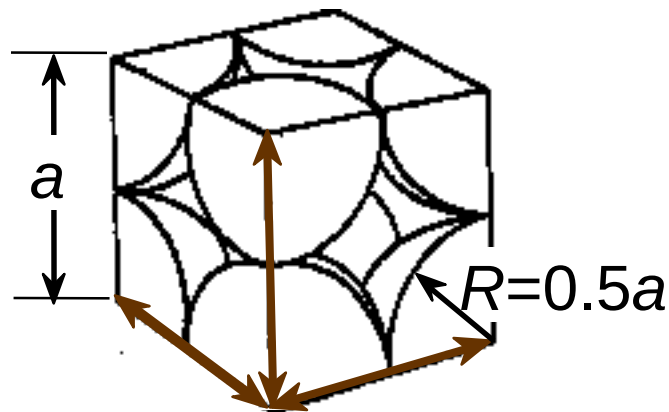
Bcc – ion cores touch along a cube diagonal eg bottom front left to top back right



Atomic Packing Factor (APF) (SC)

$$APF = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

- APF for a simple cubic structure = 0.52



close-packed

contains $8 \times 1/8 =$

1 atom/unit cell

Adapted from Fig. 3.43,
Callister & Rethwisch 4e.

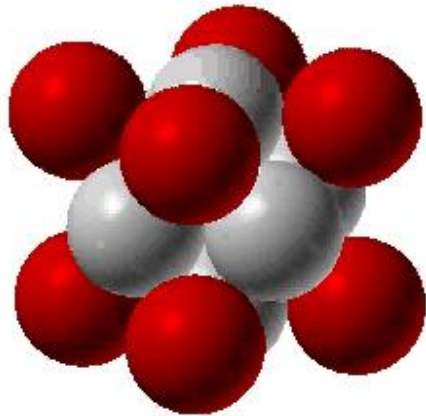
$$APF = \frac{\overbrace{1}^{\text{atoms}} \overbrace{\frac{4}{3} \pi (0.5a)^3}^{\text{volume atom}}}{\underbrace{a^3}_{\text{volume unit cell}}}$$

Face Centered Cubic Structure (FCC)

- Atoms touch each other along face.

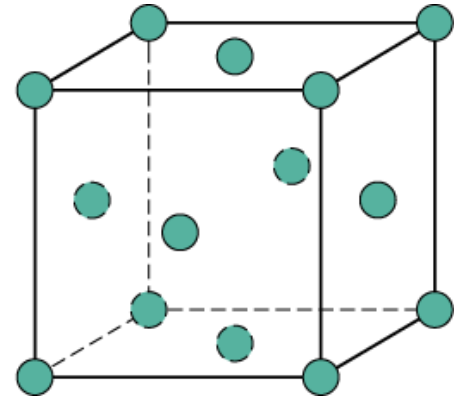
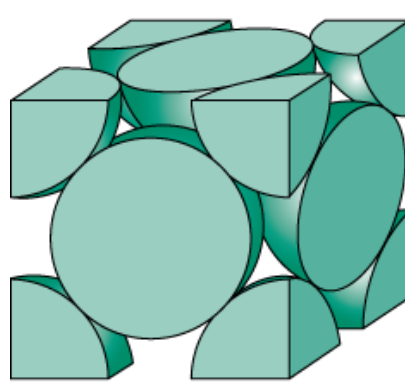
ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12



Click once on image to start animation

(Courtesy P.M. Anderson)

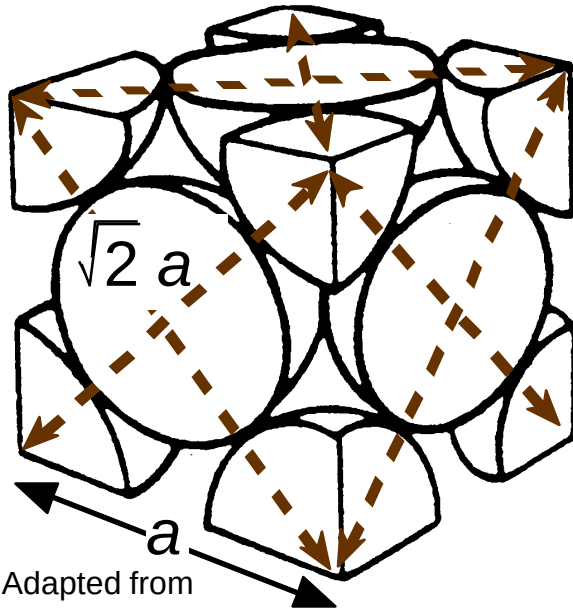


Adapted from Fig. 3.1, *Callister & Rethwisch 4e*.

4 atoms/unit cell: $6 \text{ face} \times \frac{1}{2} + 8 \text{ corners} \times \frac{1}{8}$

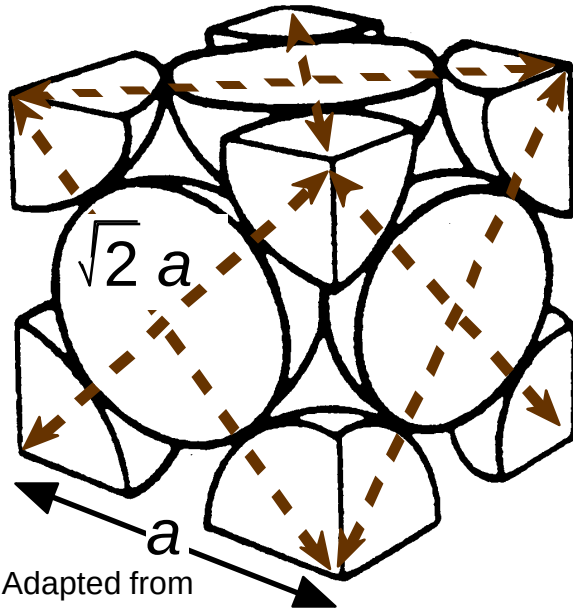
Atomic Packing Factor: FCC

Calculate the APF for a face-centered cubic structure



Adapted from
Fig. 3.1(a),
*Callister &
Rethwisch 4e.*

Atomic Packing Factor: FCC



Adapted from
Fig. 3.1(a),
Callister &
Rethwisch 4e.

Close-packed directions:

$$\text{length} = 4R = \sqrt{2} a$$

Using Pythagoras

$$(4R)^2 = a^2 + a^2 = 2a^2$$

$$16R^2 = 2a^2$$

$$R = \sqrt{\frac{2a^2}{16}} = \frac{a}{4}\sqrt{2}$$

$$APF = \frac{(4) \frac{4}{3} \pi \left(\frac{a}{4} \sqrt{2}\right)^3}{a^3} = 0.74$$

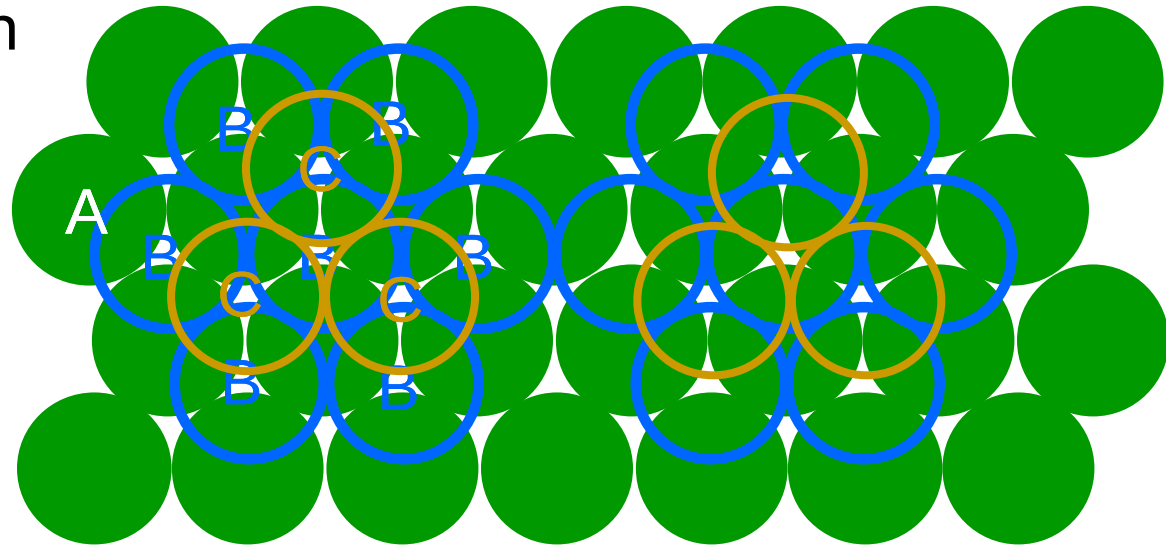
FCC Stacking Sequence

- ABCABC... _____ Sequence
- 2D Projection

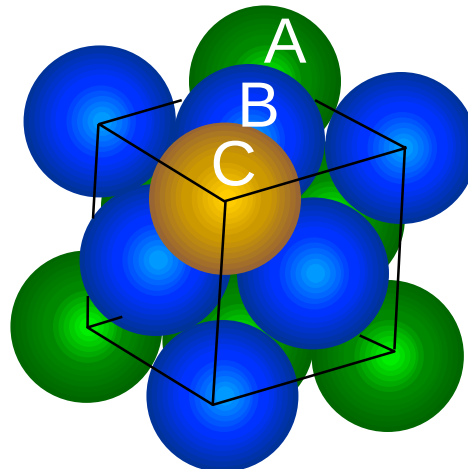
A sites

B sites

C sites



- FCC _____ Cell

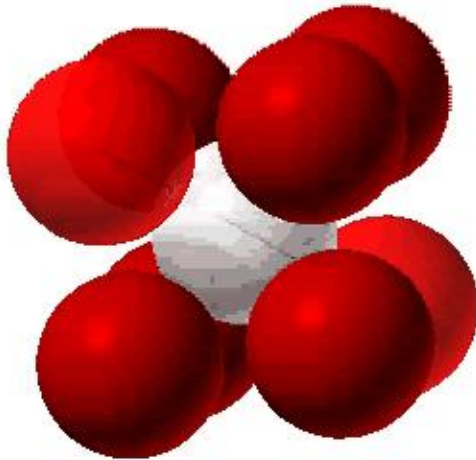


Body Centered Cubic Structure (BCC)

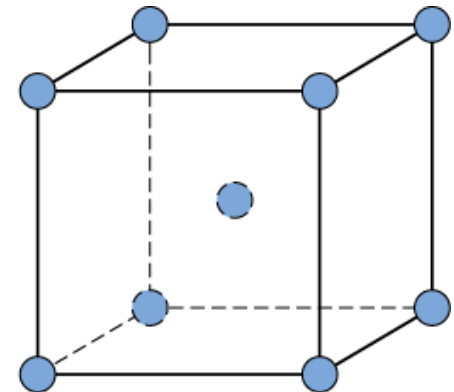
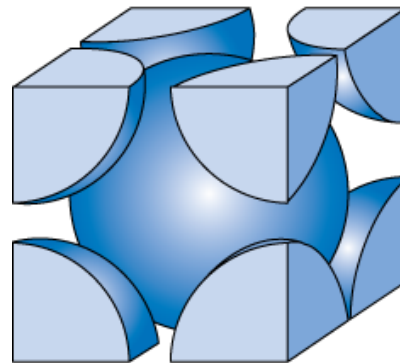
- Atoms touch each other along cube.
 - Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum

- Coordination # = 8



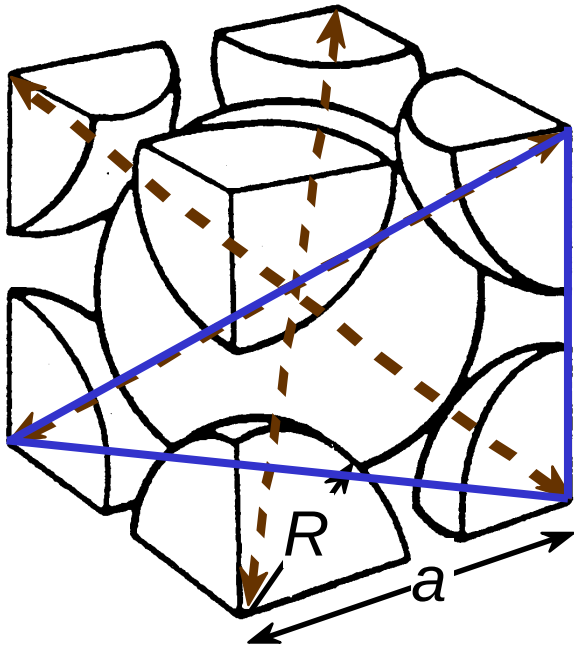
Click once on image to start animation
(Courtesy P.M. Anderson)



Adapted from Fig. 3.2,
Callister & Rethwisch 4e.

