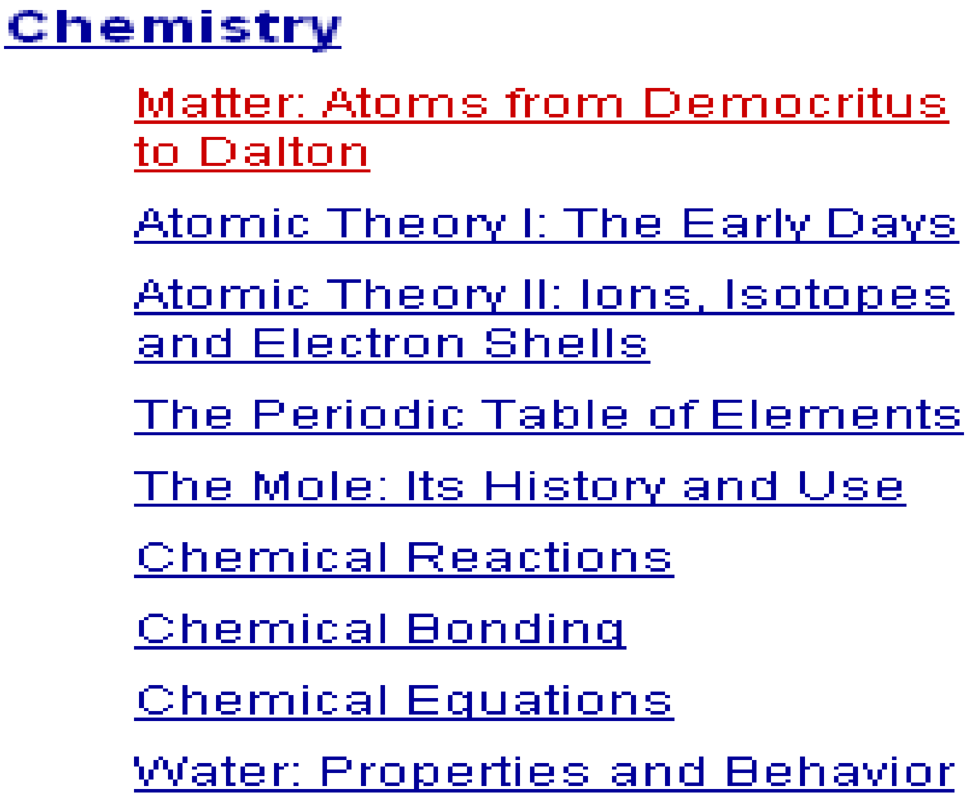
CHAPTER-2
ATOMIC STRUCTURE

Review your chemistry notes

- http://visionlearning.com/library/



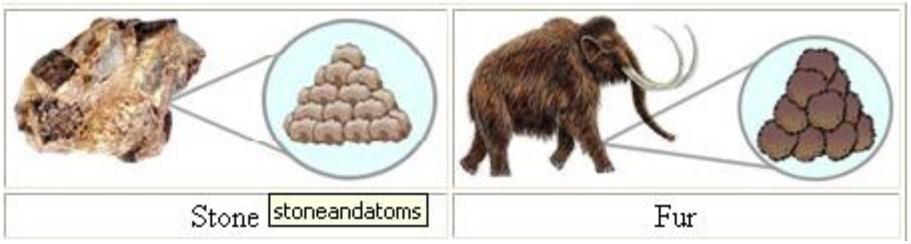
Chemistry

- Matter: Atoms from Democritus to Dalton
- Atomic Theory I: The Early Days
- Atomic Theory II: Ions, Isotopes and Electron Shells
- The Periodic Table of Elements
- The Mole: Its History and Use
- Chemical Reactions
- Chemical Bonding
- Chemical Equations
- Water: Properties and Behavior

Structure of Matter

- Empedocles (492 b.c. and 432 b.c.): All matter is composed of four main elements

- Democritus (460 b.c. to 370 b.c.) : Infinitesimally small pieces of matter called *atomos*, meaning "indivisible."



- Aristotle and Plato rejected Democritus and supported Empedocles
- Dalton first proposed part of his atomic theory in 1803

Atoms are the smallest structural units of all solids, liquids & gases.

Atom: The smallest unit of an element that retains the chemical properties of the element. Atoms can exist alone or in combinations with other atoms forming molecules.

Element: One of less than 118 pure chemical substances. An element is a substance composed of atoms with identical atomic number.

Molecule: A particle formed by the chemical bonding of two or more atoms. The molecule is the smallest particle of a chemical compound that retains the chemical properties of the compound.

Compound: A material formed by the chemical combination of elements in defined proportions. Compounds can be chemically decomposed into simpler substances.

Proton: A sub-atomic particle with a positive charge of $1.60x10^{-19}$ coulombs and a mass of $1.672x10^{-27}$ kg. Protons are found in the nucleus of atoms.

Neutron: A sub-atomic particle with no charge and a mass of $1.675x10^{-27}$ kg. Neutrons are found in the nucleus of atoms.

Electron: A sub-atomic particle with a negative charge of 1.60×10^{-19} coulombs and a mass of 9.11×10^{-31} kg. Electrons are generally found in orbit around the nucleus of an atom, but may be gained or lost during ion formation.

INTERATOMIC BONDING

- ❑ Atoms link to form materials. When this linkage is self-sufficient, the resultant will be a gas, a liquid or a solid.

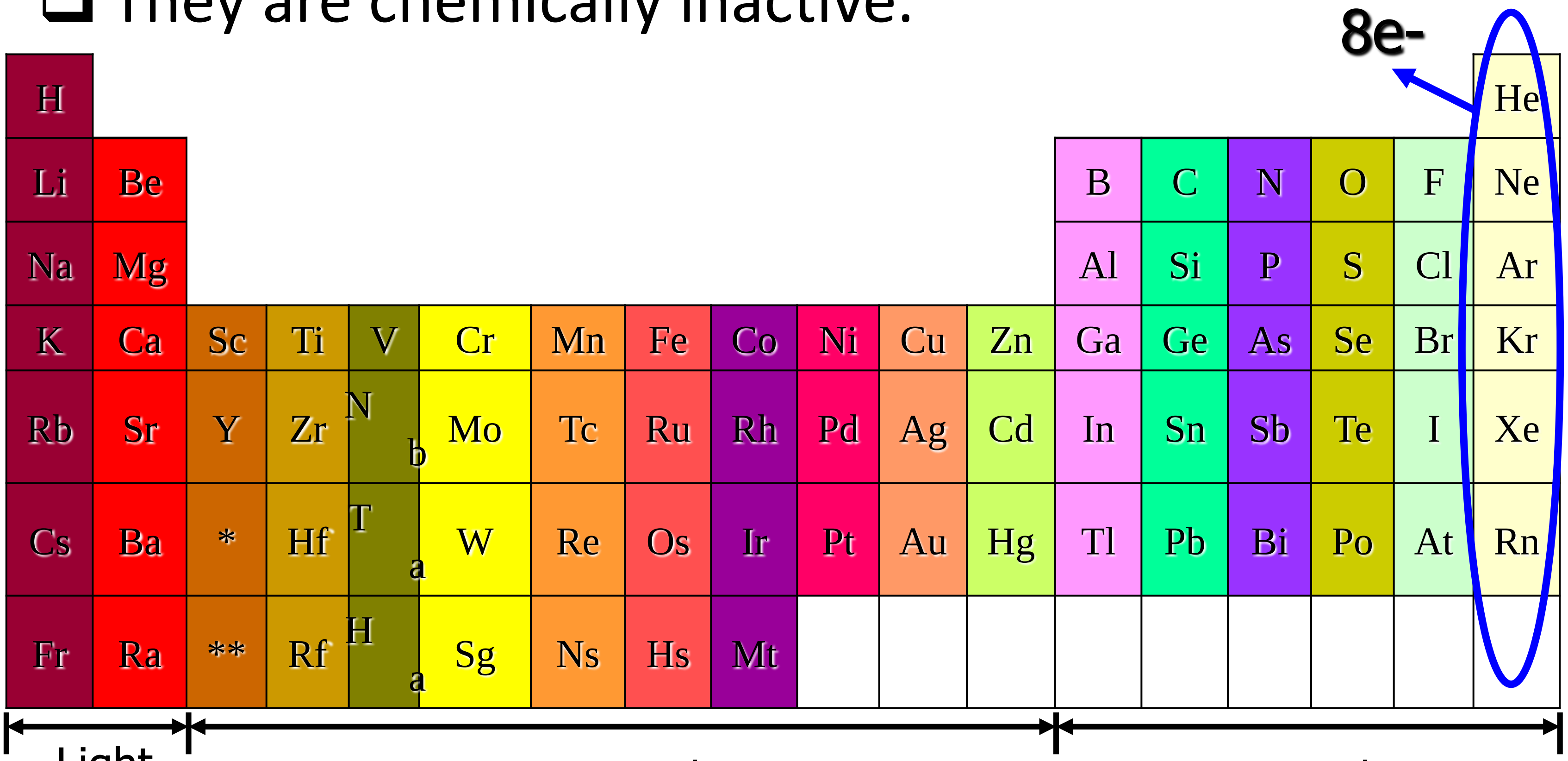
For example;

Atoms bond to form long chains→Polymers

Atoms bond in regular 3-D arrays→Metals

- ❑ The bonding b/w atoms is the result of the universal tendency of all systems to take up their lowest energy state. Atoms achieve their lowest energy level by the possession of 8 electrons in their outer most shell (except for the first shell which is stable only with $2e^-$)

- ☐ Considering the periodic table, the elements having 8e⁻ in their outermost shell are inert gases.
- ☐ They are chemically inactive.



8e-

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	**	Rf	Ha	Sg	Ns	Hs	Mt									

Light Metals

Transient Metals

Non Metals

Electropositivity increases ←

Electronegativity increases →

*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

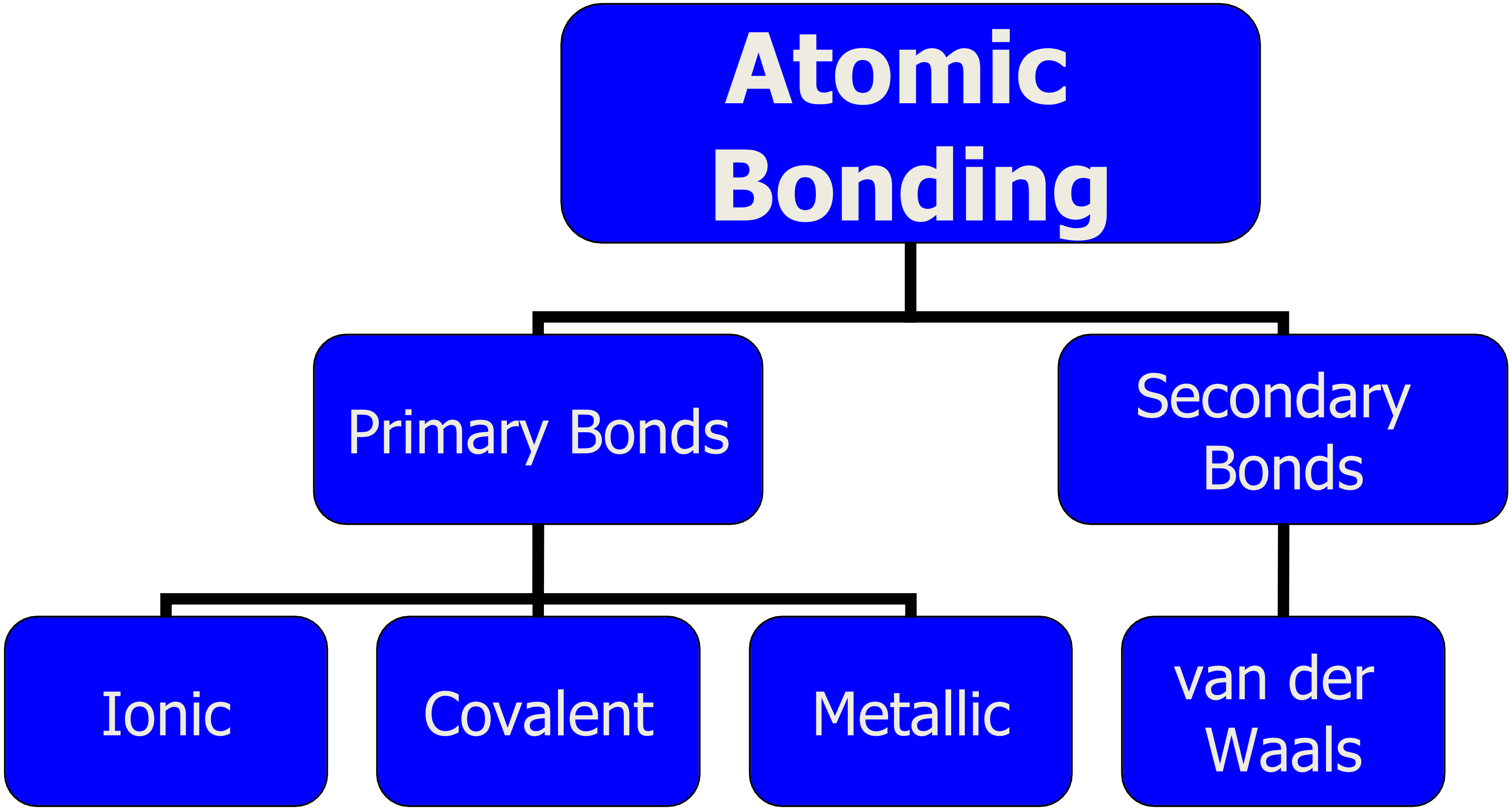
- Atoms of the elements having 5, 6, 7 e^- in their outermost shell accept 3, 2, 1 electrons respectively.

- Those having 1, 2 or 3 e^- give up their outermost shell electrons to remain with 8 e^- in their underlaying shell.

- Atoms having 4 <u>valance electrons</u> may behave in either way.

- Valance electrons: The electrons at the outermost shell.

ATOMIC BONDING



Atomic Bonding

Primary Bonds

Secondary Bonds

Ionic

Covalent

Metallic

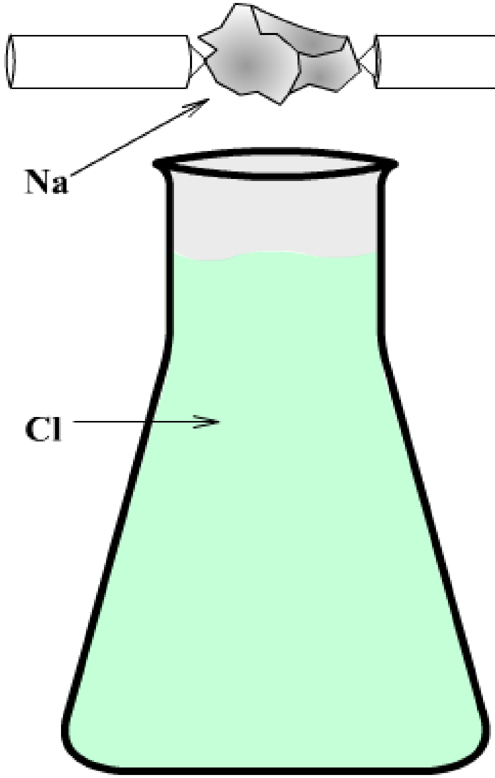
van der Waals

1. IONIC BONDING

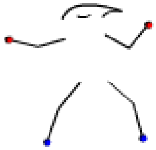
- ${}_{11}$Na & ${}_{17}$Cl These two ions are attracted to each other by the electrostatic force developed b/w them and an ionic compound (NaCl) forms.

- The ionic bonding b/w the two atoms results from the transfer of an electron from an electropositive atom to an electronegative one, so a strong electrostatic attraction is set up b/w the ions.

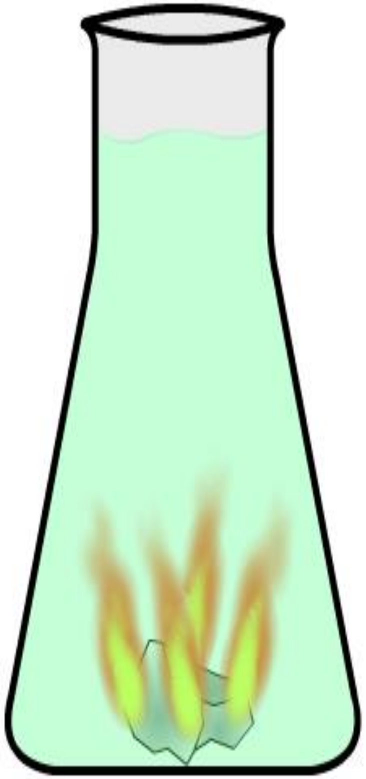
The Reaction of Sodium with Chlorine



The element sodium is a silver-colored metal while chlorine is a green-colored, toxic gas.



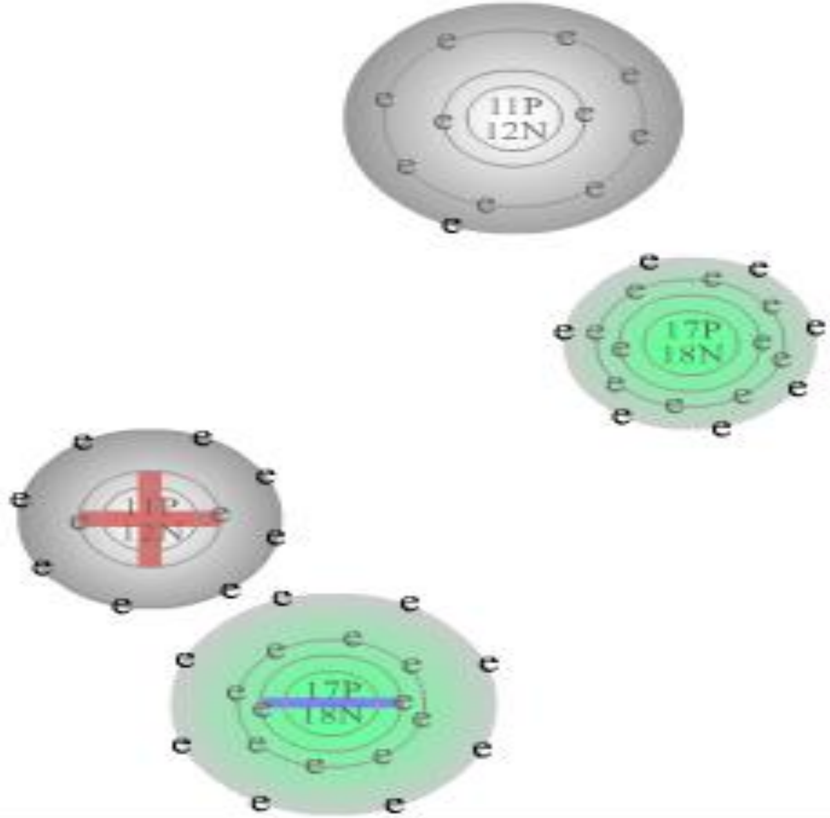
Drop the sodium into the chlorine gas

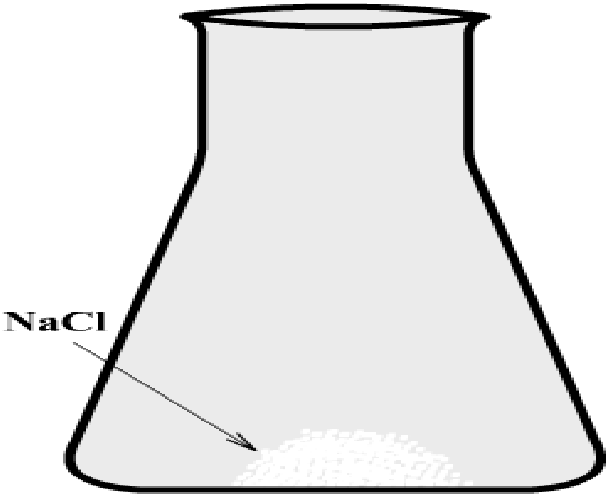


Upon contact, sodium violently reacts with chlorine. Let's take a more detailed look at this reaction.

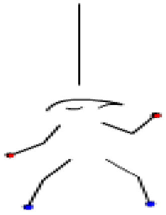
Magnify the reaction

When the sodium atoms contact the chlorine, an ionic reaction occurs in which each sodium atom loses one electron to each chlorine atom. This electron transfer releases energy. The resulting compound is held together by electrical charges.

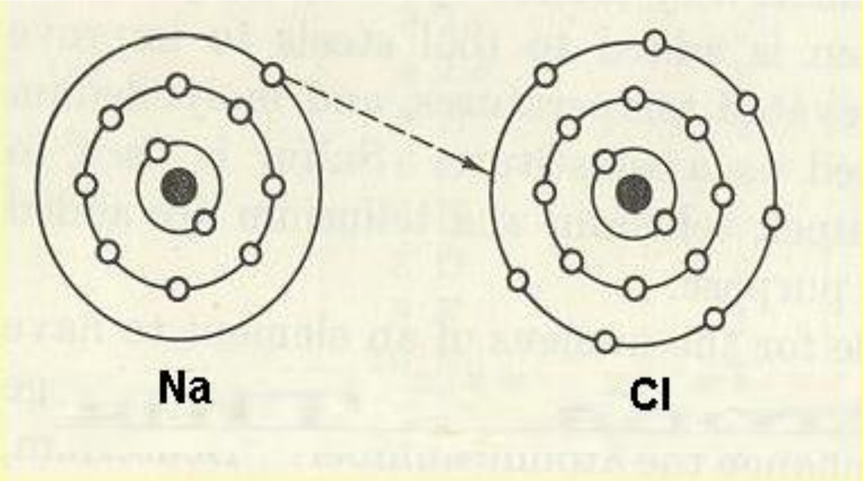




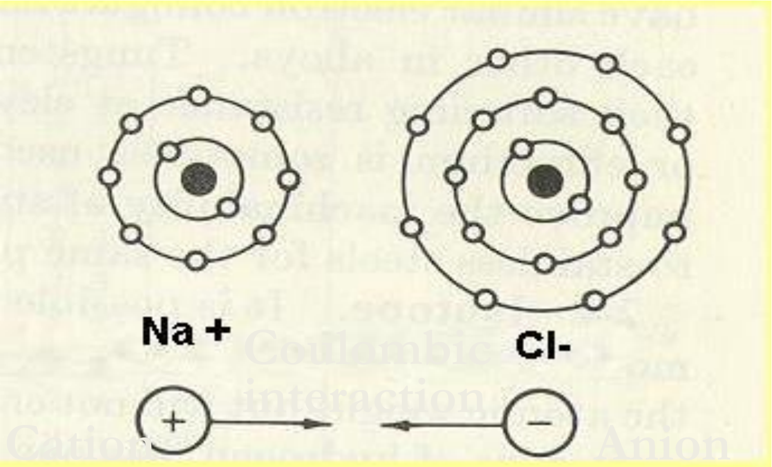
The ionic compound formed by this reaction is a hard, white solid called sodium chloride, or common table salt!



Replay

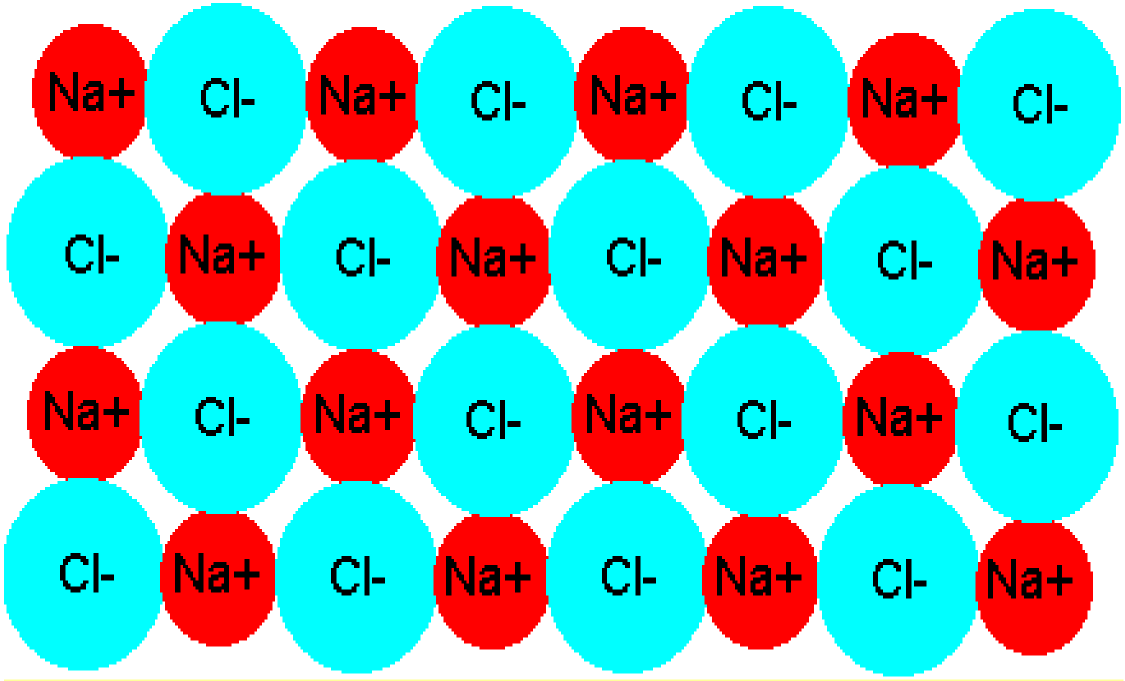


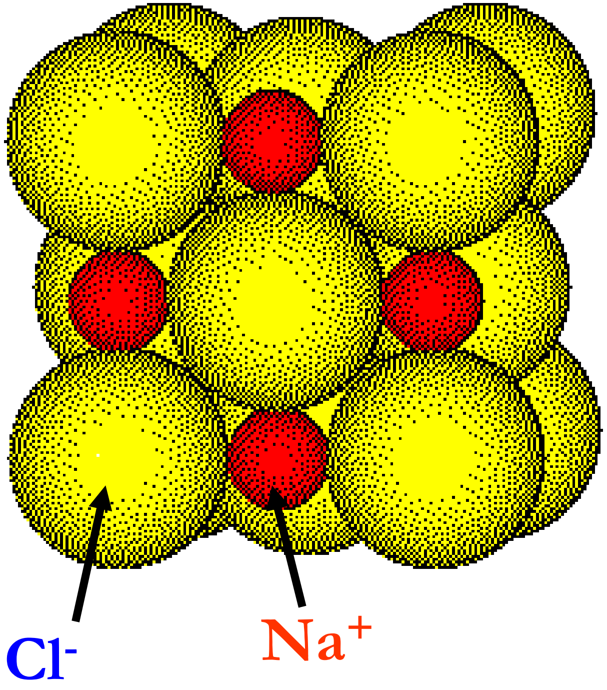
Ionic Bonds are nondirectional !



<u>**Note the relative sizes of ions**</u>

Na^+ shrinks and Cl^- expands





Properties of Ionic Bonding

1. Force of attraction is electrostatic (coulombic)
2. Bond is non-directional (each + ion is surrounded by as many – ions as possible)
3. Bond is strong, stable, brittle
4. High melting point (as the # of e^- involved in the bond increases, melting point increases)
5. Poor electrical conductivity
6. Forms between atoms of different electronegativity values (one high, one low).
7. An obvious limitation is that it can form only b/w different atoms.

2. COVALENT BONDING

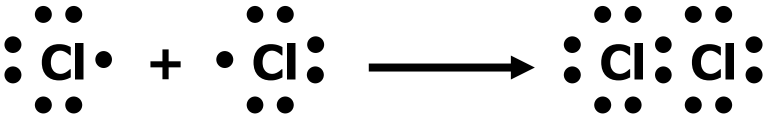
- Covalent bond is the bond in which e^- are shared b/w atoms.

The elements showing covalent bond obey (8-N) rule.

- (8-N) rule: The number of the closest neighbors to each atom is equal to (8-N)

  N is the valance e^-.

- When N=7, such as Cl



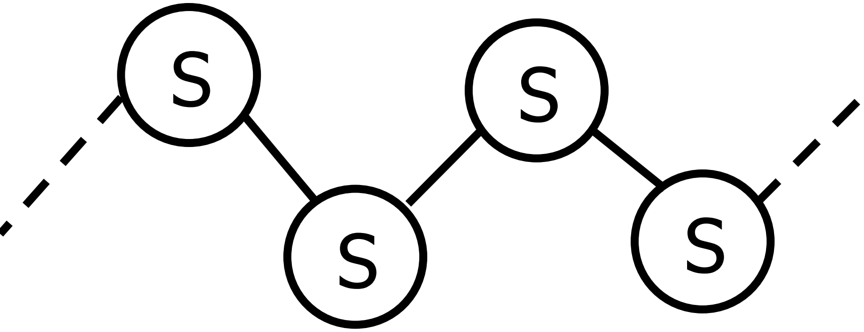
8-7=1 → the atoms pair off as diatomic molecules.

- When N=6 such as S

$${}_{16}S : 1s^2\ 2s^2\ 2p^6\ \boxed{3s^2\ 3p^4} \rightarrow 6$$

8-6=2

- each atom has two closest neighbors so they form long chains.



O, Se, Te behave like S.