2 atoms/unit cell: 1 center + $8 \times 1/8$

Atomic Packing Factor: BCC



To find the base of the triangle x:

$$x^2 = a^2 + a^2 = 2a^2$$

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

Considering 'blue' triangle

To find the diagonal through the cube $4R$ "

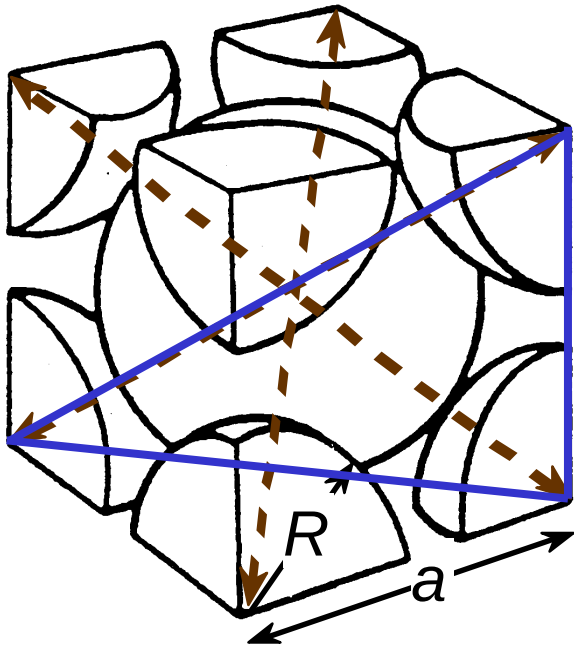
$$4R^2 = (\sqrt{2}a)^2 + a^2$$

$$4R = \sqrt{(2a + a)} = \sqrt{3}a$$

Atomic Packing Factor: BCC

So

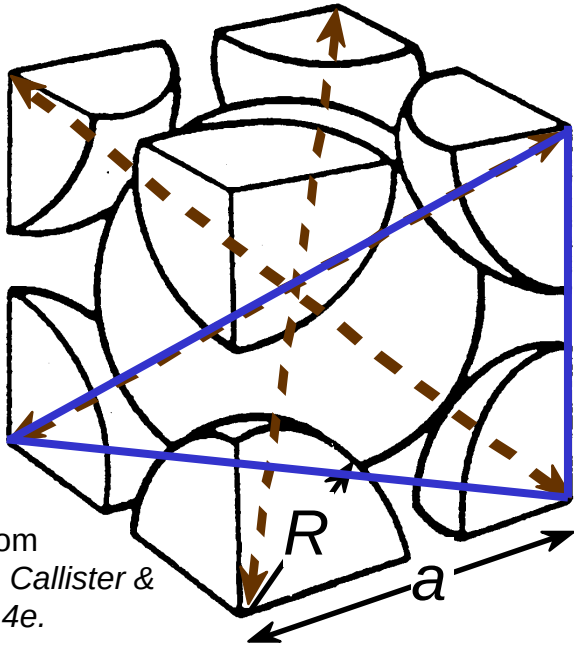
$$R = \frac{\sqrt{3}a}{4}$$



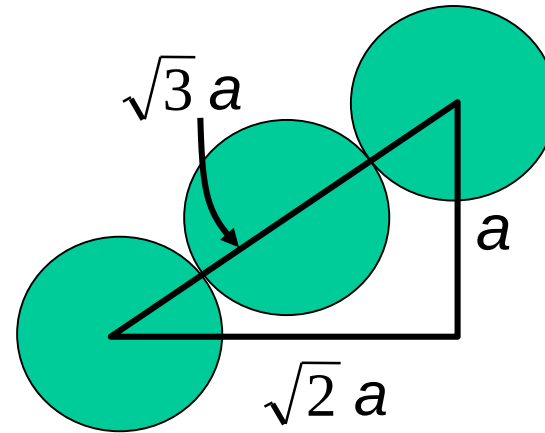
$$APF = \frac{(2) \frac{4}{3} \pi \left(\frac{a}{4} \sqrt{3}\right)^3}{a^3} = 0.68$$

Atomic Packing Factor: BCC

- APF for a body-centered structure = 0.68



Adapted from
Fig. 3.2(a), Callister &
Rethwisch 4e.

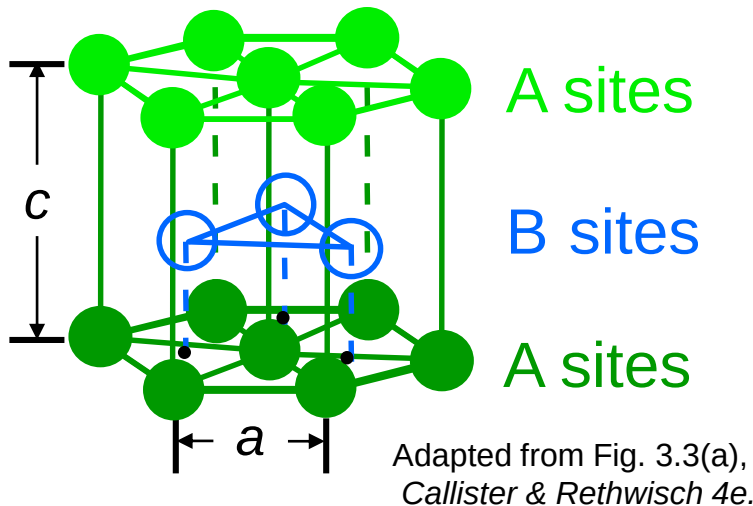


Close-packed _____ :
length = $4R = \sqrt{3}a$

$$\text{APF} = \frac{\begin{array}{c} \text{atoms} \\ \text{unit cell} \end{array} \quad 2 \quad \begin{array}{c} \text{volume} \\ \text{atom} \end{array} \quad \frac{4}{3} \pi (\sqrt{3}a/4)^3}{\begin{array}{c} \text{volume} \\ \text{unit cell} \end{array} \quad a^3}$$

Hexagonal Close-Packed Structure (HCP) (*not a cube*)

- ABAB... Stacking Sequence
- 3D Projection



- Coordination # = 12
- APF = 0.74

- 2D Projection



6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

Questions

Unit Cells

Metallic Crystal Structures

- 3.2** If the atomic radius of lead is 0.175 nm, calculate the volume of its unit cell in cubic meters.
- 3.3** Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius R are related through $a = 4R/\sqrt{3}$.

Table 3.1 Atomic Radii and Crystal Structures for 16 Metals

<i>Metal</i>	<i>Crystal Structure^a</i>	<i>Atomic Radius^b (nm)</i>	<i>Metal</i>	<i>Crystal Structure</i>	<i>Atomic Radius (nm)</i>
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 ($\text{\AA}$), multiply the nanometer value by 10.



Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

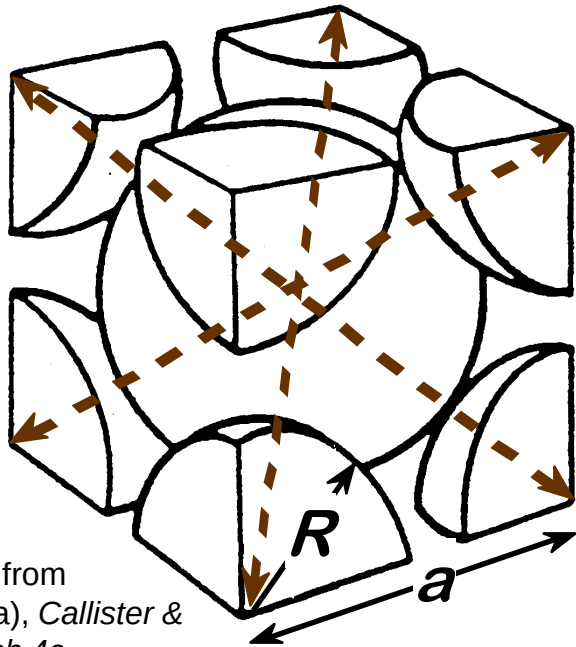
$$\rho = \frac{n A}{V_C N_A}$$

where

- n = number of atoms in each cell
- A = atomic weight
- V_C = unit cell volume
- N_A = Avogadro's number
= 6.022×10^{23} atoms/mol



Theoretical Density, ρ



Adapted from
Fig. 3.2(a), Callister &
Rethwisch 4e.

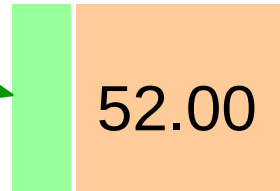
- Ex: Cr (BCC)

$$A = 52.00 \text{ g/mol}$$

$$n = 2 \text{ atoms/unit cell}$$

$$a = 4R/\sqrt{3} = 0.2887 \text{ nm}$$

atoms
unit cell



g
mol

$\rho =$

volume
unit cell

$$\frac{52.00}{a^3 \cdot 6.022 \times 10^{23}}$$

atoms
mol

$$\rho_{\text{theoretical}} = 7.18 \text{ g/cm}^3$$

$$\rho_{\text{actual}} = 7.19 \text{ g/cm}^3$$

Densities of Material Classes

In general

ρ_{metals} — ρ_{ceramics} — ρ_{polymers}

Why?

Metals have...

- close-packing (metallic bonding)
- often higher atomic masses

Ceramics have...

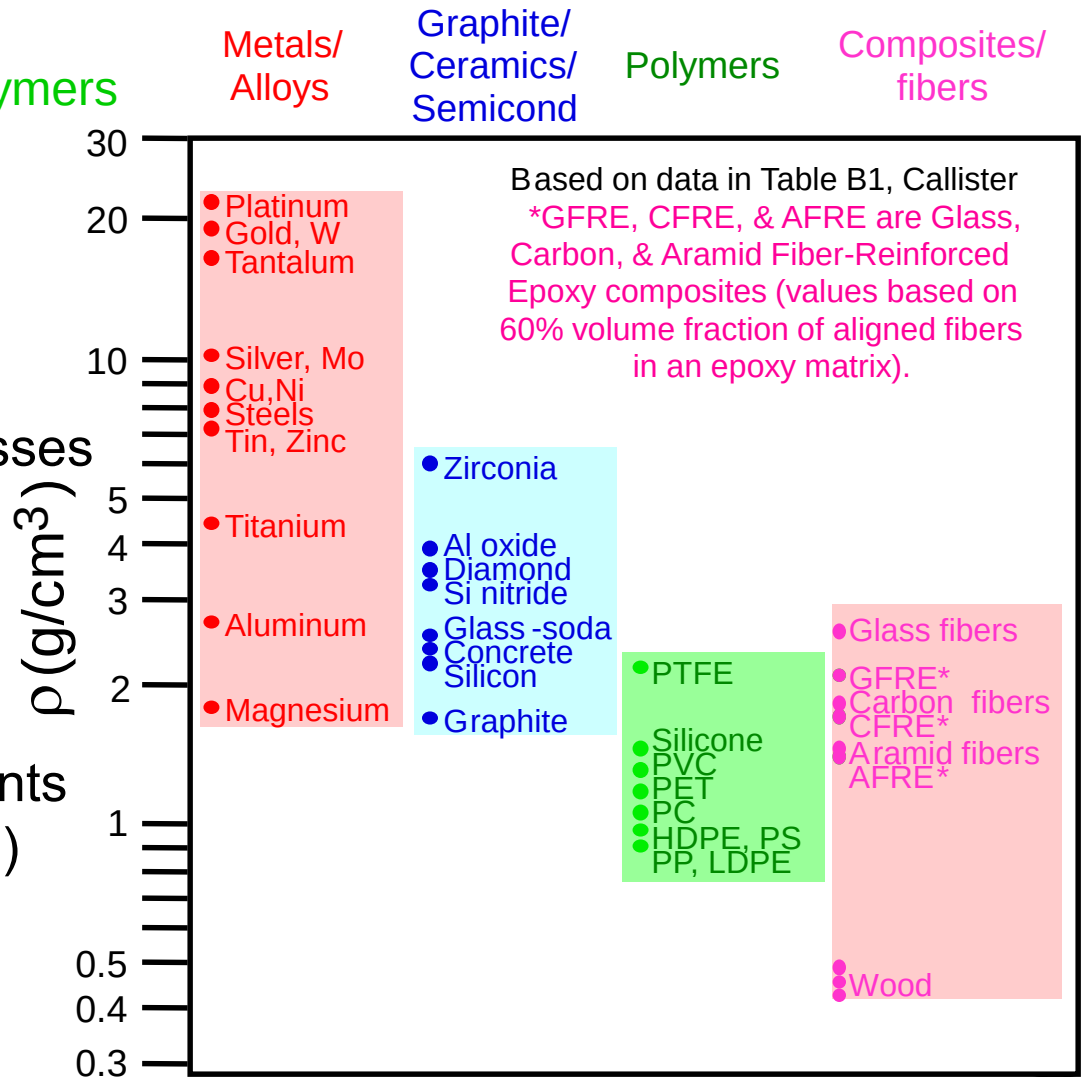
- less dense packing
- often lighter elements

Polymers have...

- low packing arrangements
- lighter elements (C,H,O)

Composites have...

- varying values



Data from Table B.1, Callister & Rethwisch, 8e.



Example

Copper has an atomic radius of 0.128nm, an FCC structure and an atomic weight of 63.5g/mol. Show that its density is 8.94 gCm⁻³

For FCC, n = 4 atoms and $R = \frac{a}{4}\sqrt{2}$. Also, given $A_{\text{Cu}}=63.5\text{g/mol}$ we can say that

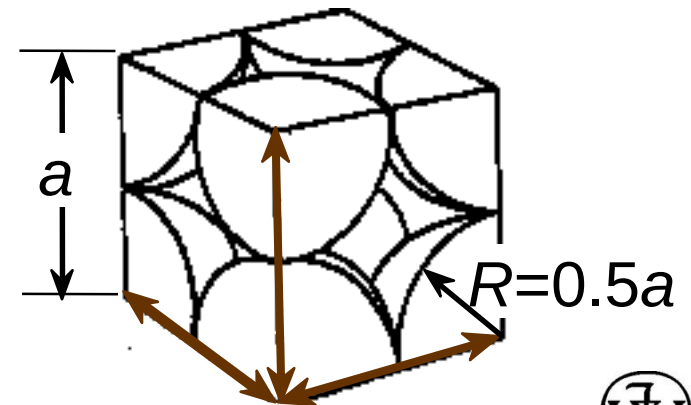
$$\rho = \frac{(4)(63.5)}{(6.02 \times 10^{23})} V, \text{ where } v = \frac{4}{3}\pi R^3 \text{ and } R = \frac{a\sqrt{2}}{4}$$



Questions

Density Computations

- 3.7** Molybdenum has a BCC crystal structure, an atomic radius of 0.1363 nm, and an atomic weight of 95.94 g/mol. Compute and compare its theoretical density with the experimental value found inside the front cover.
- 3.8** Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm^3 , and an atomic weight of 106.4 g/mol.
- 3.9** Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3 , and an atomic weight of 180.9 g/mol.
- 3.10** Some hypothetical metal has the simple cubic crystal structure shown in Figure 3.23. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.