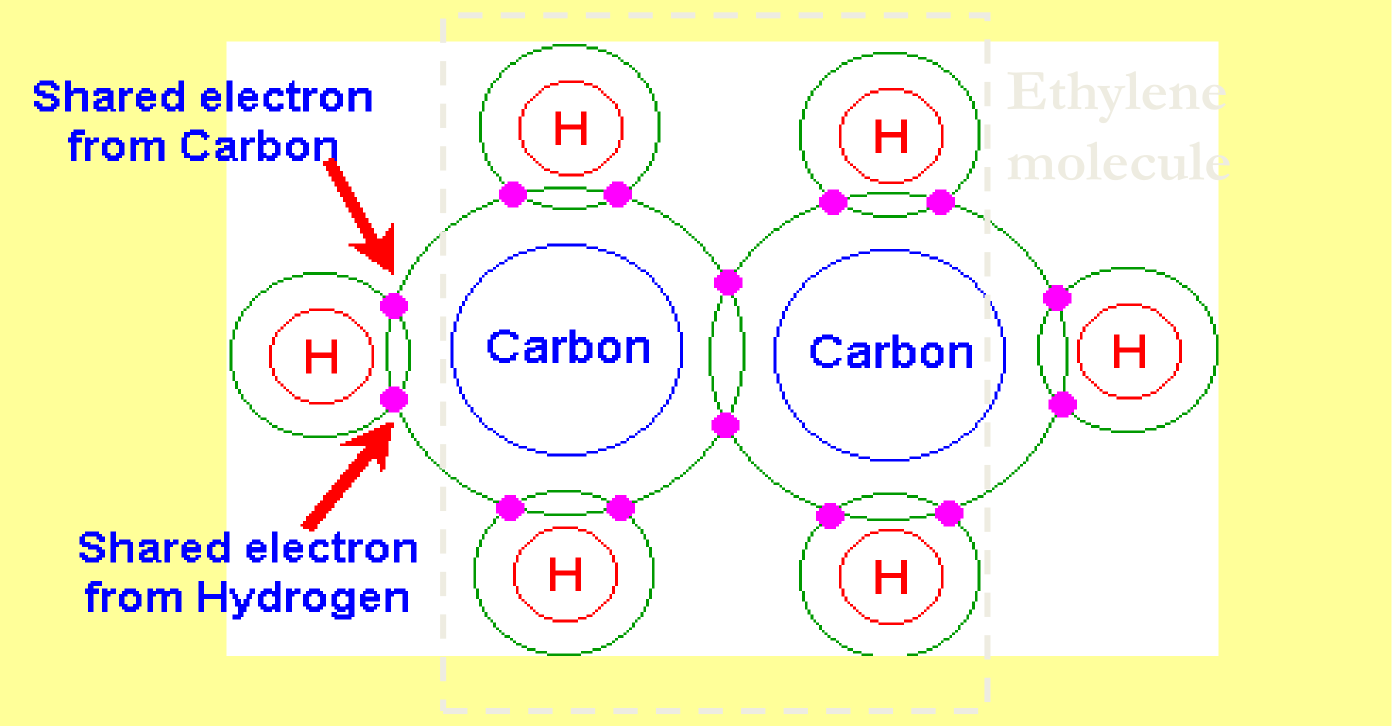
- ❑ When N=5, such as

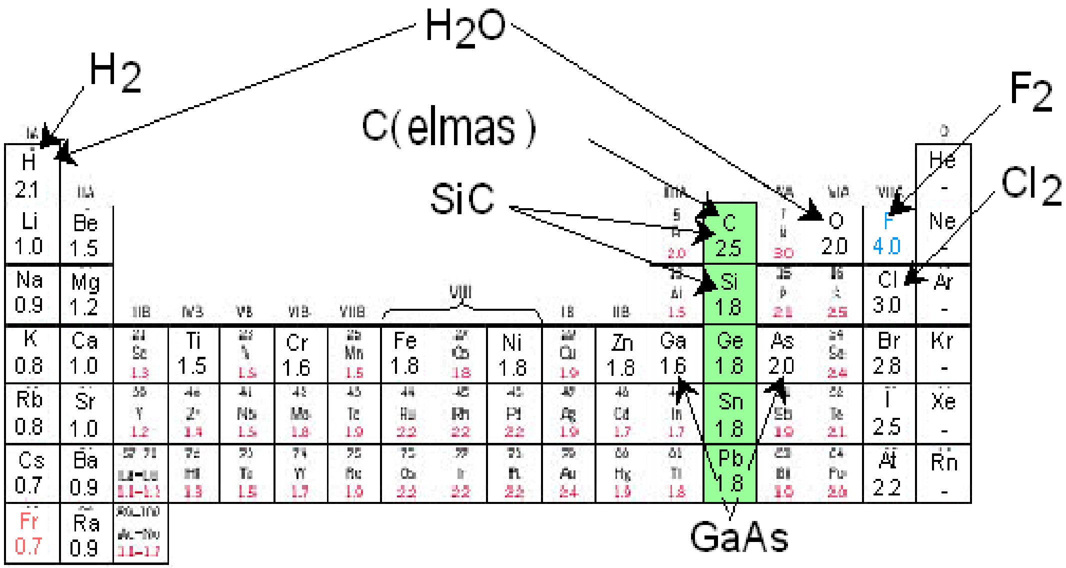
$_{33}As$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^3$

8-5=3 → They require 3 closest neighbors so they form sheets of atoms.

- ❑ When N=4, such as $_6C$: $1s^2\ 2s^2\ 2p^2$

8-4=4 → They form 3-D structures.


Shared electron from Carbon
Shared electron from Hydrogen
Ethylene molecule
Carbon
Carbon
H
H
H
H
H
H


H2
H2O
C(elmas)
SiC
F2
Cl2
GaAs
H 2.1
Li 1.0
Be 1.5
Na 0.9
Mg 1.2
K 0.8
Ca 1.0
Ti 1.5
Cr 1.6
Fe 1.8
Ni 1.8
Zn 1.8
Ga 1.6
Ge 1.8
As 2.0
Br 2.8
Kr -
Rb 0.8
Sr 1.0
Sn 1.8
I 2.5
Xe -
Cs 0.7
Ba 0.9
Pb 1.8
At 2.2
Rn -
Fr 0.7
Ra 0.9
C 2.5
Si 1.8
O 2.0
F 4.0
Cl 3.0
He -
Ne -
Ar -
VIII

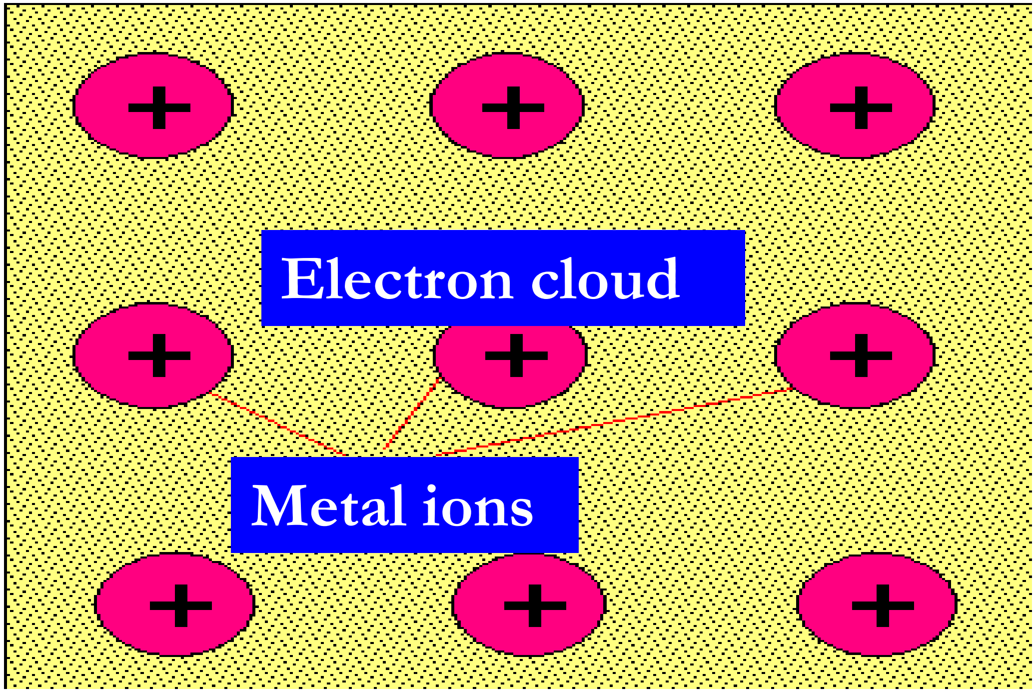
Properties of Covalent Bonding

1. It is based on electron sharing.
2. Bond is directional (each atom is surrounded by a definite amount of other atoms)
3. Bond is hard and strong (slightly less than ionic)
4. Very high melting point.
5. Poor electrical conductivity.
6. Forms b/w atoms with high electronegativity. Covalent bonding is not limited to elements; many compounds are covalent, like HCl, H_2O.

3. METALLIC BONDING

- Covalent bonding occurs in low electronegative atoms where they want to give away electrons.
- Metallic bond can be considered as a special type of covalent bond in which instead of sharing particular valance electrons, general sharing of valance e^- is responsible for the bond.
- Valance electrons are detached from atoms, and spread in an “electron cloud” that holds the ions together.

- The positive metal ions are arranged regularly in a "crystal lattice" and a cloud of valance electrons surround them.



Properties of Metallic Bond

1. It is based on electron sharing. Electrons are shared among all atoms.
2. Non directionality - desire for the largest number of nearest neighbors.
3. High thermal and electrical conductivity.
4. Moderately lower melting point.
5. Weakest primary bond.
6. Forms between atoms with <u>low electronegativity</u>.

High thermal and electrical conductivity ?

Since the valance e^- are not bound to any particular atom, they can move through the lattice under the application of an electric potential causing a current flow.

Also by a series of collisions with neighboring electrons they transmit thermal energy rapidly through the lattice.

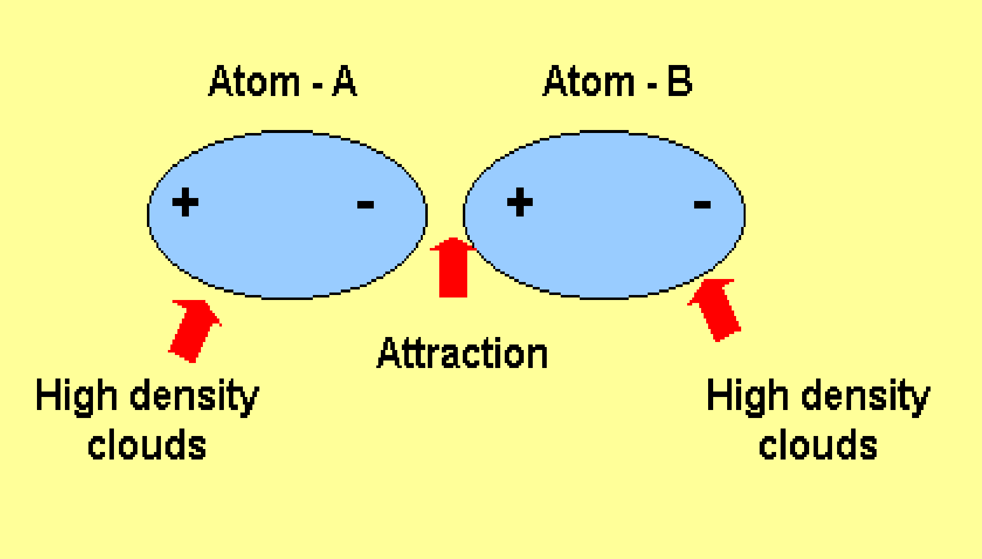
SECONDARY BONDS

(VAN DER WAALS BONDS)

- Secondary bonds are universal to all atoms and molecules, but as it is a very weak bond, it may be neglected when primary bonds exist.
- It can also be termed as a physical bond as opposite to chemical bonding that involves e^- transfer.
- Describes a dipolar attraction b/w neutral atoms.

- Since electrons move around nucleus (electronic charge is in motion), it is possible for electrons to be located unsymmetrically with respect to nucleus at a moment.
- In this way a dipole will be formed.
- Van der Waals bonding is a result of an attraction b/w opposite poles of these dipoles.

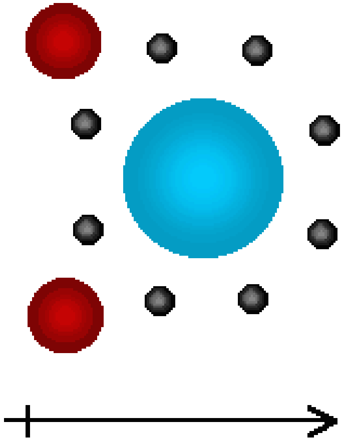
Dipole: Pair of equal and opposite electric charges.



EX: HYDROGEN BOND

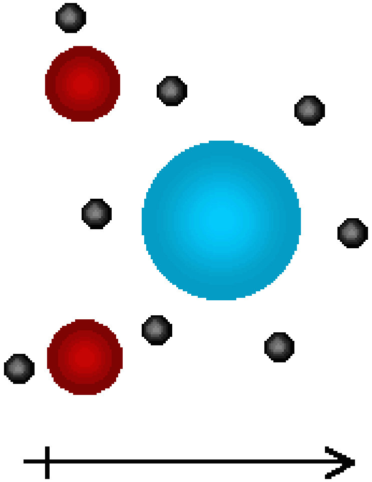
- As the valance electrons of water molecule spend more of its time around Oxygen atom than the Hydrogen atom, a dipole is formed.
  - The oxygen end of the molecule develops a partial negative charge (because of the negative charge on the electrons).
  - For the same reason, the hydrogen end of the molecule develops a partial positive charge.

- Negative end of each water molecule is attracted by a positive end of another water molecule.
- Ions are not formed; however, the molecule develops a partial electrical charge across it called a dipole.



A simulation of polar covalent bonding in the H_2O molecule

(Only valence electrons are shown)



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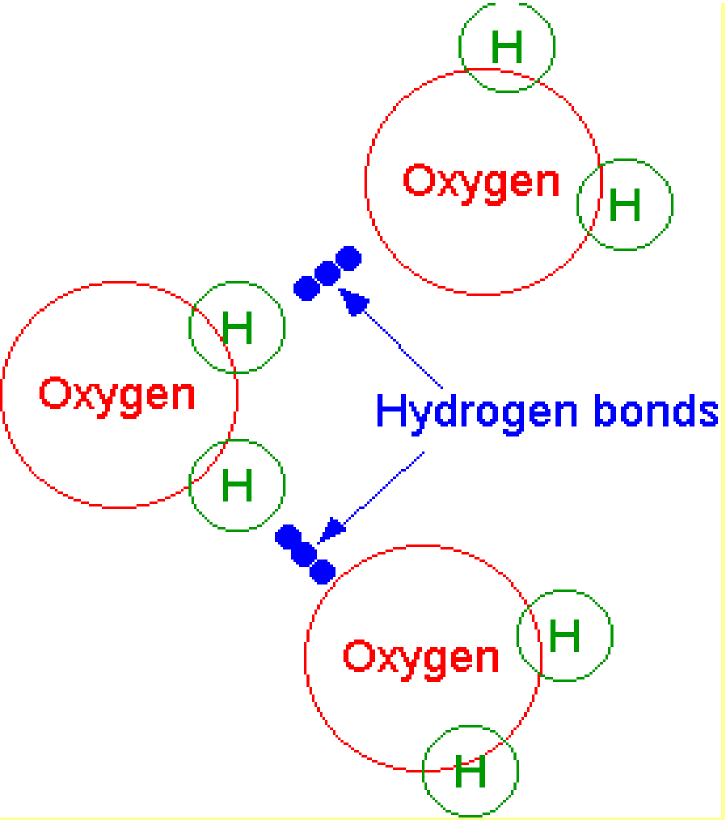
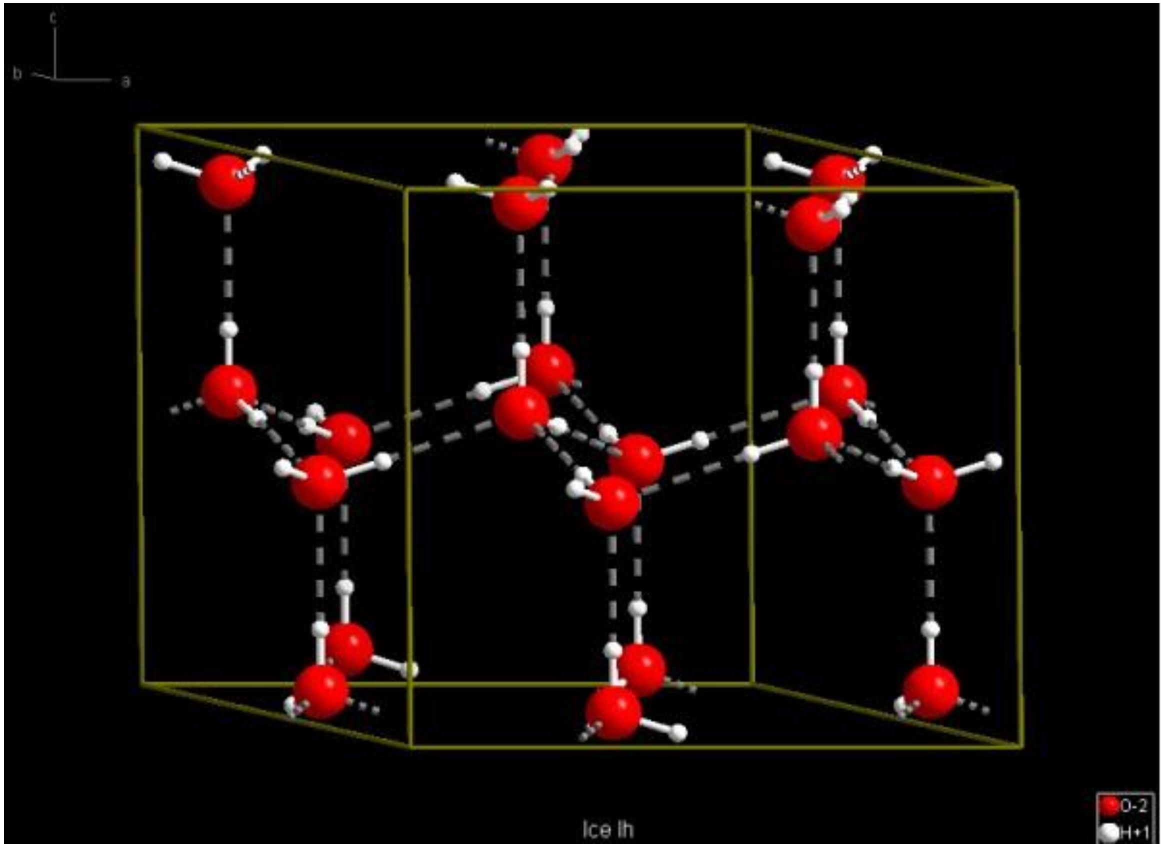
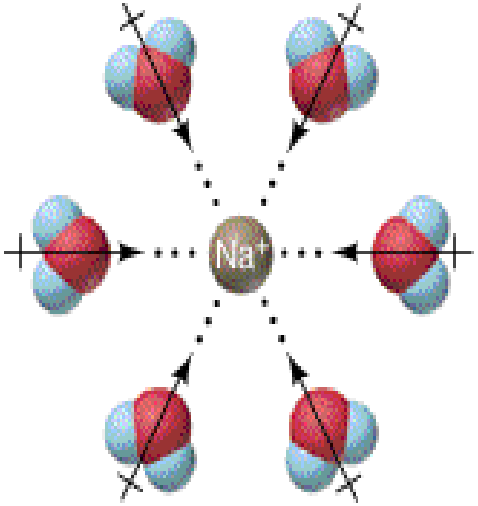
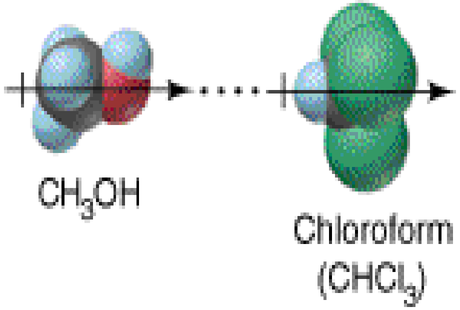




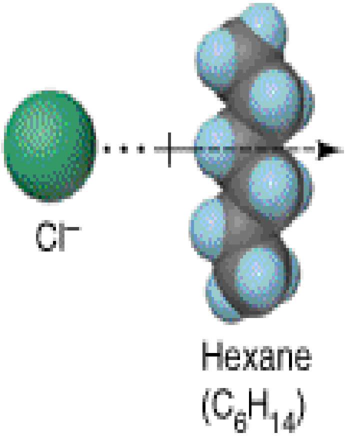


Ion-dipole

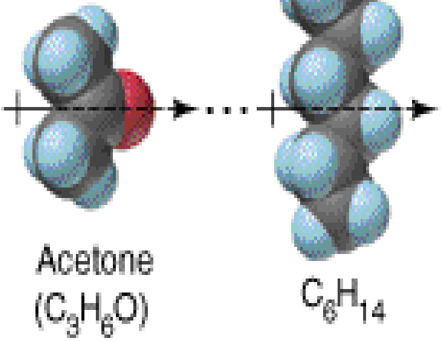
H bond



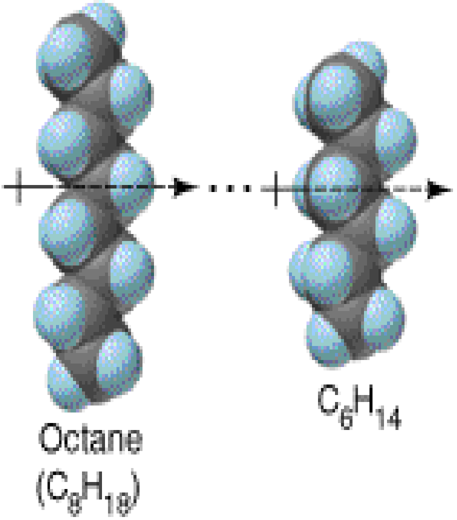
Dipole-dipole



Ion-induced dipole

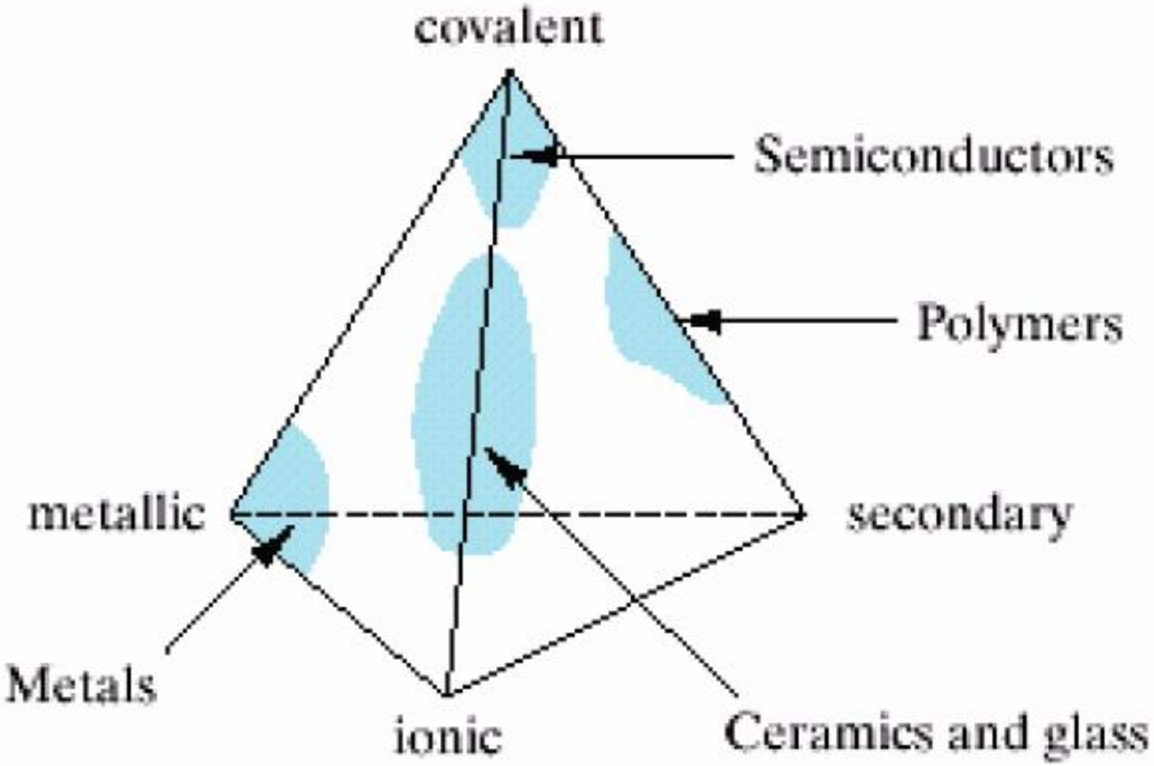


Dipole-induced dipole



Dispersion

- **Metals:** Metallic bond
- **Ceramics:** Ionic / Covalent bonds
- **Polymers:** Covalent and Secondary bonds
- **Semiconductors:** Covalent / Ionic bonds



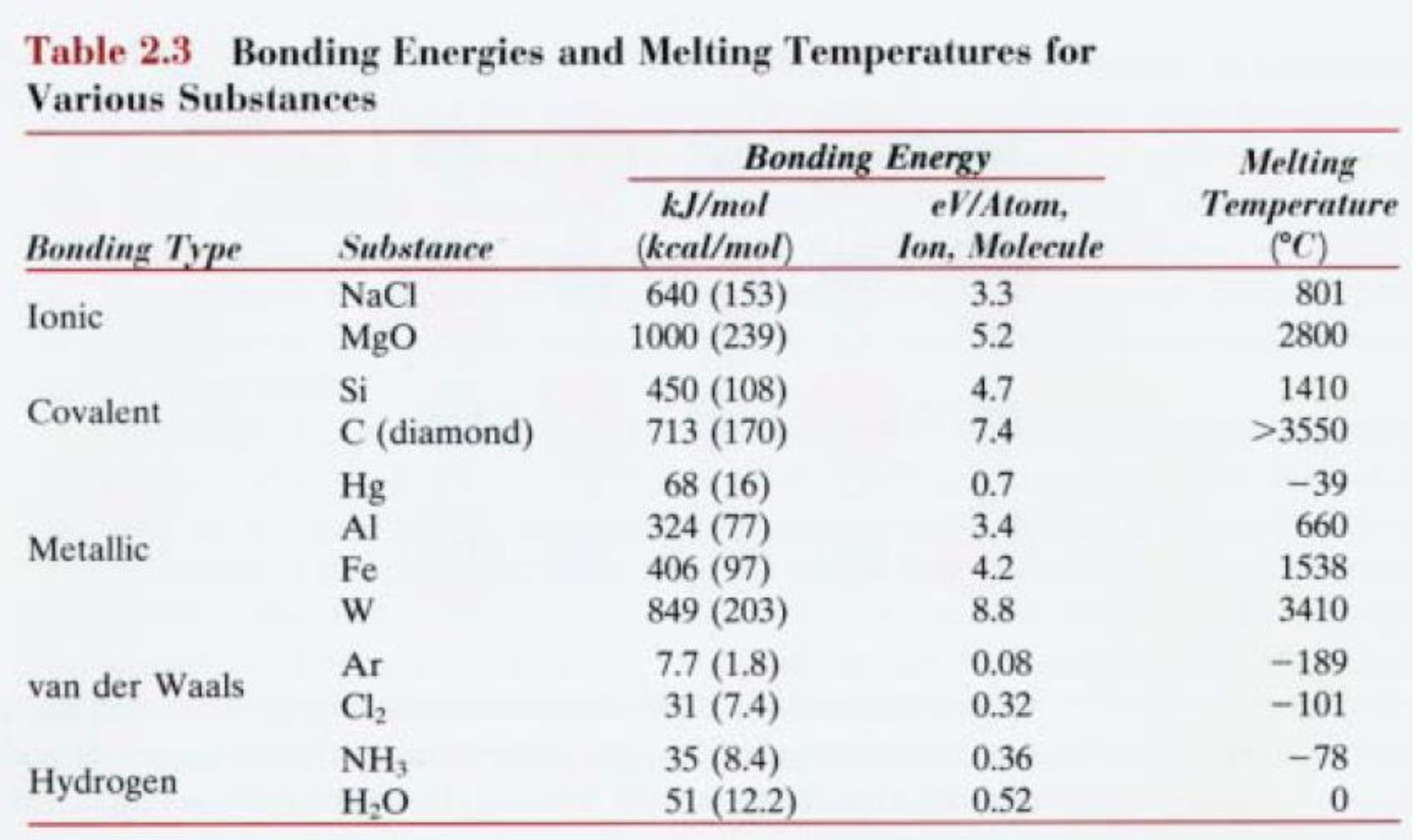


Table 2.3 Bonding Energies and Melting Temperatures for Various Substances

		Bonding Energy		*Melting*
Bonding Type	*Substance*	*kJ/mol (kcal/mol)*	*eV/Atom, Ion, Molecule*	*Temperature (°C)*
Ionic	NaCl	640 (153)	3.3	801
	MgO	1000 (239)	5.2	2800
Covalent	Si	450 (108)	4.7	1410
	C (diamond)	713 (170)	7.4	>3550
Metallic	Hg	68 (16)	0.7	−39
	Al	324 (77)	3.4	660
	Fe	406 (97)	4.2	1538
	W	849 (203)	8.8	3410
van der Waals	Ar	7.7 (1.8)	0.08	−189
	Cl_2	31 (7.4)	0.32	−101
Hydrogen	NH_3	35 (8.4)	0.36	−78
	H_2O	51 (12.2)	0.52	0

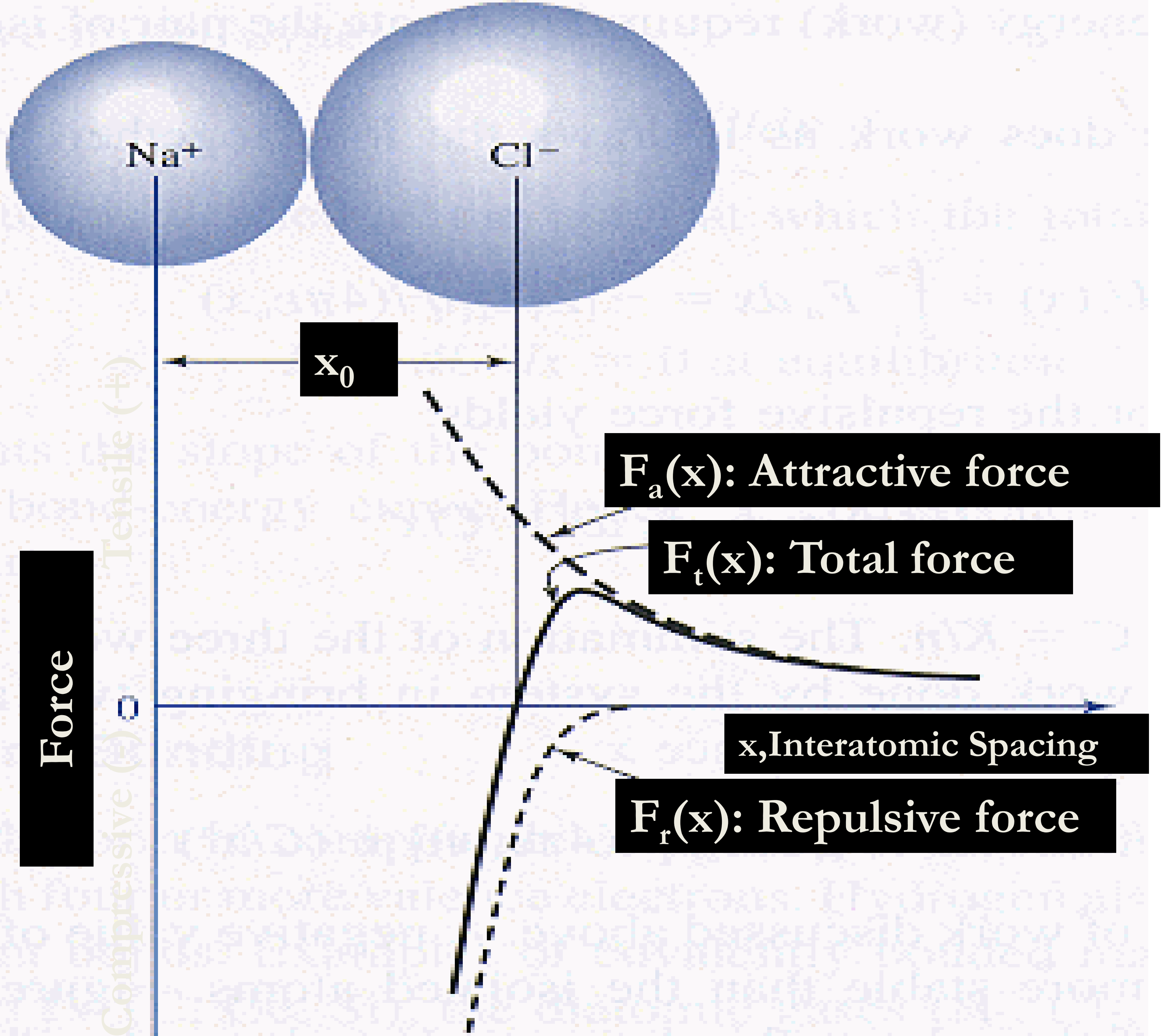
ATOMIC BONDING
IN SOLIDS

BONDING ENERGY, INTERATOMIC SPACING

- For two ions to come closer to each other, two types of forces are in effect.