Crystal Systems

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

7 crystal systems

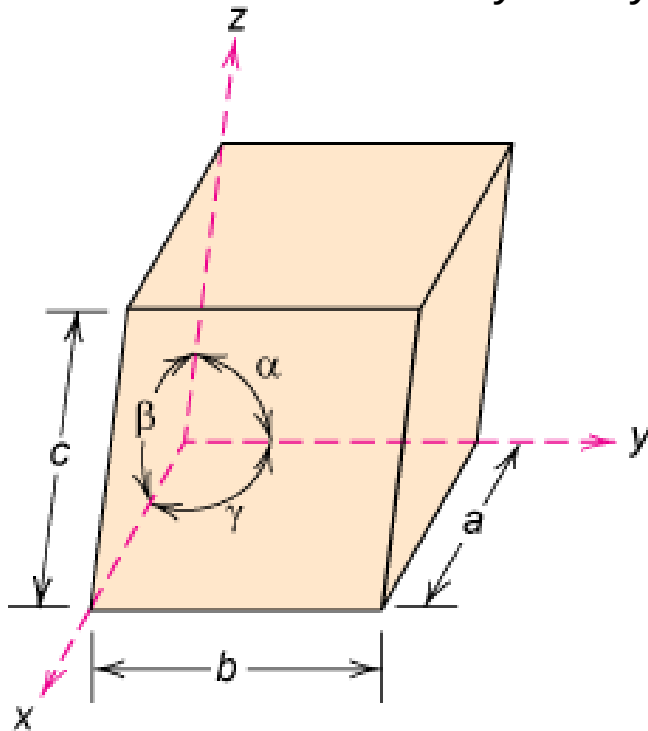
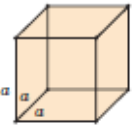
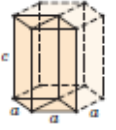
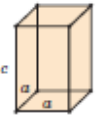
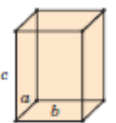
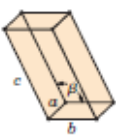
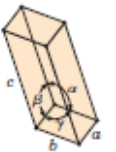
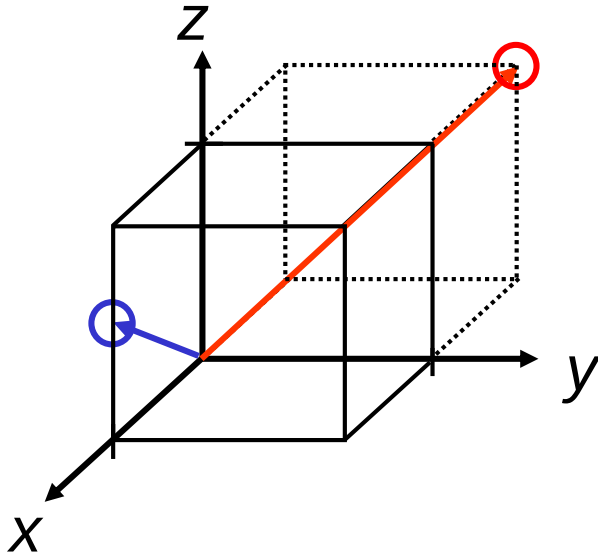


Fig. 3.20, Callister & Rethwisch 4e.

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

To Calculate Crystallographic Directions



1. Vector (if necessary) to pass through origin.
2. Read off in terms of unit cell dimensions a , b , and c
3. Adjust to smallest values
4. Enclose in square brackets, with no commas $[uvw]$

Find the indices of the blue line?

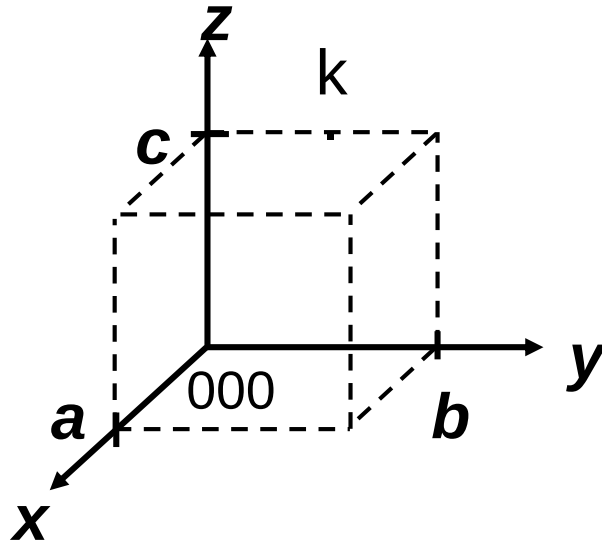
$a, 0, c/2$

$2a, 0, c$

$[201]$

Find the indices of the red line?

Point Coordinates



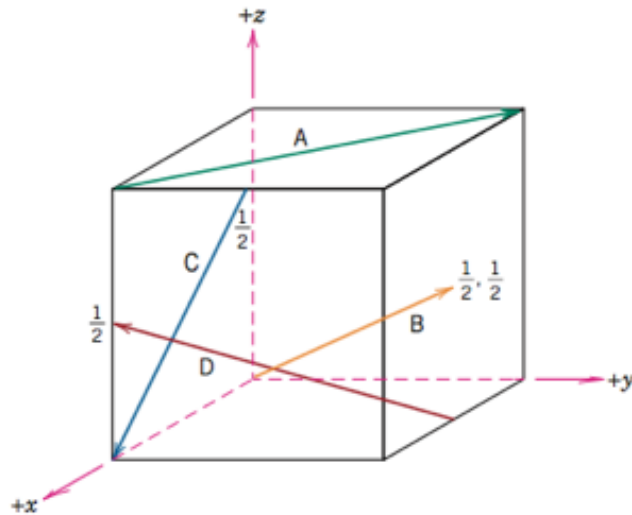
Draw the vectors for:

1. $[111]$
2. $[222]$
3. $[021]$
4. The point labelled k



Example (A)

3.31 Determine the indices for the directions shown in the following cubic unit cell:



Head point
011

Tail point
101

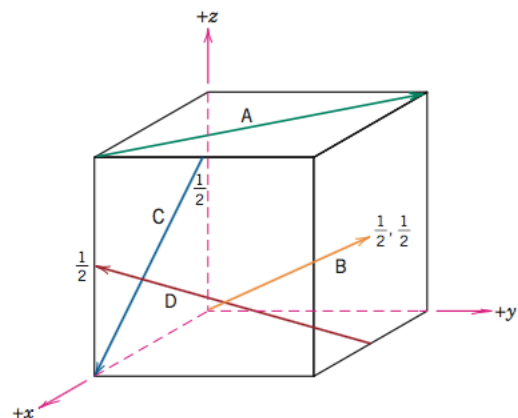
Head – Tail
(0-1)(1-0)(1-1)
[-110]

3.30 Within a cubic unit cell, sketch the following directions:

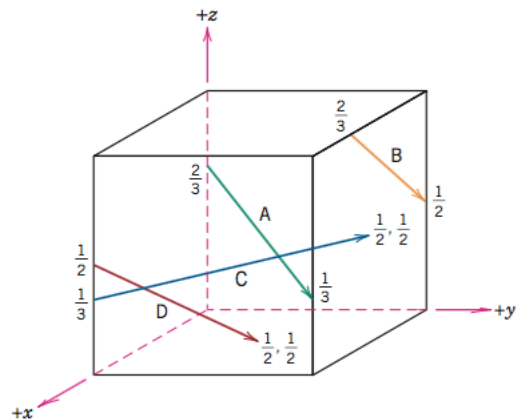


- (a) $[101]$, (e) $[\bar{1}1\bar{1}]$,
 (b) $[211]$, (f) $[\bar{2}12]$,
 (c) $[10\bar{2}]$, (g) $[3\bar{1}2]$,
 (d) $[3\bar{1}3]$, (h) $[301]$.

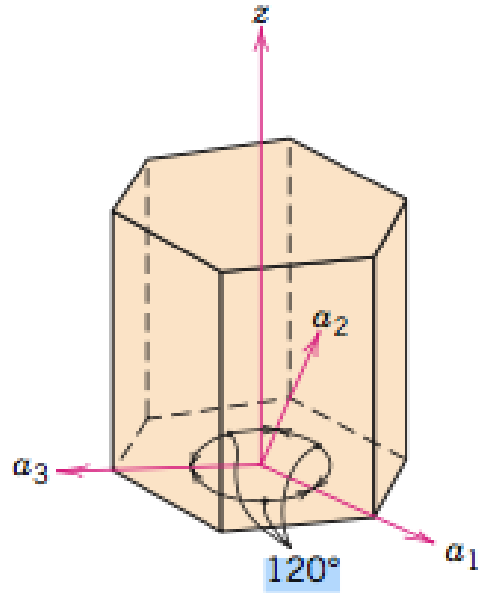
3.31 Determine the indices for the directions shown in the following cubic unit cell:



3.32 Determine the indices for the directions shown in the following cubic unit cell:



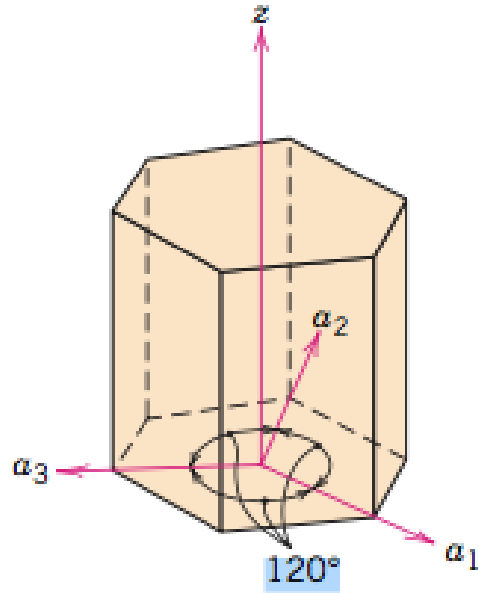
Drawing HCP Crystallographic Directions (i)



For Hexagonal close packed systems (HCP) we have to introduce a four-axis, or *Miller–Bravais*, coordinate system.

The three a_1 , a_2 , and a_3 axes are all contained within a single plane (basal plane) and are at 120° angles to one another and the z axis is perpendicular to this basal plane, in Miller-Bravais a_1 , a_2 , a_3 and z become $[uv tw]$

Drawing HCP Crystallographic Directions (i)



To convert from the 3 axis system to the 4 axis system use the following formulae

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

NB a1, a2 and z become u' , v' and w' respectively

Example

To find the direction of the green arrow.

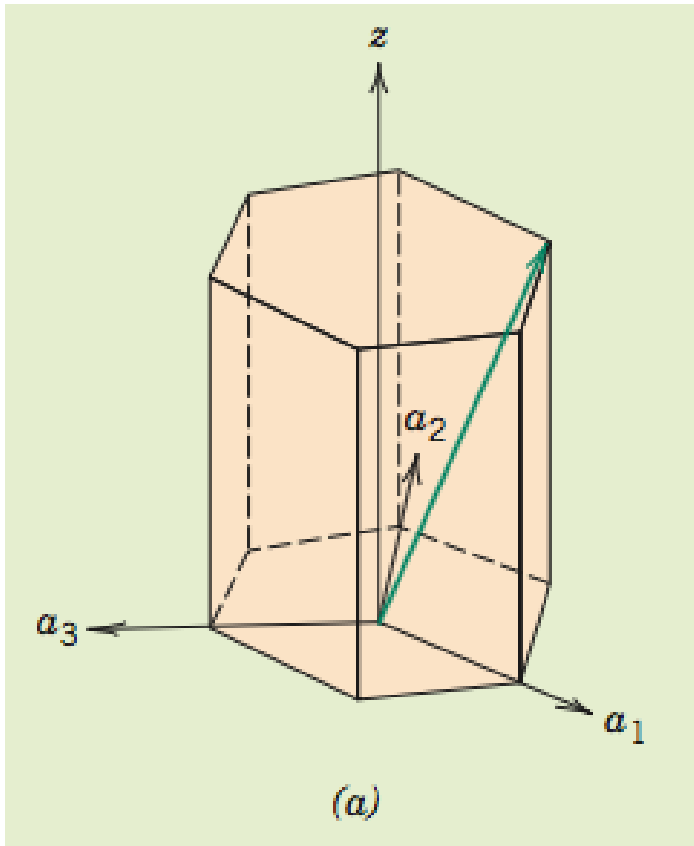
The first thing we do is neglect a_3 and just consider a_1 , a_2 and z .