Attractive Forces (+) pull atoms together

Repulsive Forces (-) develop when atoms are brought into close proximity (~nm). There is mutual electronic repulsion between the two atoms because of the electrons around an atoms.



Force

x_0

$F_a(x)$: Attractive force

$F_t(x)$: Total force

x,Interatomic Spacing

$F_r(x)$: Repulsive force

- ☐ When two atoms approach each other they exert forces on one another.

1. **Forces of attraction (F_a)**→Attractive forces b/w atoms decrease with interatomic spacing, x.

   (is inversely proportional with x)
2. **Forces of repulsion (F_r)**→As atoms come closer, repulsive forces dominate.

   (is inversely proportional to a higher power of x than F_a)

- Total force $\Sigma F = F_a + F_r$
- When $F_a = F_r$ → Equilibrium point → @ $x = x_0$

- x_0 is also known as equilibrium spacing and is a very specific distance for a given pair of atoms or ions. A large amount of force is needed to change (stretch or compress) that distance. Therefore, generally atoms can be assumed as hard balls when atomic arrangements are considered.

- Sometimes it is more convenient to work with the potential energies between two atoms

$$E = \int F dx$$

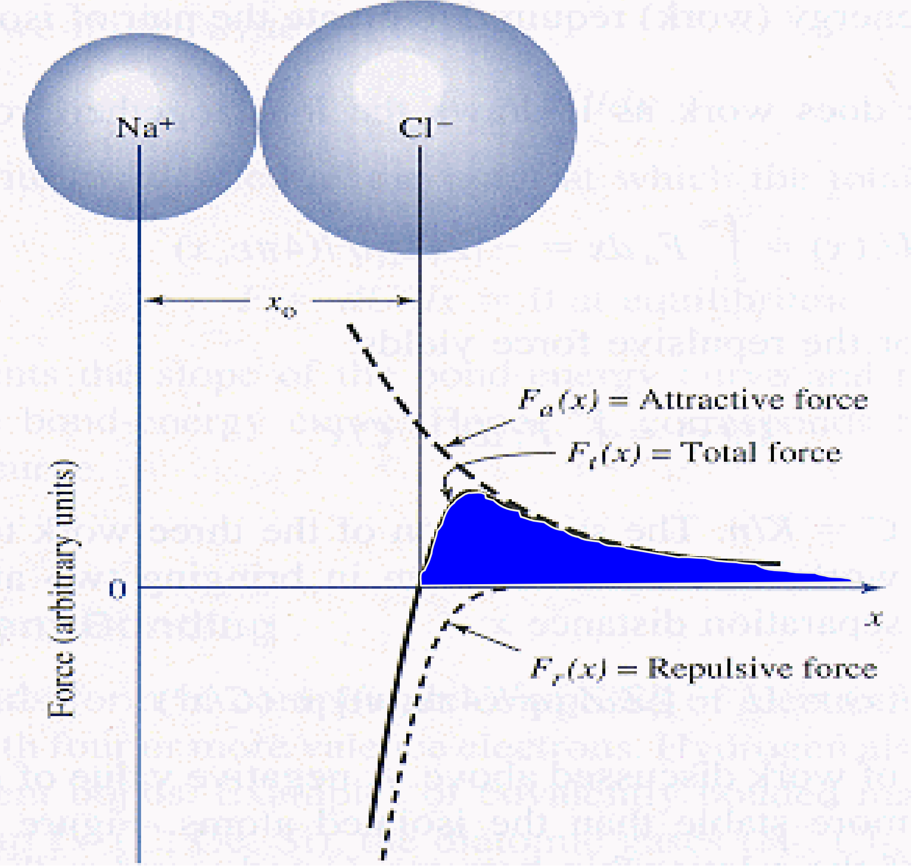
For atomic systems

$$E_n = \int_{\infty}^{x} F dx$$

$$E_n = \int_{\infty}^{x_0} (F_a + F_r) dx$$

$$E_n = E_a + E_r$$

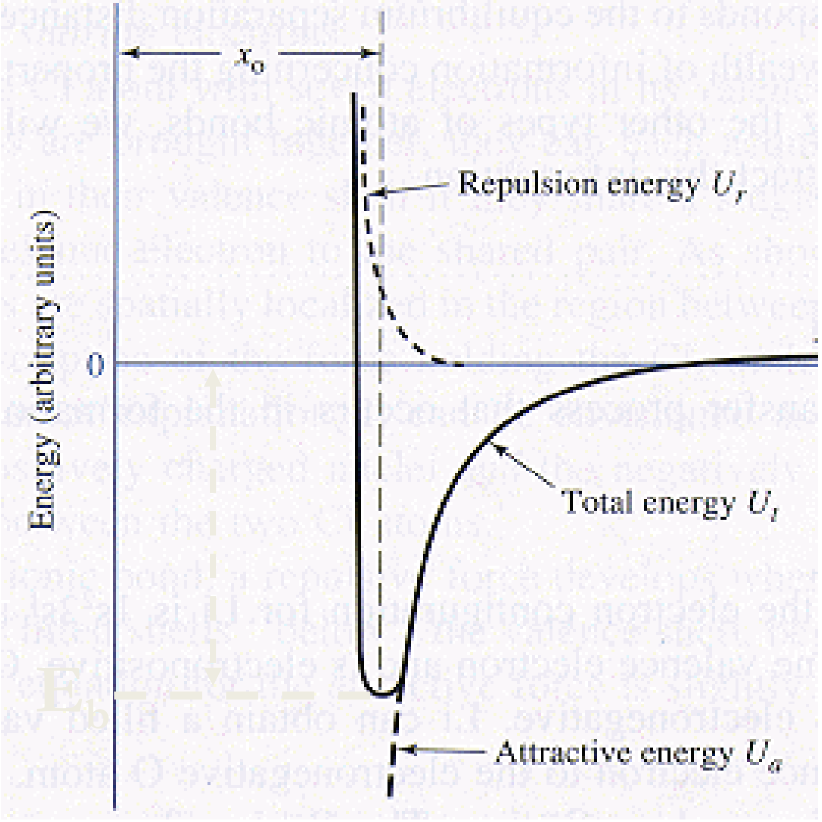
where E_n, E_a, E_r are the net, attractive and repulsive energies for two isolated and adjacent atoms.



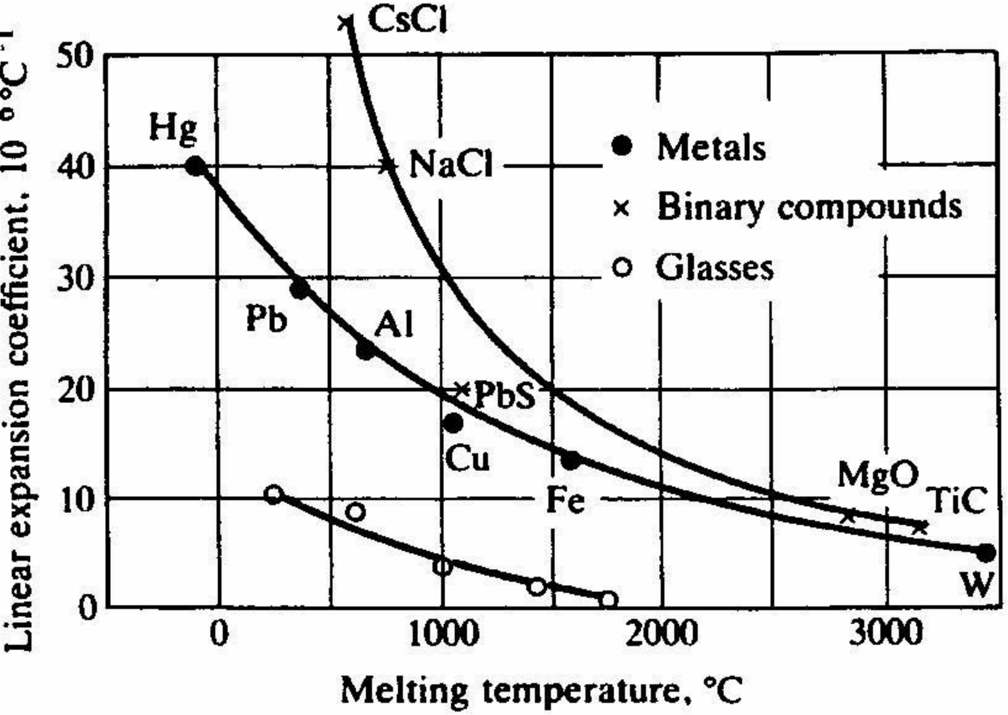
$$@\, x = x_0$$

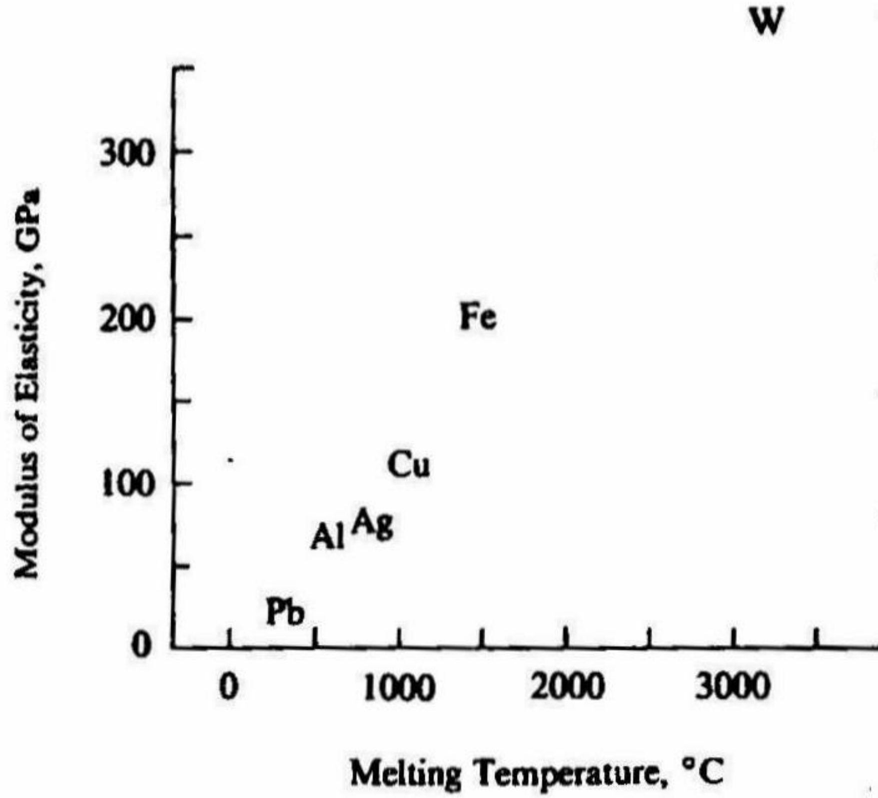
$$E_b = \int_{\infty}^{x_0} F\,dx$$

E_b is the bonding energy that represents the energy required to separate two atoms to an infinite separation.



- The magnitude of the bonding energy and the shape of E-x curve vary from material to material and they both depend on the atomic bonding.
- Furthermore a number of material properties depend on atomic relationships (E_b, curve shape and bond type).
  - Melting point
  - Hardness
  - Modulus of Elasticity→=dF/dx at $x=x_0$
  - Thermal expansion
  - Conductivity of metals

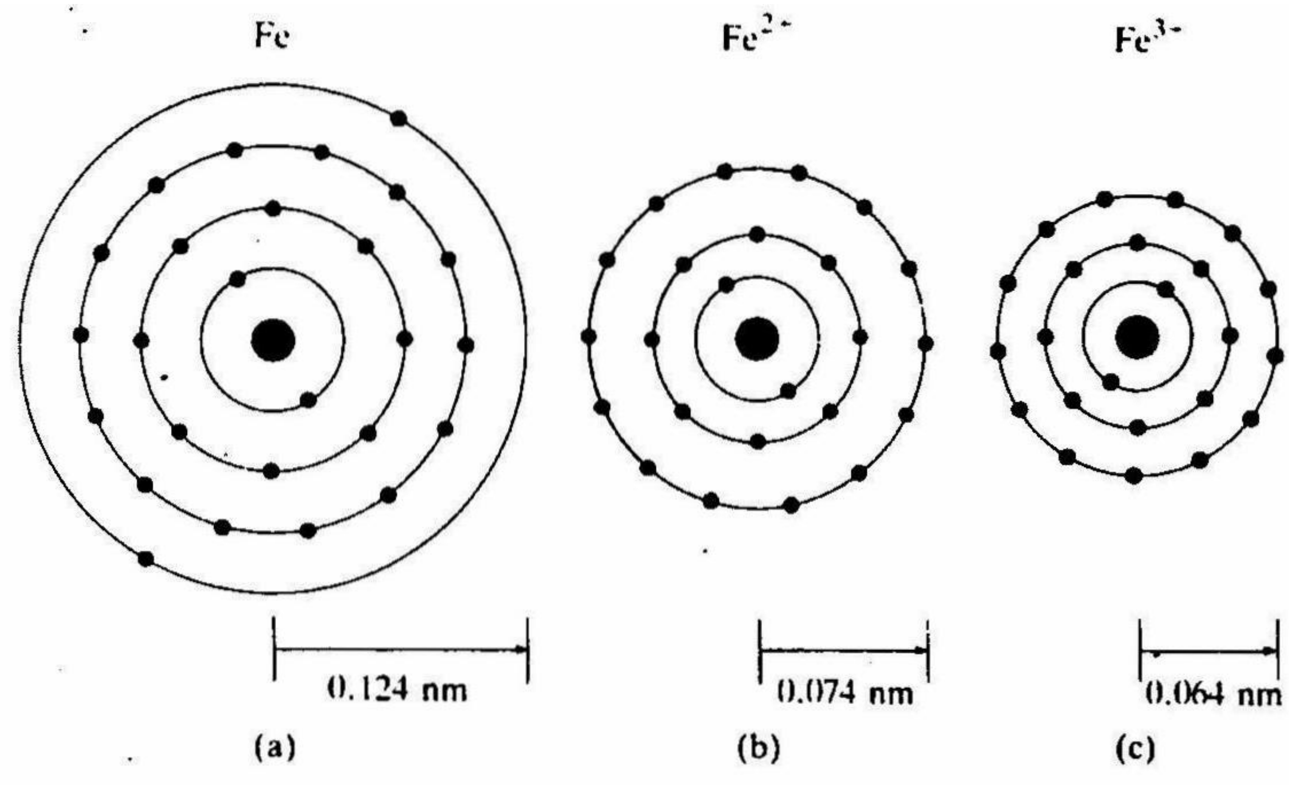




METAL	MELTING TEMPERATURE	COEFFICIENT OF LINEAR EXPANSION
Hg	−39° C	40×10^{-6} m/m · ° C
Pb	327° C	29×10^{-6} m/m · ° C
Al	660° C	22×10^{-6} m/m · ° C
Cu	1084° C	17×10^{-6} m/m · ° C
Fe	1538° C	12×10^{-6} m/m · ° C
W	3410° C	4.2×10^{-6} m/m · ° C

Factors Affecting the Atomic Radius

1. **Temperature:** As T increases, x_0 also increases.
2. **Ionic Value:** An electropositive atom (F_e^{+2}) has a smaller radius than a neutral atom (F_e).



Similarly an electronegative atom (O^{-2}) has a higher radius than a neutral atom (O).

3. **Surrounding Atoms:** As the number of surrounding atoms around a bond increases, the interatomic distance increases due to the repulsive forces developed by electrons.
4. **Covalency:** As the number of shared electrons increases, atoms will attract each other more and the radius decreases.

Example :

$$U = \frac{A}{r^m} + \frac{B}{r^n} \quad [J]$$

r: Interatomic distance in nm ($*10^{-9}$ m)

A: $-7.2 * 10^{-20}$ [J $(nm)^2$]

B: $9.4 * 10^{-25}$ [J $(nm)^{10}$]

$m = 2, n = 10$

$$U = \frac{-7.2 * 10^{-20}}{r^2} + \frac{9.4 * 10^{-25}}{r^{10}}$$

Find r_0 where the bond is most stable? → Energy is minimum

Calculate the net energy?

$$\frac{dU}{dr} = 0$$

$$U = A\, r^{-m} + B\, r^{-n}$$

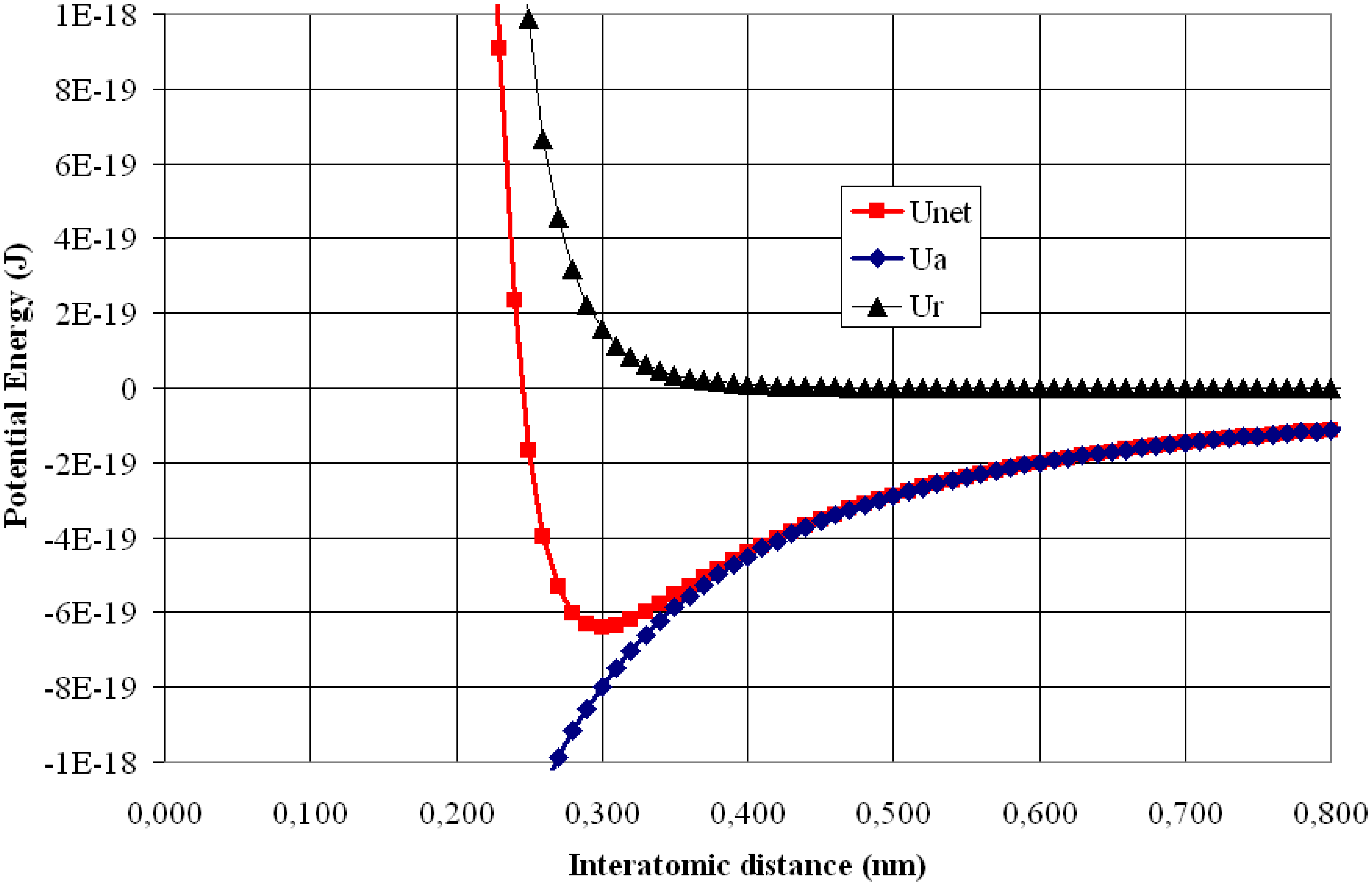
$$\frac{dU}{dr} = -m\, A\, r^{-m-1} - n\, B\, r^{-n-1}$$

$$\frac{dU}{dr} = -2 * (-7.2*10^{-20}) * r^{-3} - 10*(9.4*10^{-25})*r^{-11} = 0$$

$$\frac{14.4*10^{-20}}{r^{3}} = \frac{9.4*10^{-25}}{r^{11}} \rightarrow \quad r^{8} = 6.53*10^{-5}$$

$$r = 0.299 \text{ nm}$$

$$U_{min} = \frac{-7.2*10^{-20}}{(0.299)^{2}} + \frac{9.4*10^{-25}}{(0.299)^{10}} = -6.40*10^{-19} \text{ [J]}$$


1E-18
8E-19
6E-19
4E-19
2E-19
0
-2E-19
-4E-19
-6E-19
-8E-19
-1E-18
Potential Energy (J)
0,000
0,100
0,200
0,300
0,400
0,500
0,600
0,700
0,800
Interatomic distance (nm)
Unet
Ua
Ur

STATES OF AGGREGATION
AND
CRYSTAL STRUCTURES

- ❑ Any material may be in either of the following state.
  - Gas state
  - Liquid state
  - Solid state
- The state of a material is governed by:
  - Type of bond
  - Energy of bond
  - Stability of bond
  - Sizes of atoms
  - Temperature
  - Pressure

GAS STATE

- Each individual molecule of a gas has an order. However, the overall structure has no order.

- Intermolecular bonding in gases is built by Van der Waals bonding which is a weak bond.

- Atoms are in continuous motion at high speeds which prevents them of having a fixed shape.

- The random movement of atoms will lead the gas to fill any container into which it is introduced.

LIQUID STATE

- Liquids have more orderly structure than gases. However, this order is short ranged.

- The bond b/w particles is weak & limited. So, liquids can take the shape of the container easily.

- The thermal expansion of liquids is less than that of gases.

1. Liquids derived from Crystalline solids:

   These consist of small group of atoms still arranged in a crystalline structure. However, bonds are not strong enough for them to form a rigid mass.

2. Liquids derived from amorphous solids:

   These are composed of large molecules which are flexible & mobile. The major difference b/w two liquid types is their melting point. First one has a definite melting point because all the bonds in the crystalline structure have the same strength & break down at the same temperature.

SOLID STATE

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

- Crystalline Solids
- Amorphous Solids

- In crystalline materials atoms are situated in a repeating or periodic array over large atomic distances. (long range order)

- In amorphous materials long range order do not exist

Upon solidification of a liquid the atoms will position themselves in a repetitive 3-D pattern in which each atom is bonded to its nearest atoms.

Therefore, speed of solidification has a great effect on the type of solid.

- Solidification occurs gradually → Crystalline
- Solidification occurs suddenly → Amorphous

- The type of bond also affects the type of solid
  - Ionic and Metallic Bonds → Crystalline
  - Covalent Bonds → Amorphous

- While passing from liquid state to solid state there is no definite dividing line. (Gels are in between)

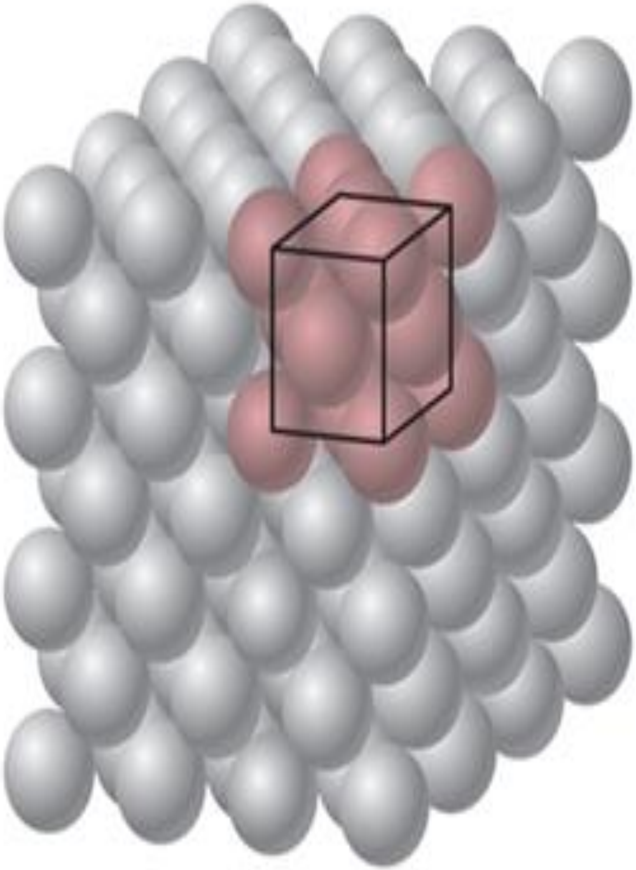
- Gels are formed by very fine particles of solid trapping liquid molecules within themselves. According to the type, strength and number of bonds, gels may be more liquid or more solid.

CRYSTALLINE SOLIDS

- In a crystalline solid, particles which may be (atoms, molecules or ions) are surrounded by like neighbors according to a definite geometrical repetitive pattern.

- When describing crystalline structures, atoms or ions are thought of as being solid spheres having well-defined diameters.

An example of the hard sphere model is the atomic arrangement of some common elemental metals shown in the figure.



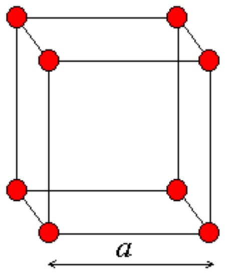
In this example:

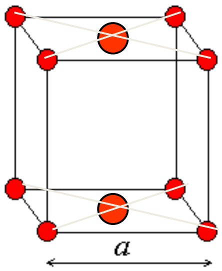
- All atoms are identical.
- Sometimes the term "lattice" is used in the context of crystal structures.
- **Space-Lattice:** 3-D arrays of points in space coinciding with atom positions.

- ❑ **Unit cell:** is the smallest unit of a space lattice which repeats itself to form the lattice.
- ❑ In other words space-lattice is formed by face to face packing of unit cells.

Unit Cell Configurations

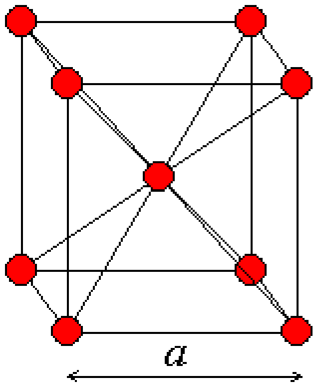
1. Simple Unit Cell: Lattice points are at every corner of the cell.

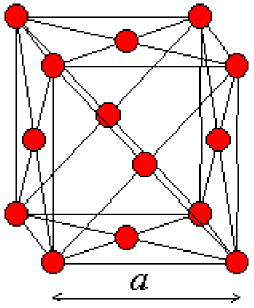




2. Base Centered Unit Cell: Extra lattice points in the center of two parallel faces.

3. Body Centered Unit Cell: An extra lattice points in the interior.





4. Face Centered Unit Cell: Extra lattice points at the center of each face.

CRYSTAL SYSTEMS

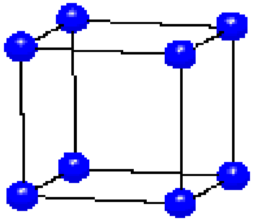
Based on unit cell configurations and atomic arrangements

CUBIC

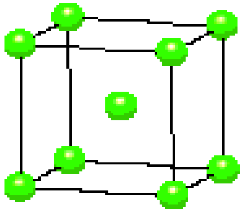
$a = b = c$

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

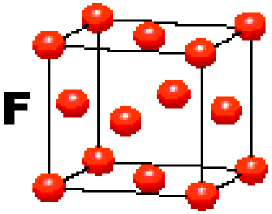
P



I



F

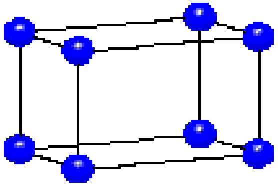


TETRAGONAL

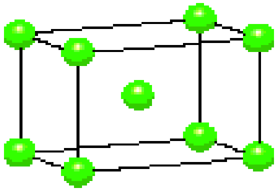
$a = b \neq c$

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

P



I

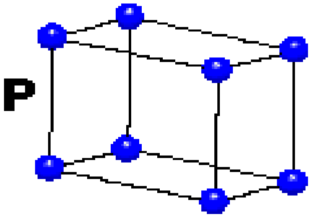


ORTHORHOMBIC

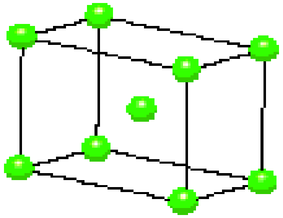
$a \neq b \neq c$

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

P



I



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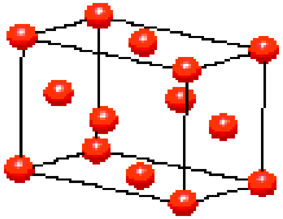
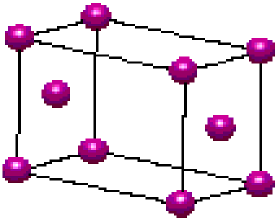


C



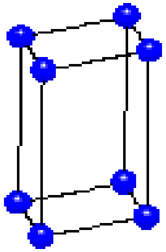
HEXAGONAL

$a = b \neq c$

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

$\gamma = 120^\circ$

P

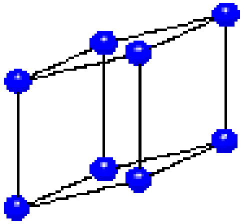


TRIGONAL

$a = b = c$

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

P



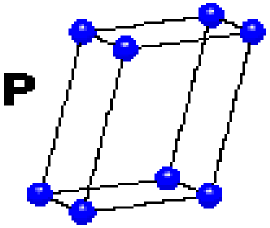
MONOCLINIC

$a \neq b \neq c$

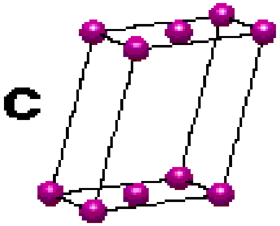
$\alpha = \gamma = 90^\circ$

$\beta \neq 120^\circ$

P



C

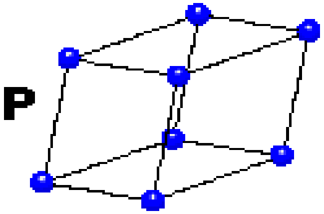


TRICLINIC

$a \neq b \neq c$

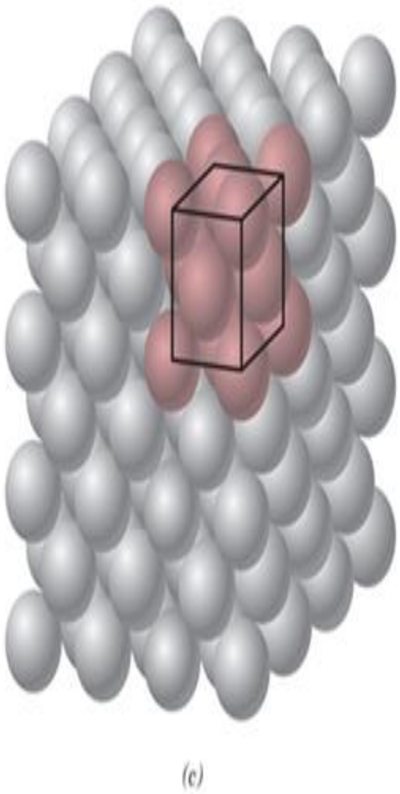
$\alpha \neq \beta \neq \gamma \neq 90^\circ$