As before

Head point
111

Tail point
000

Head – tail
111



Example

So $u'=1$, $v'=1$ and $w'=1$

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}(2(1) - (1)) = \frac{1}{3}$$

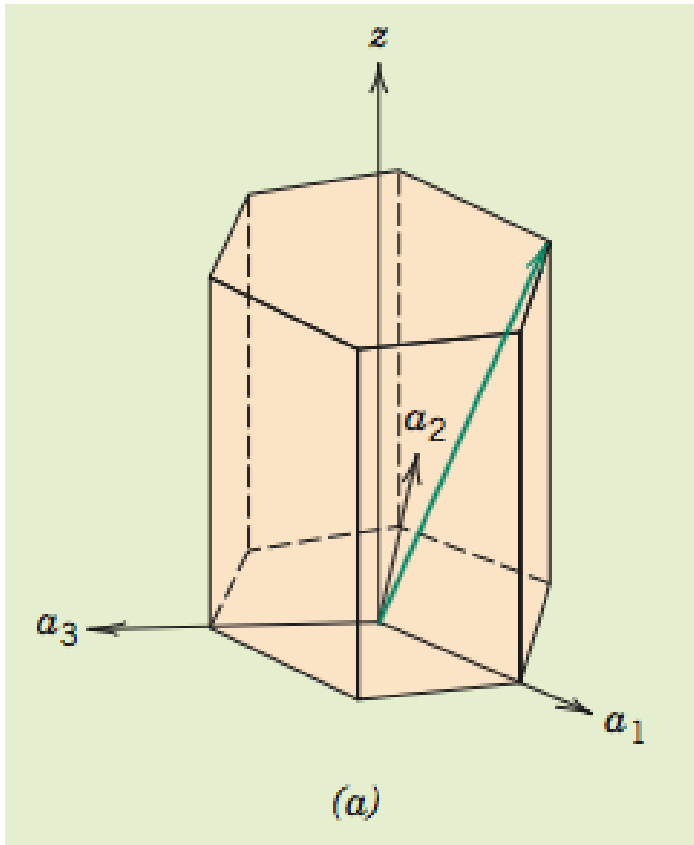
$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}$$

$$t = -(u + v) = -\left(\frac{1}{3} + \frac{1}{3}\right) = \frac{-2}{3}$$

$$w = w' = 1$$

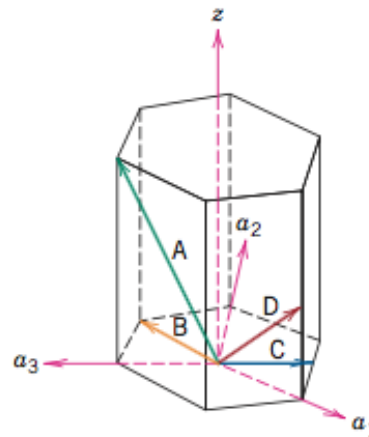
Multiply through by 3 to create integers

$$[11\bar{2}3]$$



Questions

3.35 Determine the indices for the directions shown in the following hexagonal unit cell:



3.36 Using Equations 3.6a, 3.6b, 3.6c, and 3.6d, derive expressions for each of the three primed indices set (u' , v' , and w') in terms of the four unprimed indices (u , v , t , and w).

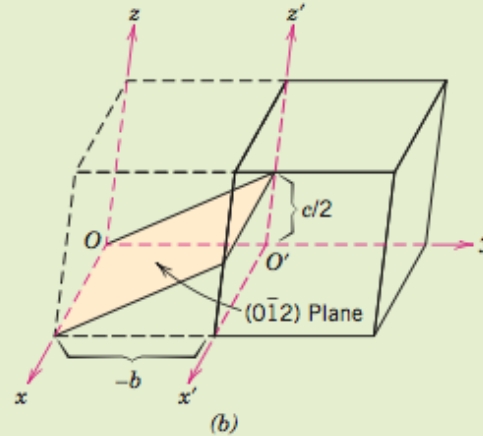
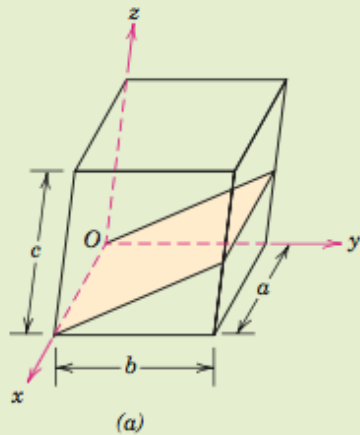
Crystallographic Planes

- 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.
- 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) .



Determination of Planar (Miller) Indices

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

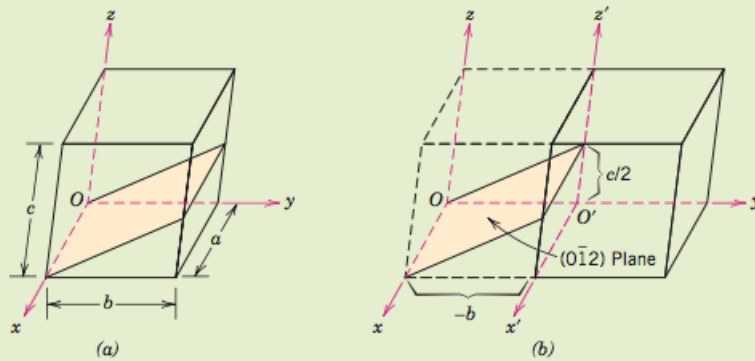


To determine Miller indices use 3 steps

1. Where do the planes intercept the axis
2. Take the inverse
3. Reduce the fractions

Determination of Planar (Miller) Indices

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



1. Where do the planes intercept the axis
2. Take the inverse
3. Reduce the fractions

It is not allowed for the plane to intercept the origin O therefore a new point O' is taken.

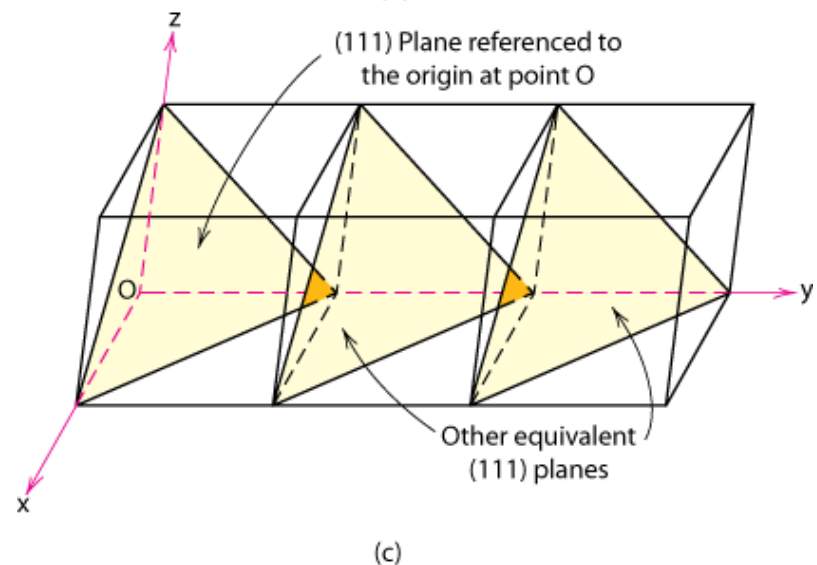
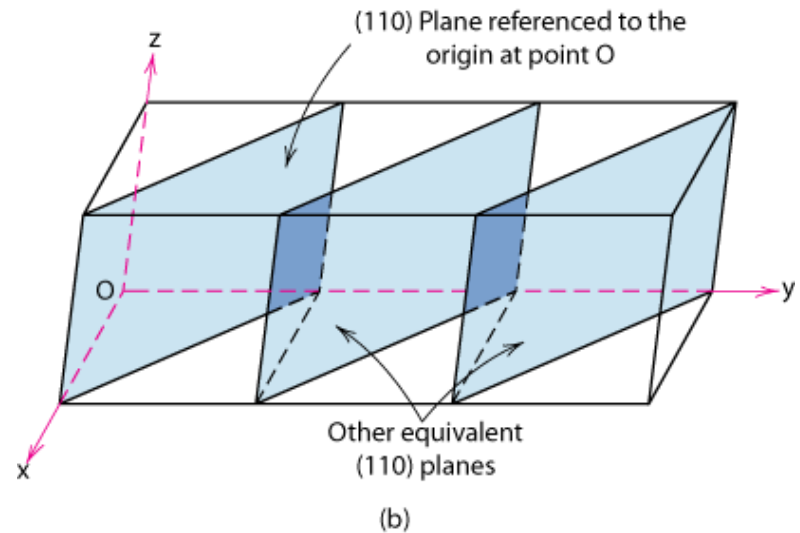
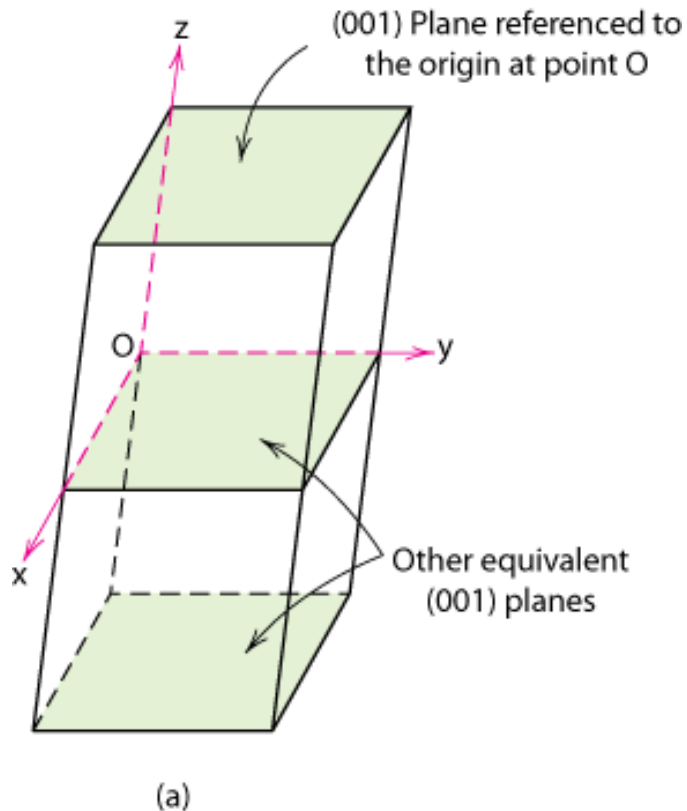
Intercepts (from O')

	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		$(0\bar{1}2)$	

- <https://www.youtube.com/watch?v=1TG456bpUk4>
- <https://www.youtube.com/watch?v=ElneDZrrL-Y>



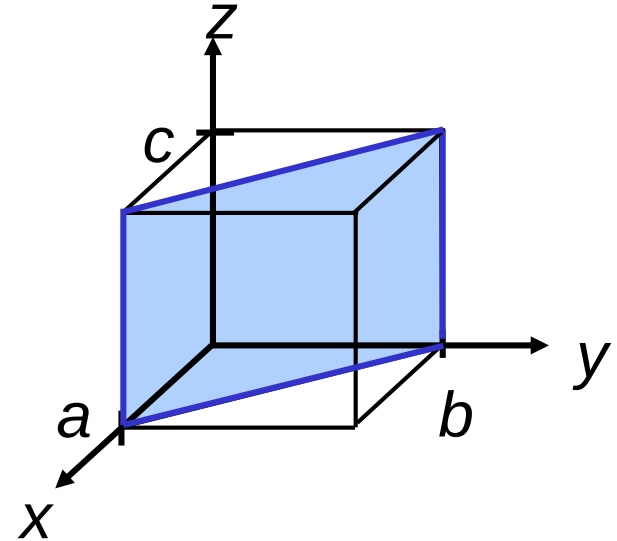
Crystallographic Planes



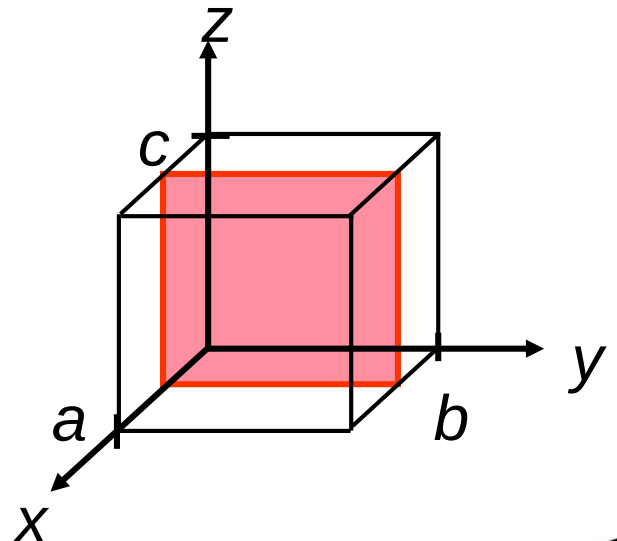
Adapted from Fig. 3.26,
Callister & Rethwisch 4e.

Crystallographic Planes

<u>example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1	1	∞
2. Reciprocals	1/1	1/1	1/ ∞
	1	1	0
3. Reduction	1	1	0
4. Miller Indices	(110)		

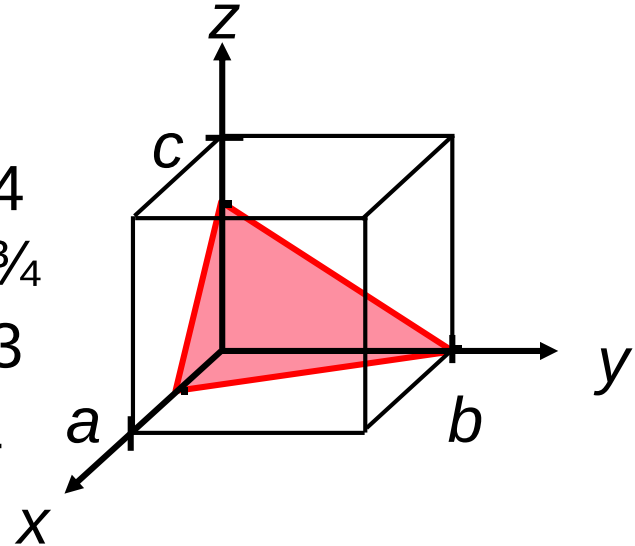


<u>example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/1/2	1/ ∞	1/ ∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		



Crystallographic Planes

<u>example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/1/2	1/1	1/3/4
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



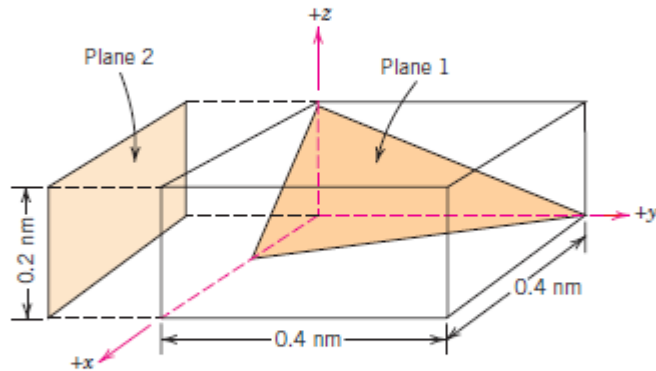
Family of Planes $\{hkl\}$

Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

Questions

Crystallographic Planes

- 3.37 (a) Draw an orthorhombic unit cell, and within that cell a $(02\bar{1})$ plane.
 (b) Draw a monoclinic unit cell, and within that cell a (200) plane.
- 3.38 What are the indices for the two planes drawn in the sketch below?

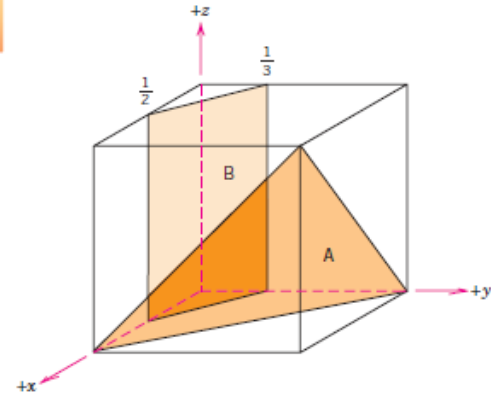


- 3.39 Sketch within a cubic unit cell the following planes:

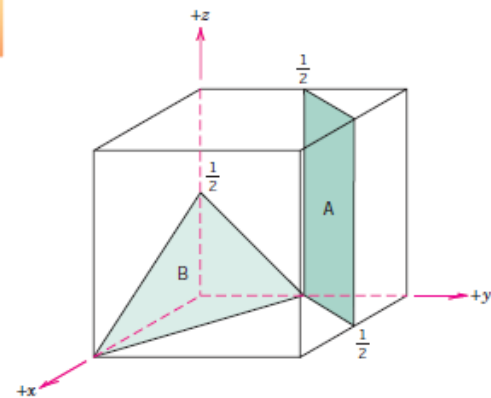


- | | |
|---------------------|---------------------------|
| (a) $(10\bar{1})$, | (e) $(\bar{1}1\bar{1})$, |
| (b) $(2\bar{1}1)$, | (f) $(\bar{2}12)$, |
| (c) (012) , | (g) $(3\bar{1}2)$, |
| (d) $(3\bar{1}3)$, | (h) (301) . |

- 3.40 Determine the Miller indices for the planes shown in the following unit cell:



- 3.41 Determine the Miller indices for the planes shown in the following unit cell:

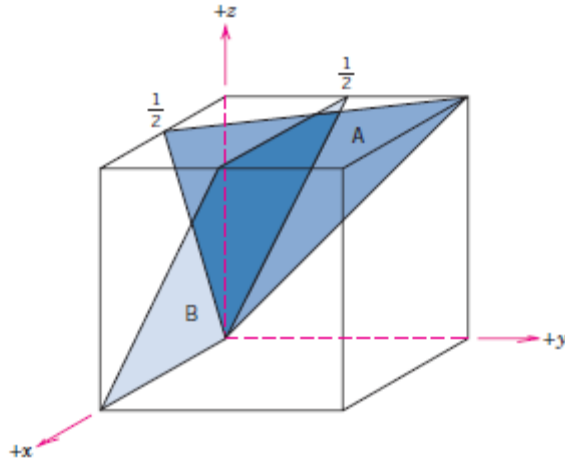


- 3.42 Determine the Miller indices for the planes shown in the following unit cell:



Questions

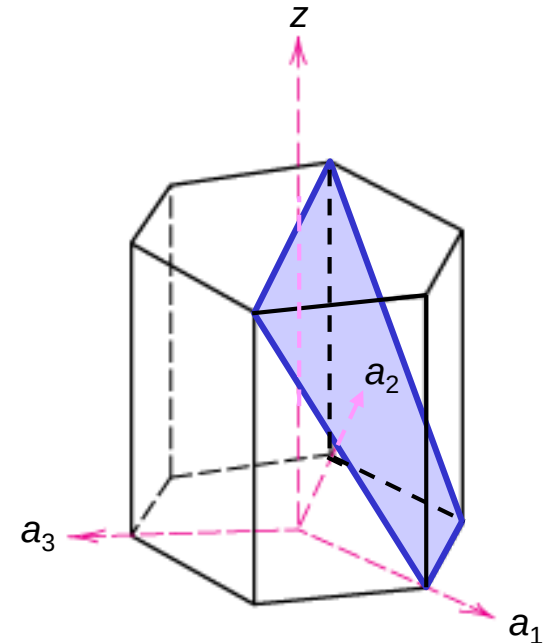
3.42 Determine the Miller indices for the planes shown in the following unit cell:



Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

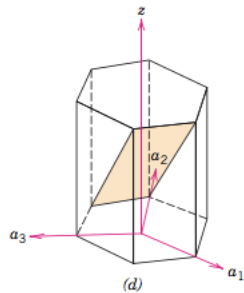
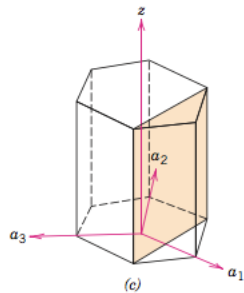
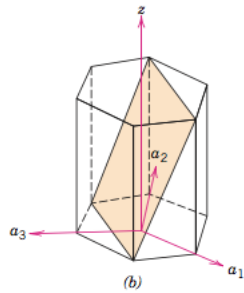
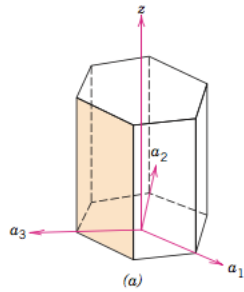
<u>example</u>	a_1	a_2	a_3	c
1. Intercepts	1	∞	-1	1
2. Reciprocals	1	$1/\infty$	-1	1
	1	0	-1	1
3. Reduction	1	0	-1	1
4. Miller-Bravais Indices	$(10\bar{1}1)$			



Adapted from Fig. 3.24(b),
Callister & Rethwisch 4e.

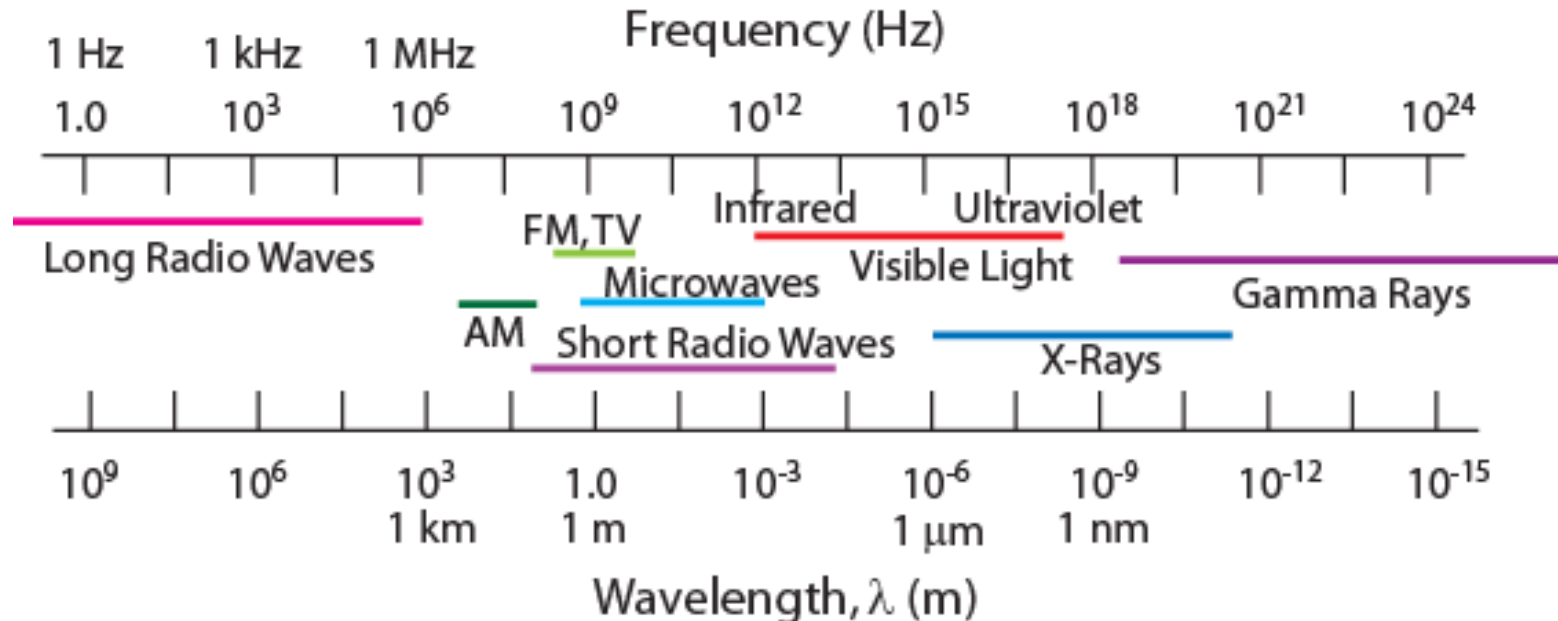
3.49 Determine the indices for the planes shown in the hexagonal unit cells below:

Questions



X-Ray Diffraction

Electromagnetic Spectrum



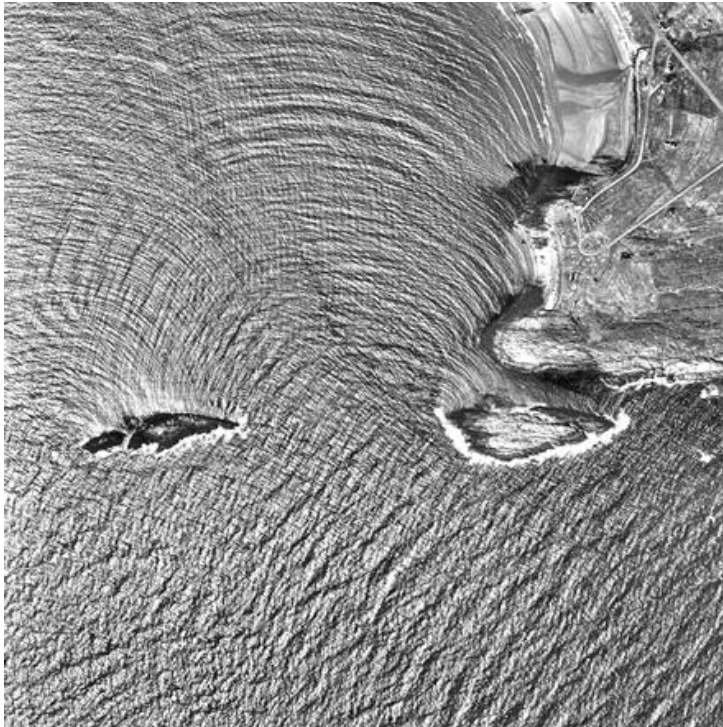
- Diffraction gratings must have spacings comparable to the wavelength of diffracted waves.
- Can't resolve wavelengths $< \lambda$
- Spacing is the distance between parallel planes of atoms.



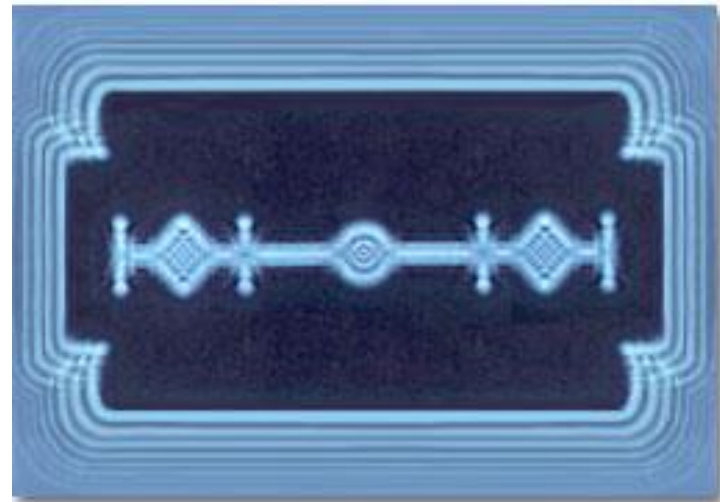
Diffraction

Diffraction occurs when waves spread out after passing through a gap or round an obstacle.