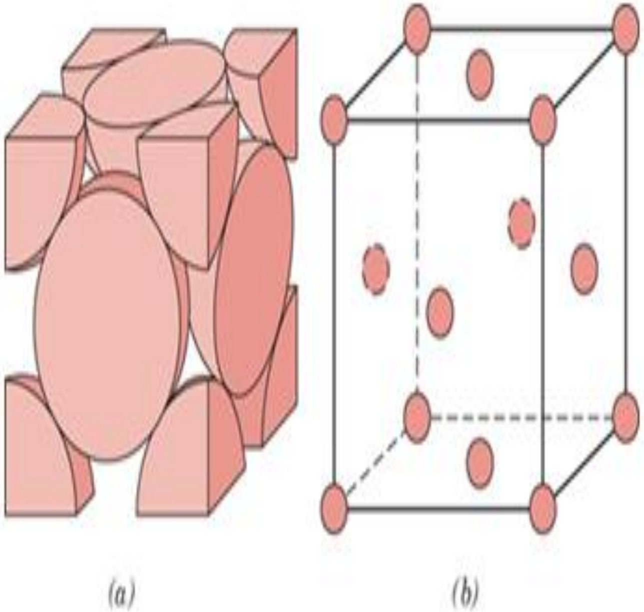
P



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Face Centered Cubic (FCC) Structure





Two representations of a unit cell

Atomic Packing Factor

Atomic packing factor shows us how dense the unit cell is:

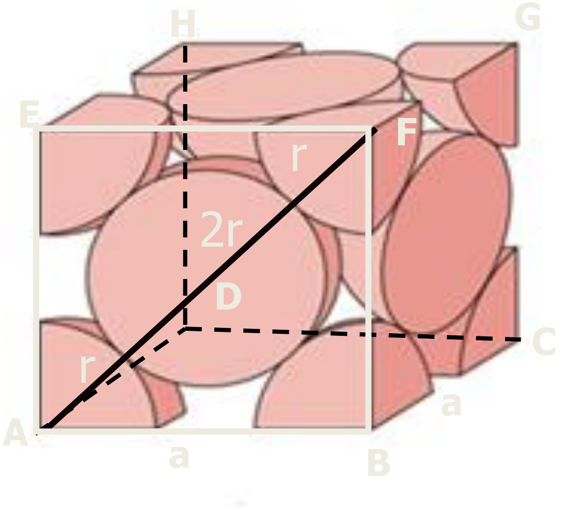
$$APF = \frac{Volume\ of\ atoms\ in\ a\ unit\ cell}{Total\ unit\ cell\ volume}$$

APF = 1 ……… Unit cell is filled with atoms

APF = 0 ……… Unit cell is empty

Atomic Packing Factor of FCC

Remember!!! Atoms are hard spheres and they touch one another along cube diagonal for an FCC structure.



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

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

Volume of unit cell, V_c

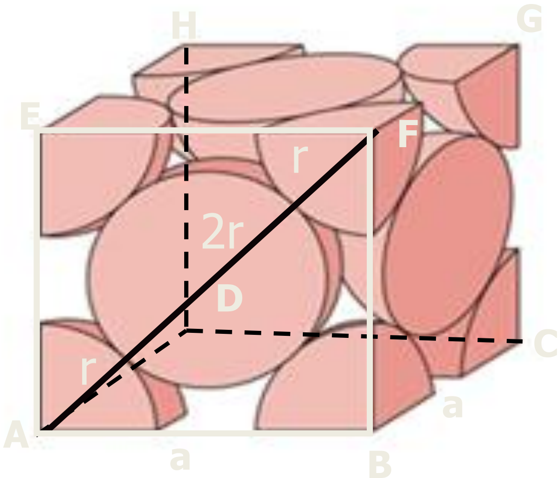
$$V_c = a^3 = (2r\sqrt{2})^3 = 16r^3\sqrt{2}$$

Number of atoms per unit cell:

- Face atoms – 6 x 1/2 = 3
- Corner atoms – 8x1/8 = 1

Total number of atoms in the unit cell = 4

Atomic Packing Factor of FCC



$$APF = \frac{Volume\ of\ atoms\ in\ a\ unit\ cell}{Total\ unit\ cell\ volume}$$

$$APF = \frac{(4)*(4/3\pi r^3)}{16r^3\sqrt{2}}$$

$$APF \cong 0.74$$

How many atoms are in the fcc unit cell?

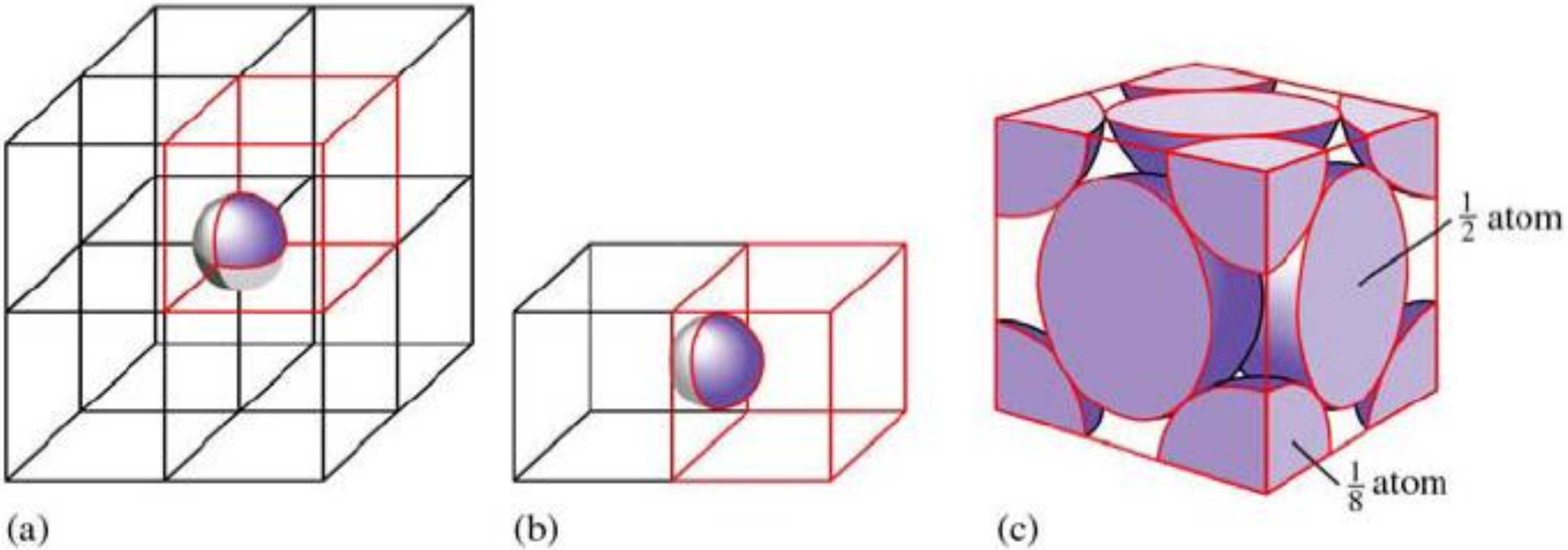


Figure 16.17

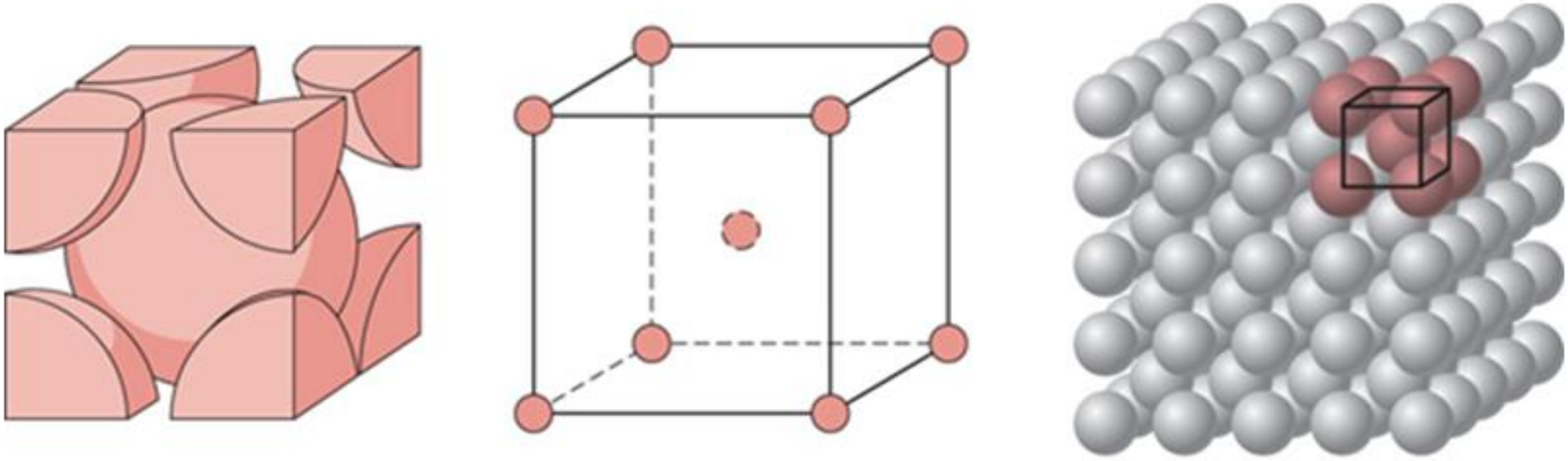
6(atoms on faces) + 8(atoms on corners)

$$= 6(1/2) + 8(1/8)$$

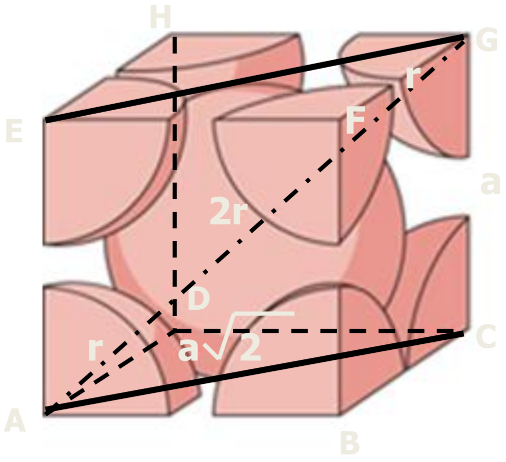
$$= 3 + 1$$

$$= 4$$

Body Centered Cubic (BCC) Structure



(a) (b) (c)



How many atoms are there in BCC structure?

APF of BCC?

DENSITY COMPUTATION

Since the entire crystal can be generated by the repetition of the unit cell, the density of a crytalline material can be calculated based on the density of the unit cell.

$$\rho = \frac{nM}{V_c}$$

ρ : Density of the unit cell

n : Number of atoms in the unit cell

M : Mass of an atom

V_c : Volume of the cell

Mass of an atom is given in the periodic table in atomic mass units (amu) or gr/mol. To convert (amu) to (gr) use avagadro's number.

DENSITY COMPUTATION

Avagadro’s number, $N_A = 6.023 \times 10^{23}$ atoms/mol

Therefore,

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

ρ : Density of the unit cell

n : Number of atoms in the unit cell

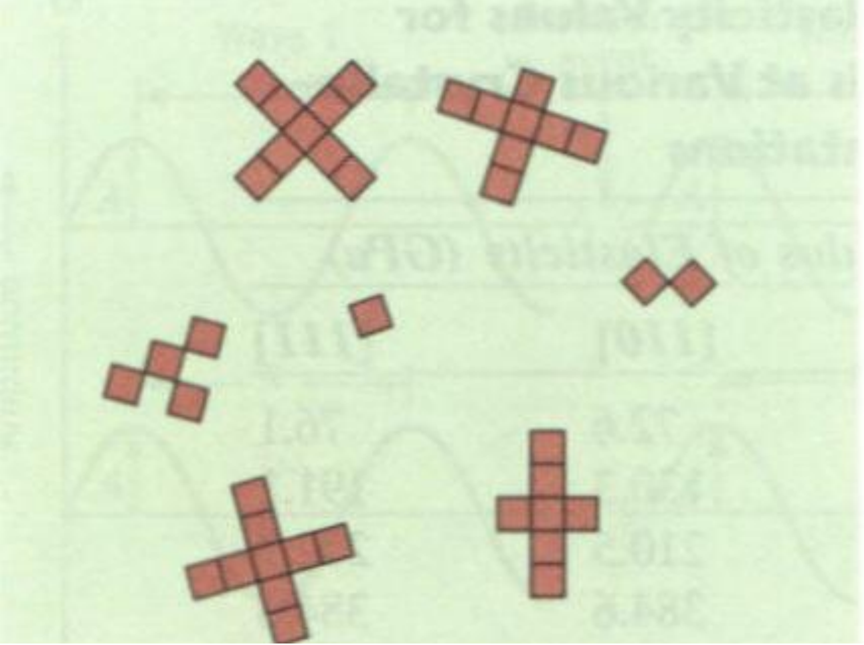
A : Atomic mass

V_c : Volume of the cell

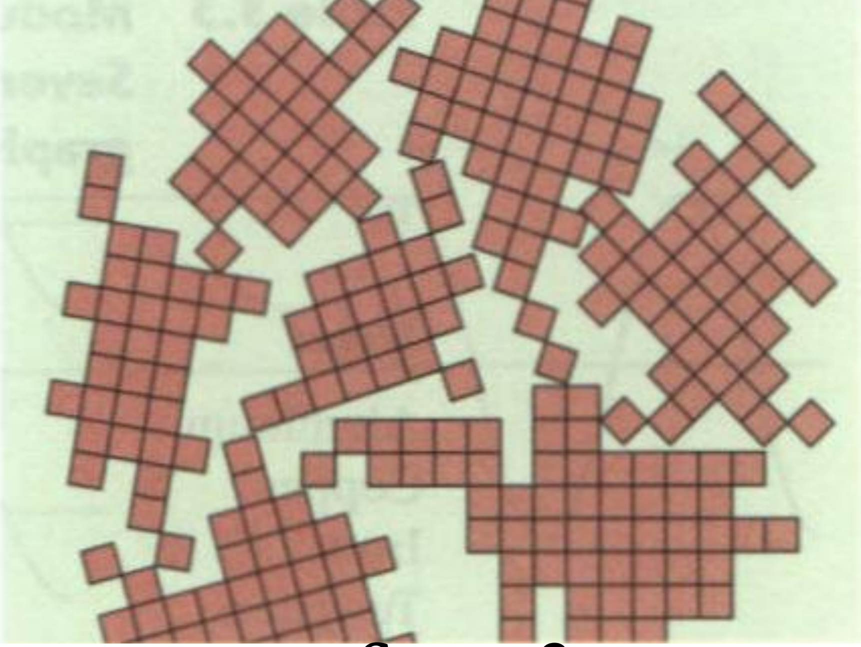
N_A : Avagadro’s number

POLYCRYSTALLINE MATERIALS

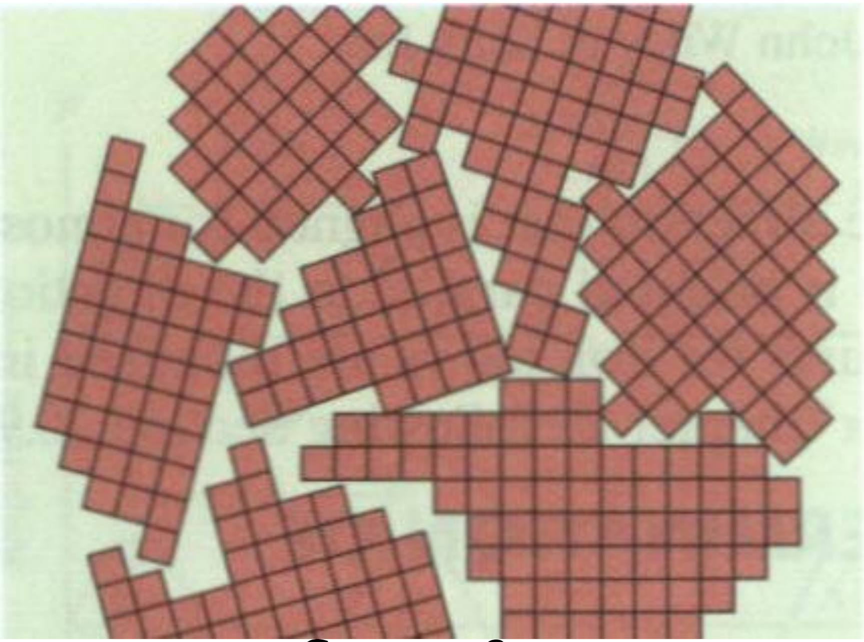
- Most crystalline solids are composed of many small crystals or grains termed as polycrystalline.
- During the solidification of a polycrystalline solids, the crystallization may start at various nuclei with random crystallographic orientations.
- Upon solidification, grains of irregular shapes may form.
- The structure will have grain boundaries that could be seen under a microscope.