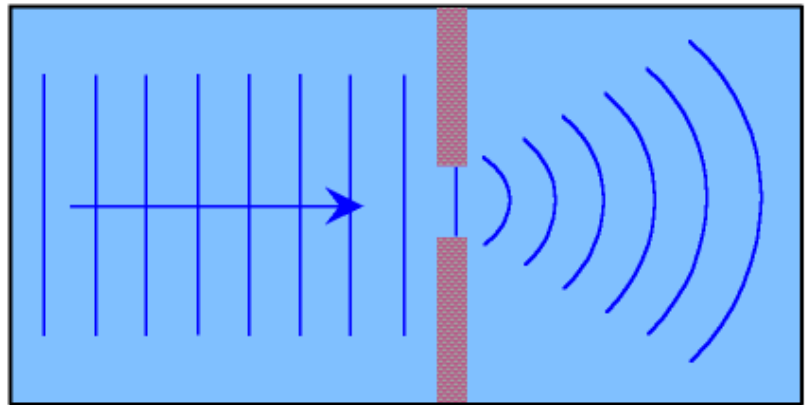
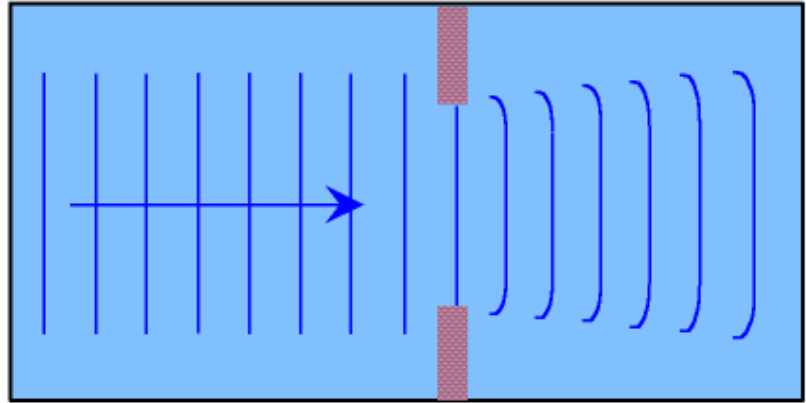
Sea wave diffraction



Light Diffraction by a Razor Blade



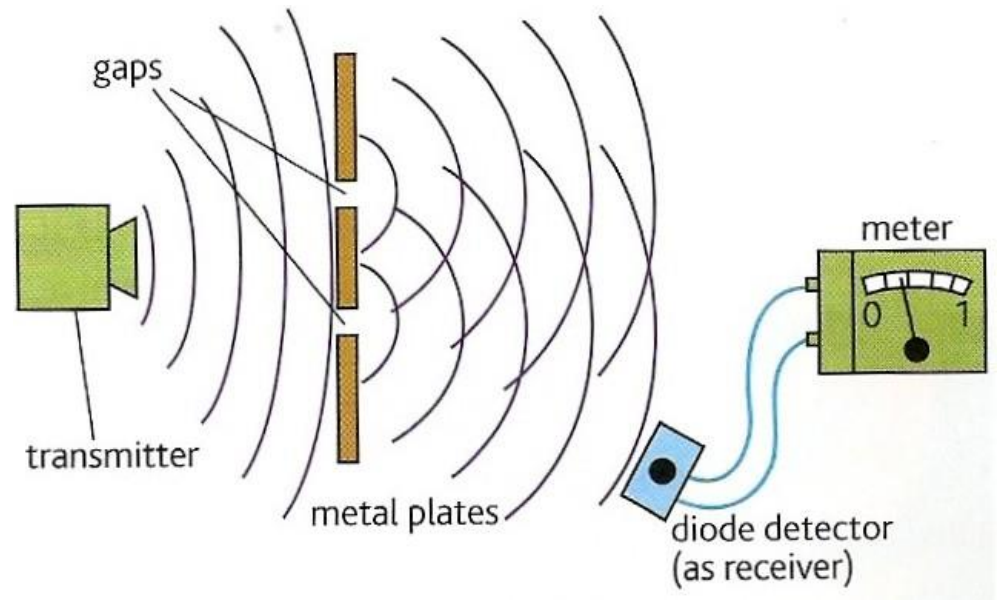
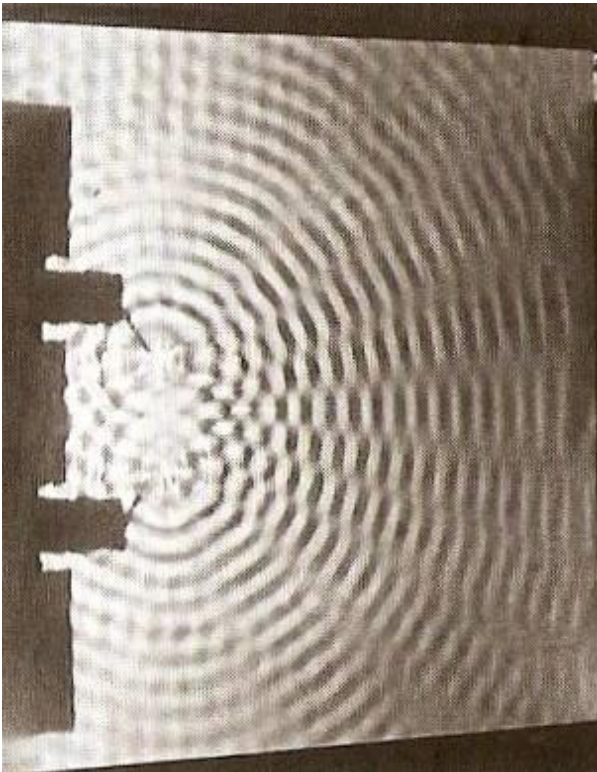
Diffraction becomes more significant when the size of the gap or obstacle is reduced compared with the wavelength of the wave.



Interference

Interference occurs when two waves of the same type (e.g. both water, sound, light, microwaves etc.) occupy the same space.

Wave superposition results in the formation of an interference pattern made up of regions of reinforcement and cancellation.



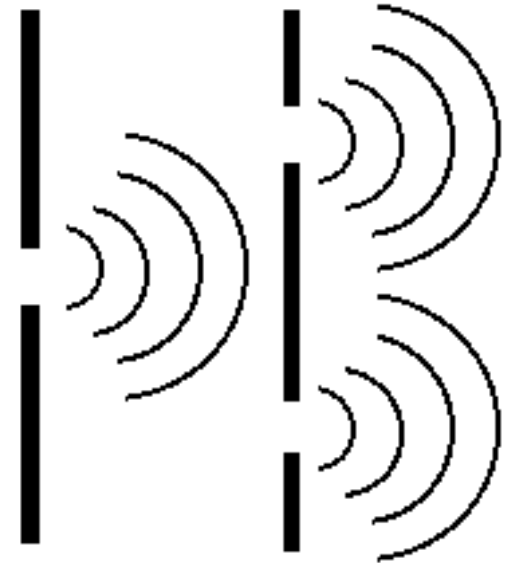
Coherence

For an interference pattern to be observable the two overlapping waves must be **coherent**.

This means they will have:

- 1. the same frequency**
- 2. a constant phase difference**

If the two waves are incoherent the pattern will continually change usually too quickly for observations to be made.



Two coherent waves can be produced from a single wave by the use of a double slit.

Path difference

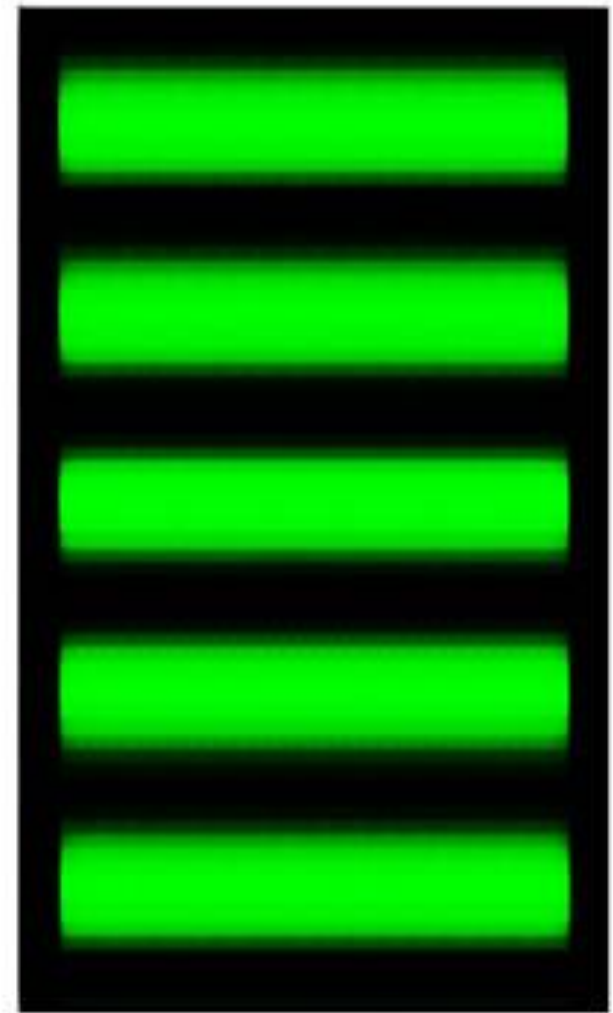
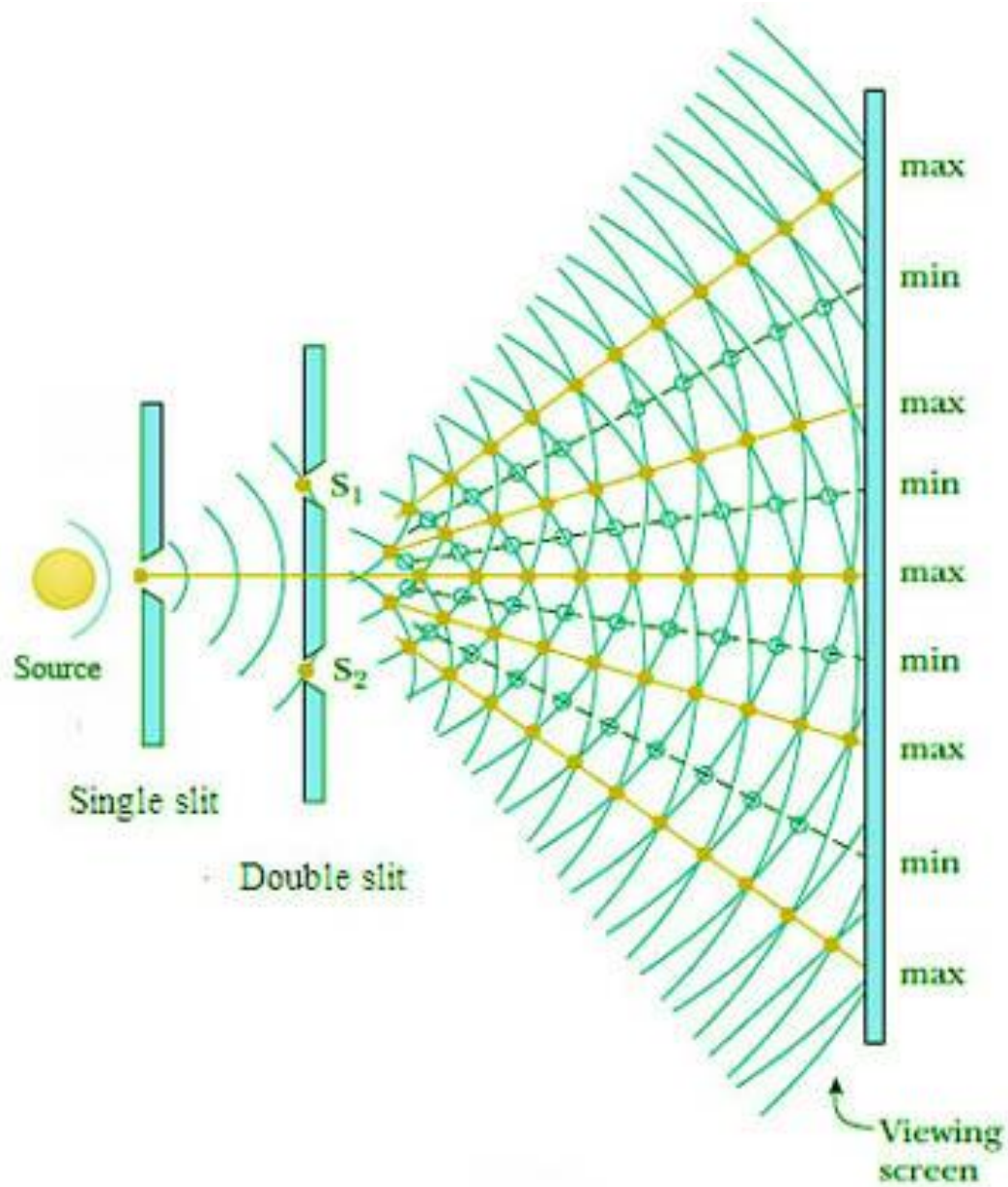
Path difference is the difference in distance travelled by two waves.

Path difference is often measured in 'wavelengths' rather than metres.

Example:

Two waves travel from A to B along different routes. If they both have a wavelength of 2m and the two routes differ in length by 8m then their path difference can be stated as '4 wavelengths' or '4 λ '





Interference pattern on screen

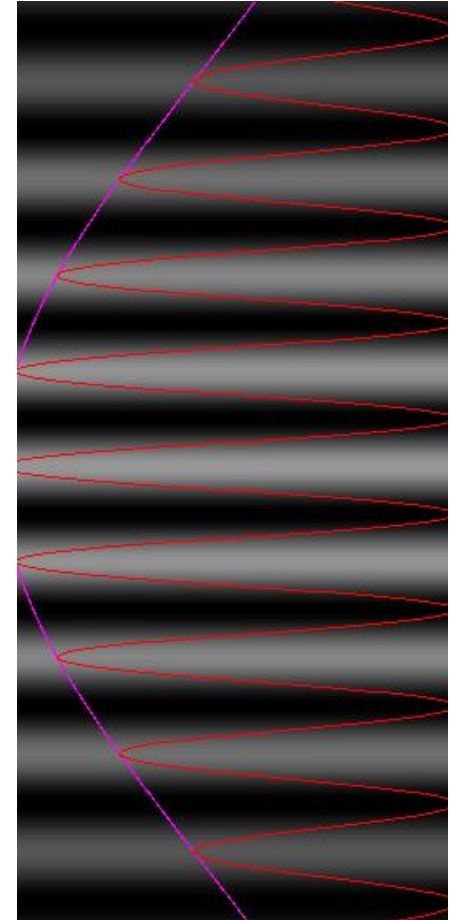
Interference fringes

Interference fringes are formed where the two diffracted light beams from the double slit overlap.

A **bright fringe** is formed where the light from one slit reinforces the light from the other slit. At a bright fringe the light from both slits will be **in phase**.

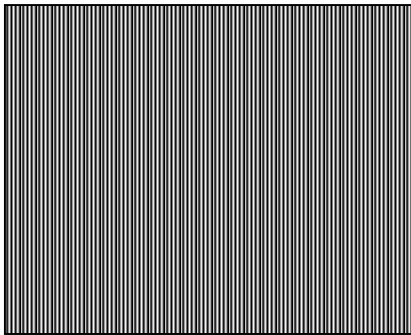
They will have path differences equal to a whole number of wavelengths: 0 , 1λ , 2λ , 3λ etc...

A **dark fringe** is formed due to cancelation where the light from the slits is **180° out of phase**. They will have path differences of: $\frac{1}{2}\lambda$, $\frac{3}{2}\lambda$, $\frac{5}{2}\lambda$ etc..

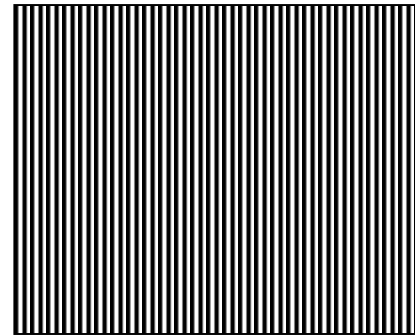


Transmission diffraction grating

A transmission diffraction grating consists of a glass or plastic slide with many closely spaced slits ruled onto it (typically 500 per mm).



**500 lines per mm
(magnified view)**



**100 lines per mm
(magnified view)**

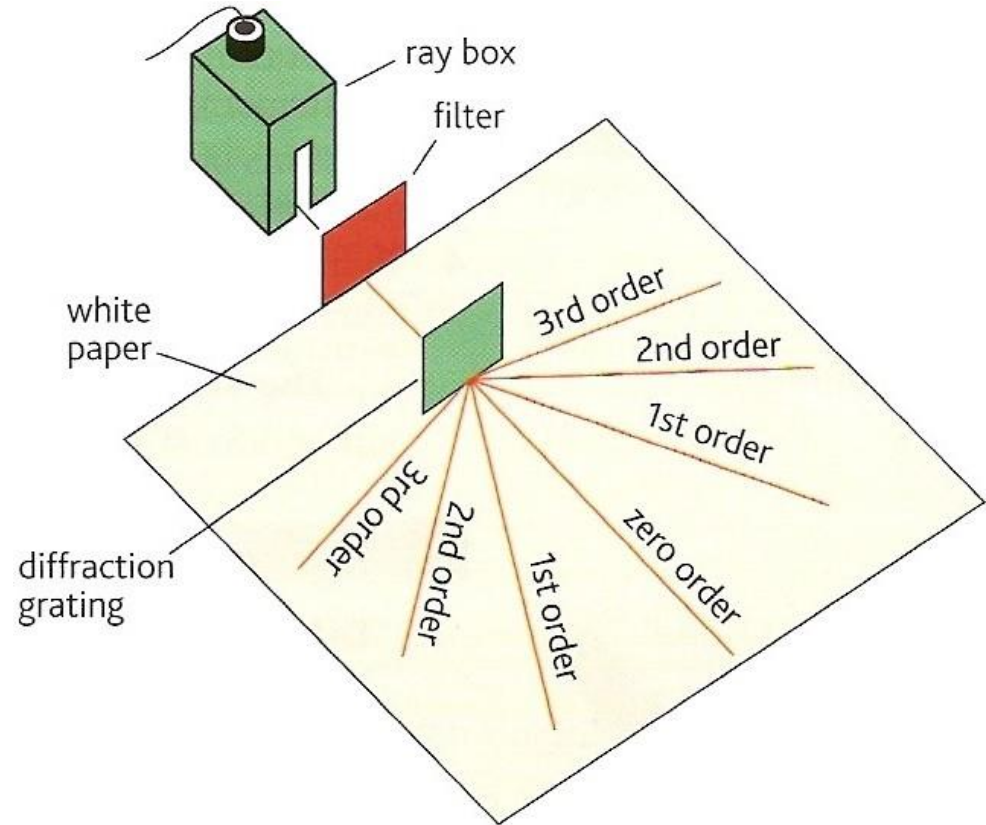
Note: A CD or DVD disc acts as a reflection diffraction grating

Grating and monochromatic light

When a parallel beam of monochromatic light is incident normally with the grating the light is transmitted in certain directions only.

This happens because:

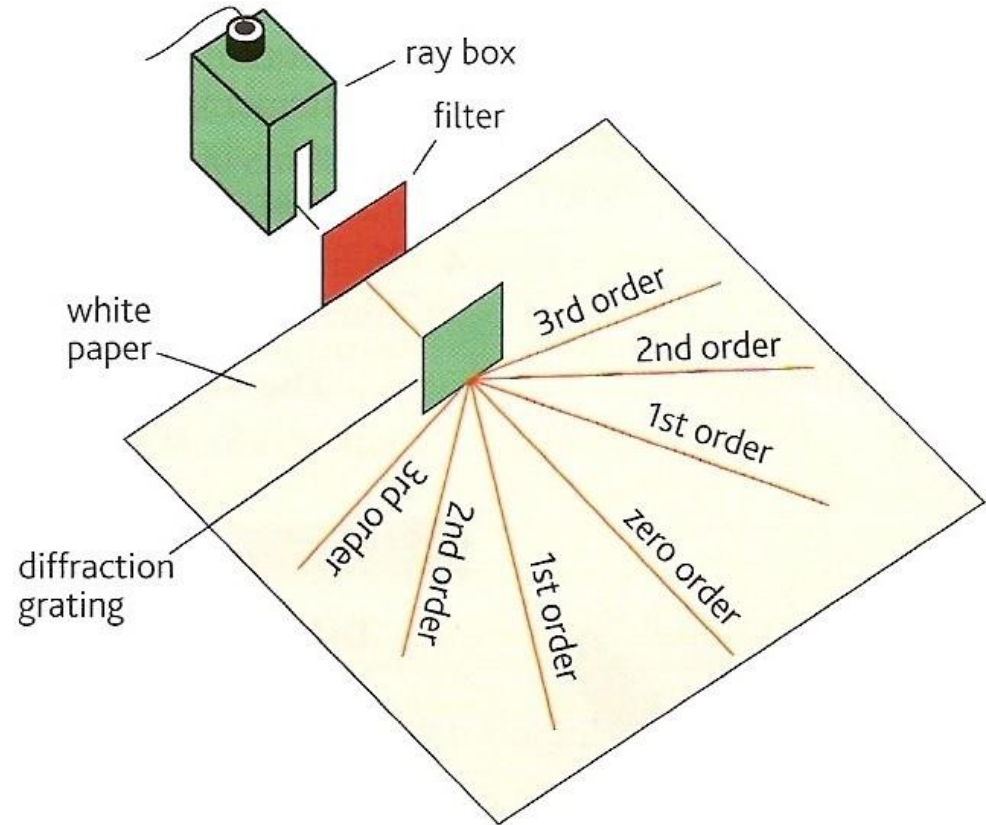
- the light is diffracted by each slit in the grating.
- the diffracted light from adjacent slits reinforces only in a few directions. In all other directions cancellation occurs.



The central beam is referred to as the 'zero order beam' and is in the same direction as the incident beam.

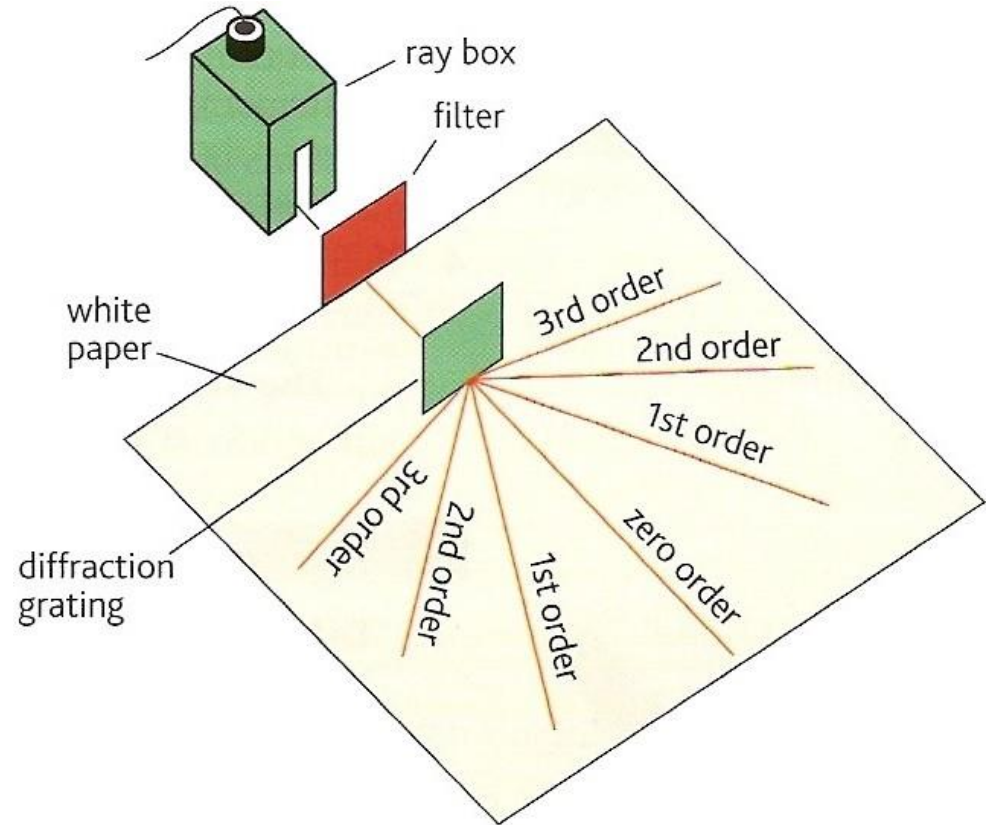
Other transmitted beams are numbered outwards from the zero order beam.

The pattern of beams is symmetric about the zero order beam.



The angle between the beams increases if:

- the wavelength of the light is increased
- the width of the slits in the grating is decreased (more lines per mm)

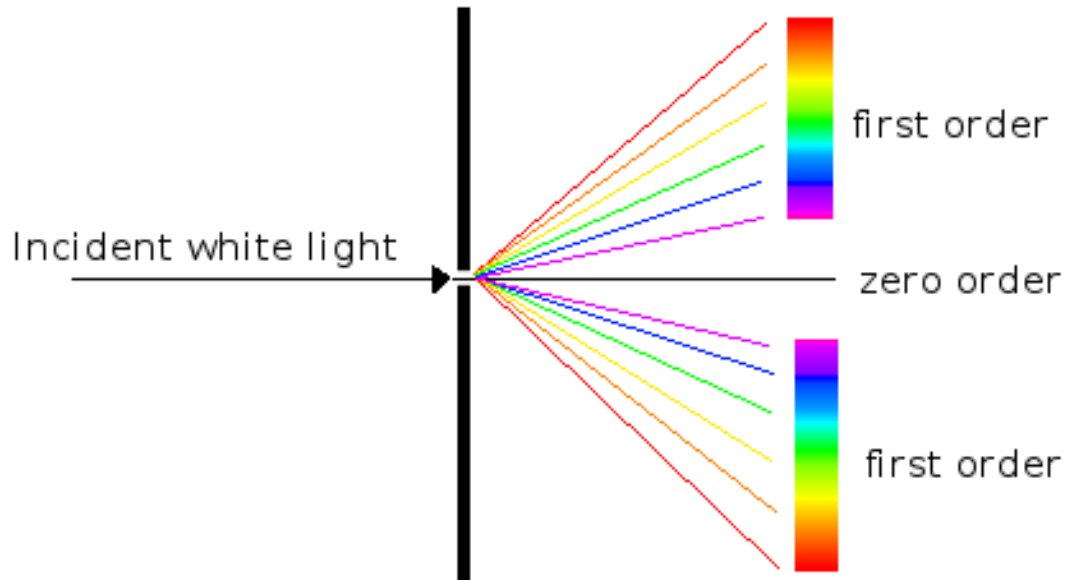


Grating and white light

Each wavelength produces its own set of lines.

The zero order beam is white.

The other beams are spectra with red showing the greatest angles



Diffraction grating equation

$$d \sin \theta = n\lambda$$

where:

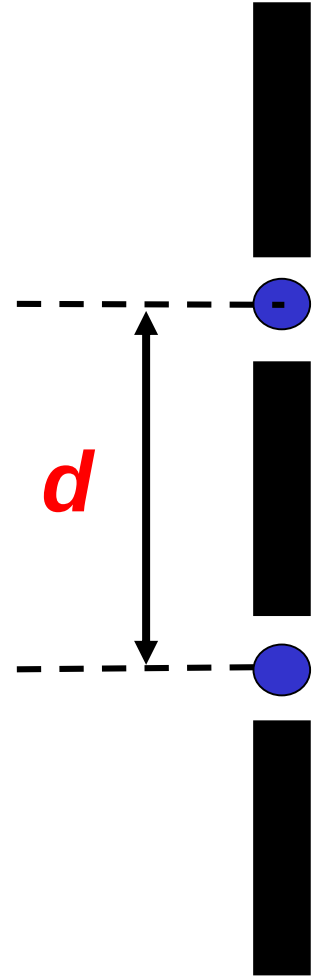
d = the grating spacing (the distance between the centres of adjacent slits drawn on the grating)

n = the beam order number (0, 1, 2 etc..)

λ = the wavelength of the light

θ = the angle between the beam in question and the zero order beam

Note: The number of slits per metre, N in the grating is given by: $N = 1 / d$



Diffraction grating equation derivation

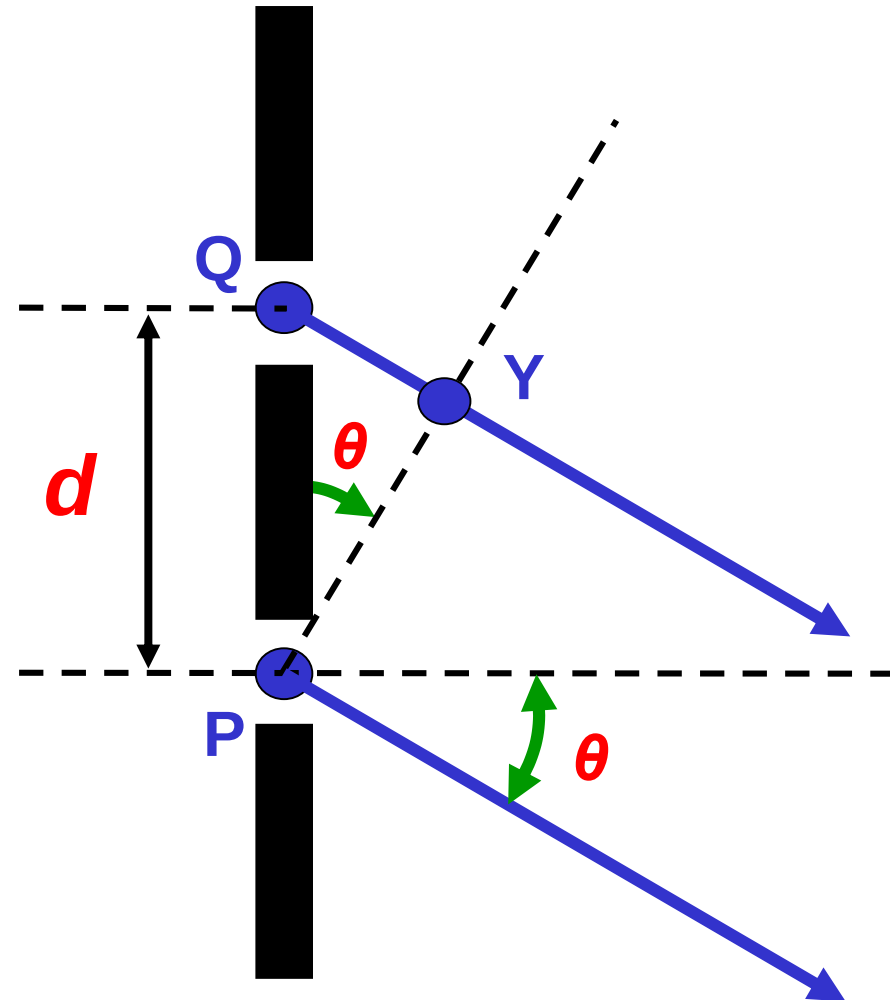
Let θ be the angle between the zero order maximum and the n^{th} order maximum.

For this to occur the path difference between the light from two adjacent slits must equal a $n\lambda$.

In the diagram opposite distance QY must equal $n\lambda$.

But: $\sin \theta = QY / QP$
 $\sin \theta = n\lambda / d$

Hence: $d \sin \theta = n\lambda$



Question 1

Calculate the angle of the first order beam when red light, wavelength 650nm is incident on a diffracting grating that has 200 lines per mm.

$$d \sin \theta = n\lambda$$

becomes: $\sin \theta = n\lambda / d$

with grating spacing, $d = 1/200 \text{ mm} = 0.005 \text{ mm}$

$$\sin \theta = (1 \times 650 \text{ nm}) / (0.005 \text{ mm})$$
$$= (650 \times 10^{-9} \text{ m}) / (5 \times 10^{-6} \text{ m})$$

$$\sin \theta = 0.13$$

First order angle, $\theta = 7.5^\circ$



Question 2

Calculate the wavelength of light that has a second order angle of 30° when used with a diffracting grating of 500 lines per mm.

$$d \sin \theta = n\lambda$$

becomes: $\lambda = d \sin \theta / n$

with grating spacing, $d = 1/500 \text{ mm} = 0.002 \text{ mm}$

$$\begin{aligned} \lambda &= (0.002 \text{ mm} \times \sin 30^\circ) / (2) \\ &= (2 \times 10^{-6} \text{ m} \times 0.5) / (2) \end{aligned}$$

$$\text{wavelength} = 5 \times 10^{-7} \text{ m} = 500 \text{ nm}$$



Question 3

How many beams are formed when blue light, wavelength 450nm is used with a diffracting grating of 400 lines per mm.

$$d \sin \theta = n\lambda$$

becomes: $n = d \sin \theta / \lambda$

grating spacing, $d = 1/400 \text{ mm} = 0.0025 \text{ mm}$

$\sin \theta$ cannot be greater than 1.0 (with $\theta = 90^\circ$)

$$n = (0.0025 \text{ mm} \times 1.0) / (450 \text{ nm})$$

$$= (2.5 \times 10^{-6} \text{ m}) / (4.5 \times 10^{-7} \text{ m})$$

$$= 5.6$$

but n must be an integer

and so max $n = 5$

There will therefore be 11 beams



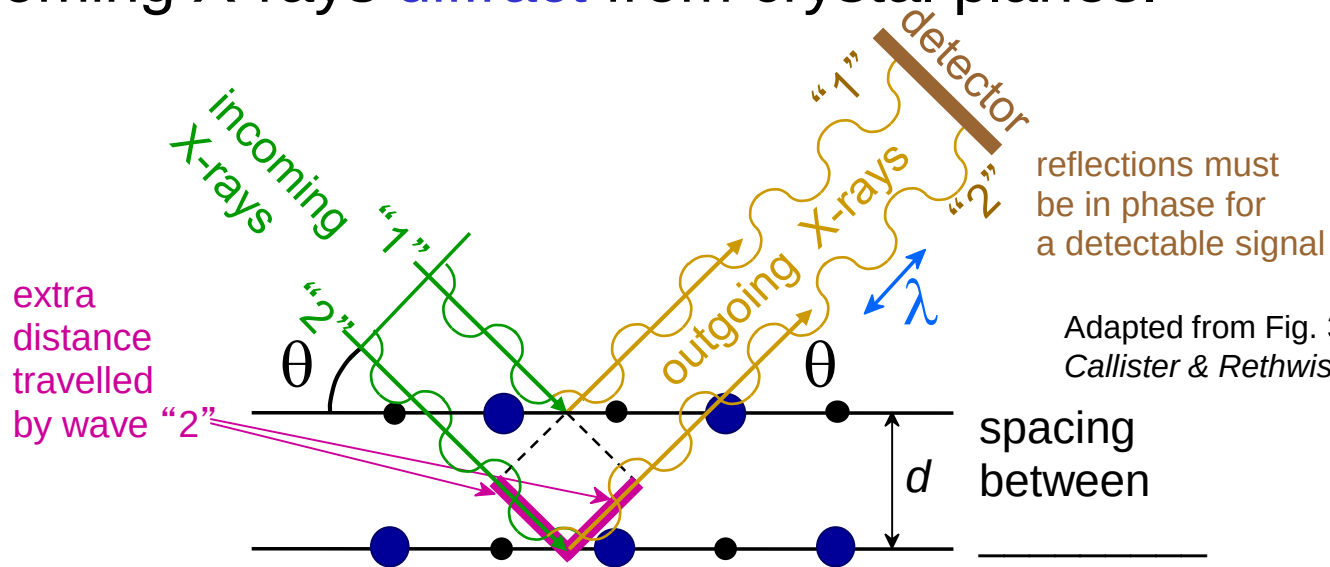
Answers:

$d / \mu\text{m}$	N / mm^{-1}	$\theta / ^\circ$	n	λ / nm
2.00	500	11.5	1	400
2.00	500	23.6	2	400
2.00	500	53.1	4	400
5.00	200	9.21	2	400
2.50	400	30	5	250



X-Rays to Determine Crystal Structure

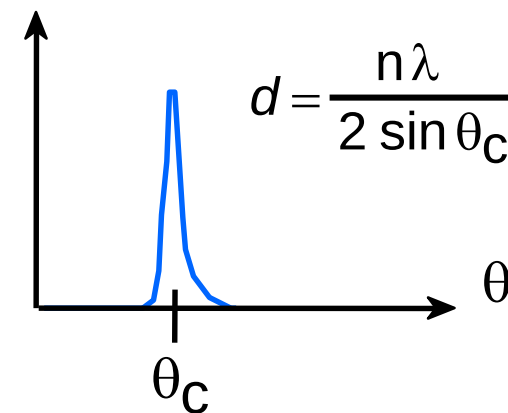
- Incoming X-rays **diffract** from crystal planes.



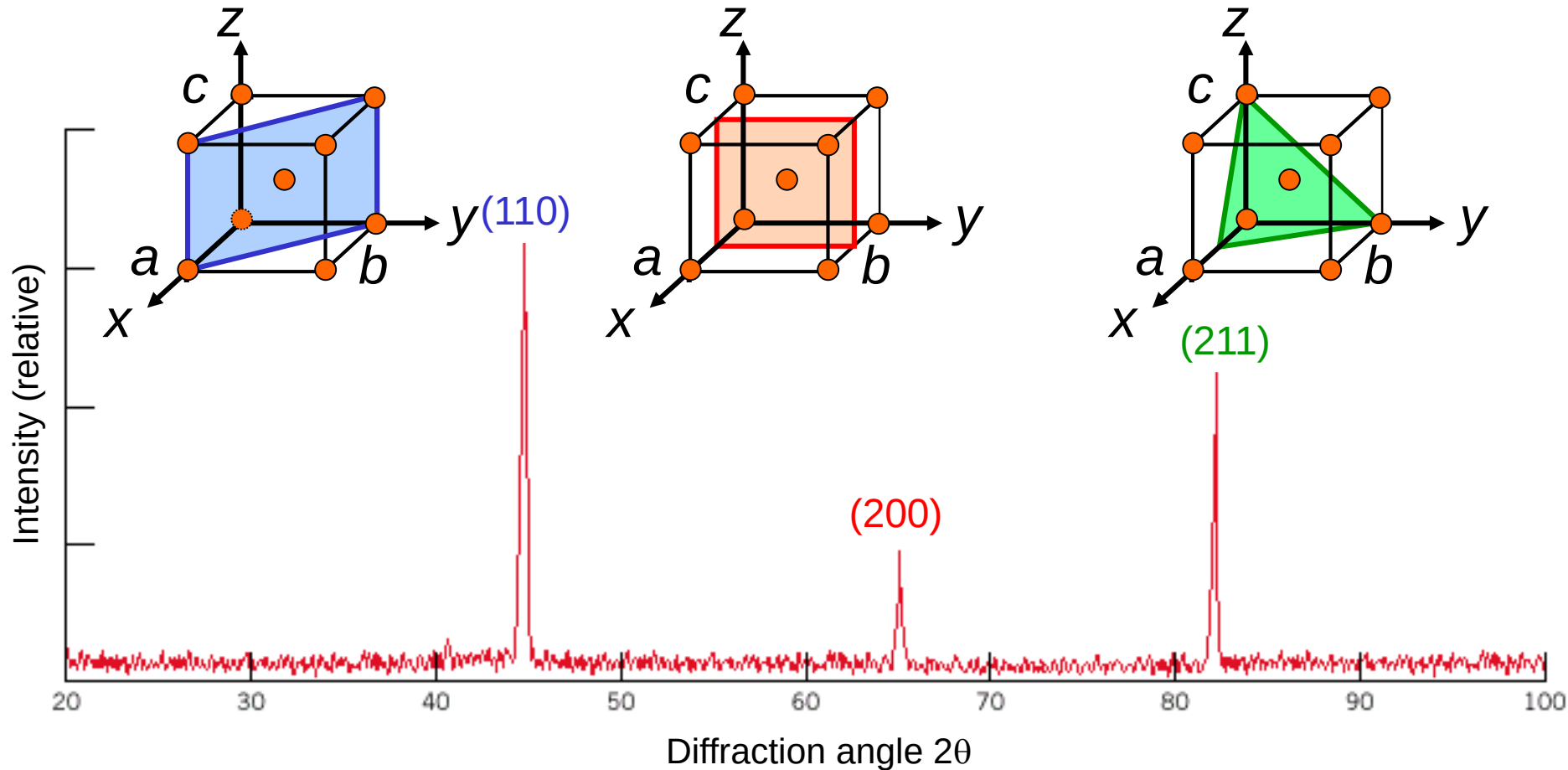
Adapted from Fig. 3.38,
Callister & Rethwisch 4e.

_____ of
critical angle, θ_c ,
allows computation of
planar _____,
 d .

X-ray
intensity
(from
detector)



X-Ray Diffraction Pattern



Diffraction pattern for polycrystalline α -iron (BCC)

Adapted from Fig. 3.40, *Callister 4e*.

SUMMARY

- Atoms may assemble into **crystalline** or **amorphous** structures.
- Common metallic crystal structures are **FCC**, **BCC**, and **HCP**.
Coordination number and **atomic packing factor** are the same for both FCC and HCP crystal structures.
- We can predict the **density** of a material, provided we know the **atomic weight**, **atomic radius**, and **crystal geometry** (e.g., FCC, BCC, HCP).
- Interatomic bonding in ceramics is ionic and/or covalent.
- Ceramic crystal structures are based on:
 - maintaining **charge neutrality**
 - cation-anion radii ratios.
- **Crystallographic points**, **directions** and **planes** are specified in terms of indexing schemes. Crystallographic directions and planes are related to **atomic linear densities** and **planar densities**.



SUMMARY

- Materials can be **single crystals** or **polycrystalline**.
Material properties generally vary with single crystal orientation (i.e., they are **anisotropic**), but are generally non-directional (i.e., they are **isotropic**) in polycrystals with randomly oriented grains.
- Some materials can have more than one crystal structure. This is referred to as **polymorphism** (or **allotropy**).
- **X-ray diffraction** is used for crystal structure and **interplanar spacing** determinations.