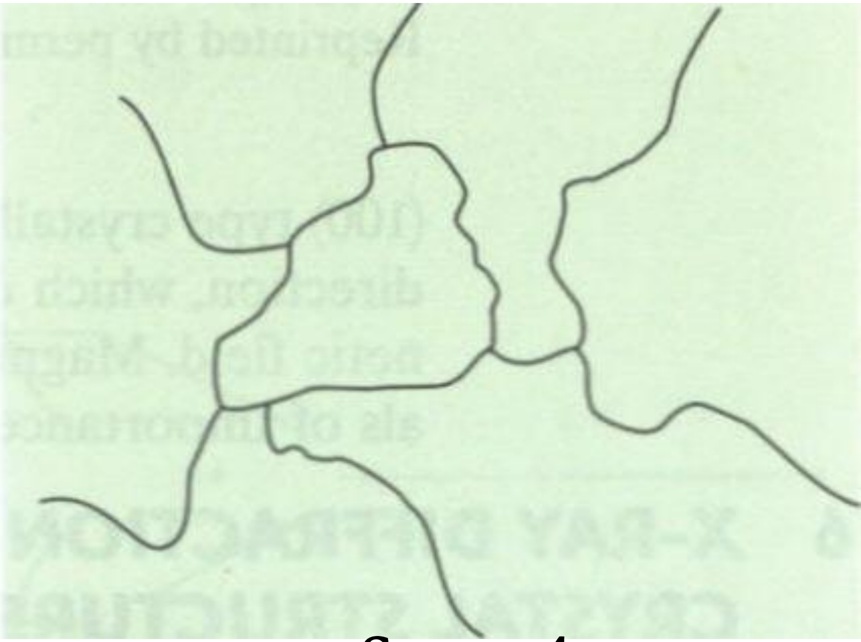
Stage 1



Stage 2



Stage 3



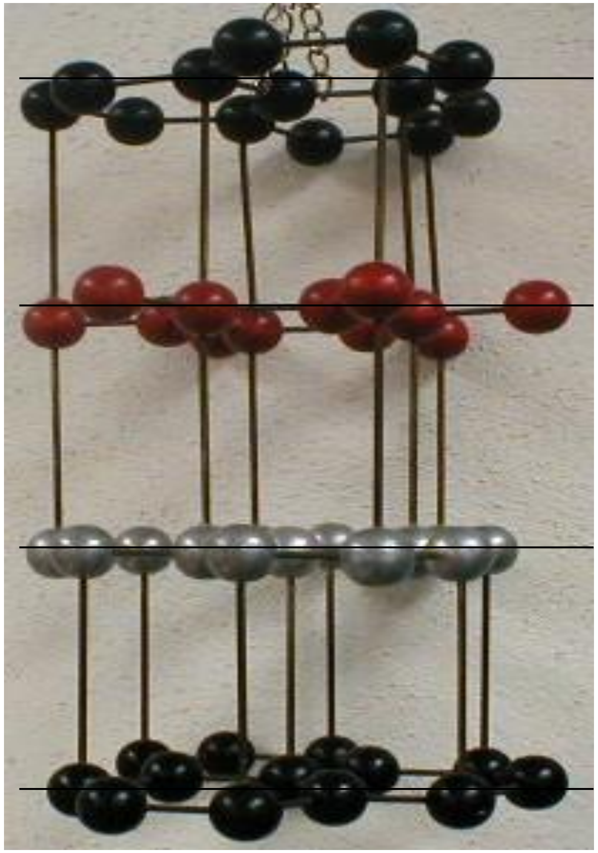
Stage 4

POLYMORPHIC TRANSFORMATION

- Materials having the same chemical composition can have more than one crystal structure. These are called allotropic or polymorphic materials.
  - **Allotropy** for pure elements.
  - **Polymorphism** for compounds.
- These transformations result in changes in the properties of materials and form the basis for the heat treatment of steels and alloys.

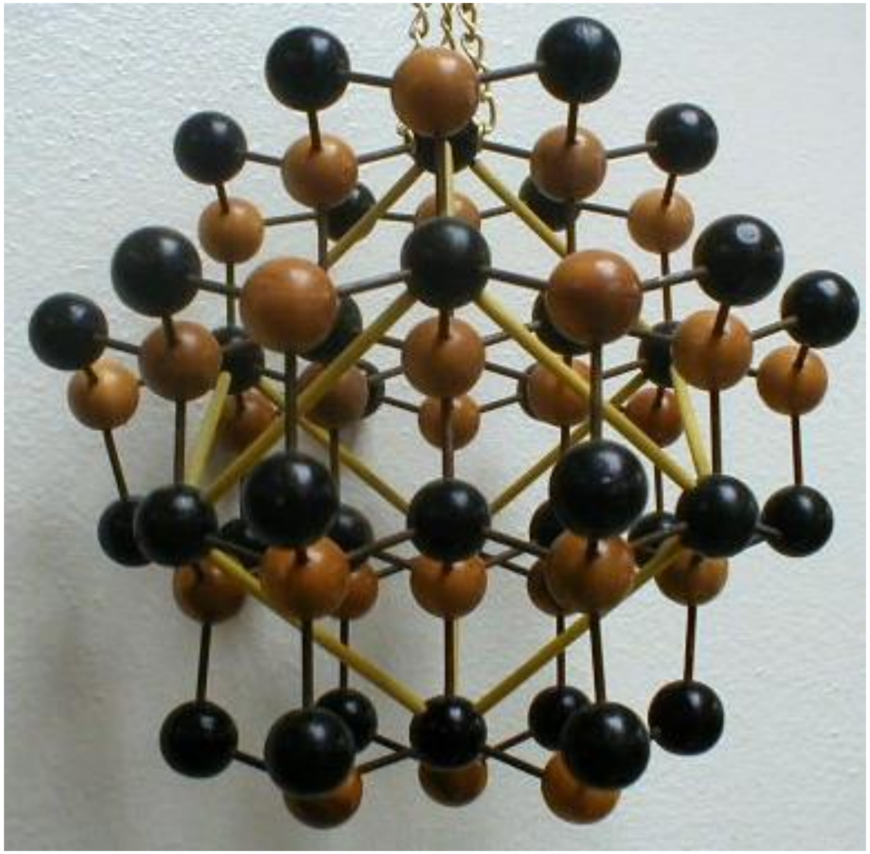
POLYMORPHISM

- Carbon may exist in two forms:



Graphite

(2D layers)



Diamond

(3D structure)

POLYMORPHISM

Iron (Fe) may also exist in several forms:

- ☐ BCC at room temperature → α iron
- ☐ FCC at 910°C → γ iron
- ☐ BCC at above 1400°C → β iron
- ☐ Above 1539°C → liquid

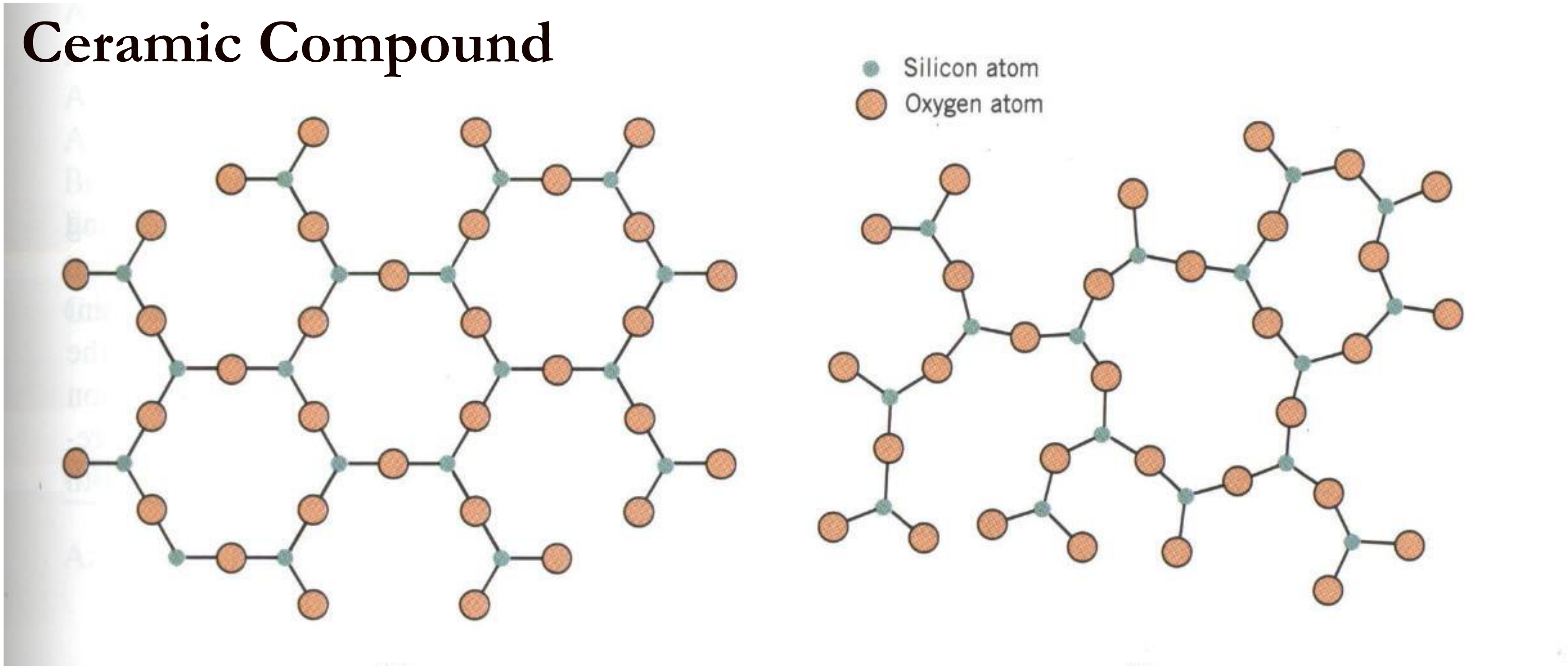
Upon heating an iron from room temperature to above 910°C, its crystal structure changes from BCC to FCC accompanied by a contraction (reduction in volume).

NONCRYSTALLINE SOLIDS

Amorphous Structures

AMORPHOUS SOLIDS

- Materials which don’t have the long range repetitive pattern of crystals are called amorphous materials. Amorphous means “without form”.



Crystalline Amorphous

AMORPHOUS SOLIDS

During the rapid cooling of a liquid, if atoms or molecules do not find sufficient time to arrange themselves in a long-range repetitive pattern amorphous solids will form unlike crystalline solids obtained by gradual cooling.

- Glasses
- Polymeric materials
- Some ceramics

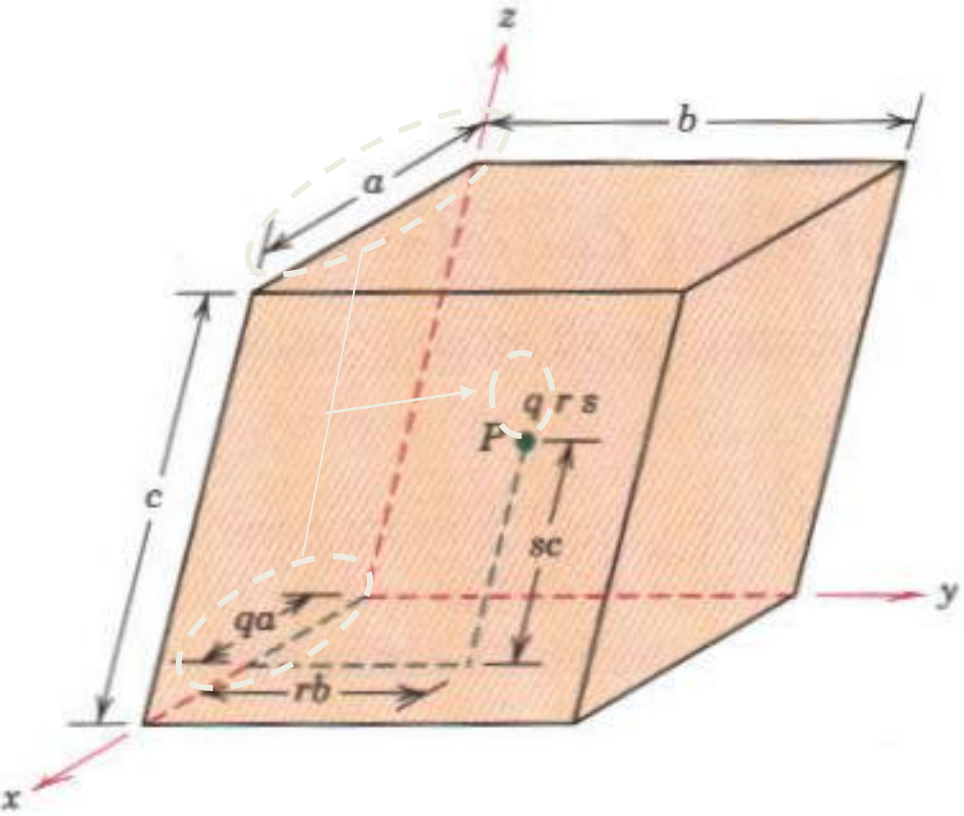
CRYSTALLOGRAPHIC POINTS, DIRECTIONS, PLANES & THE MILLER SYSTEM OF INDICES

- ☐ When dealing with crsytalline materials, it is often necessary to specify a particular point within a unit cell, a particular direction or a particular plane of atoms.
- ☐ Planes are important in crystals because if bonding is weak between a set of parallel planes, then brittle shear fracture may occur along these planes.
- ☐ Therefore, it is necessary to be able to specify individual crystal planes and in the case of shear to specify directions within these planes.

Such identification is carried out by means of

Miller Indices.

POINT COORDINATES



The position of any point located within a unit cell is specified in terms of its coordinates as fractional multiplies of the unit cell edge lengths.

To determine the point coordinates of point P, the manner in which the q, r, s coordinates of point P within the unit cell are determined.

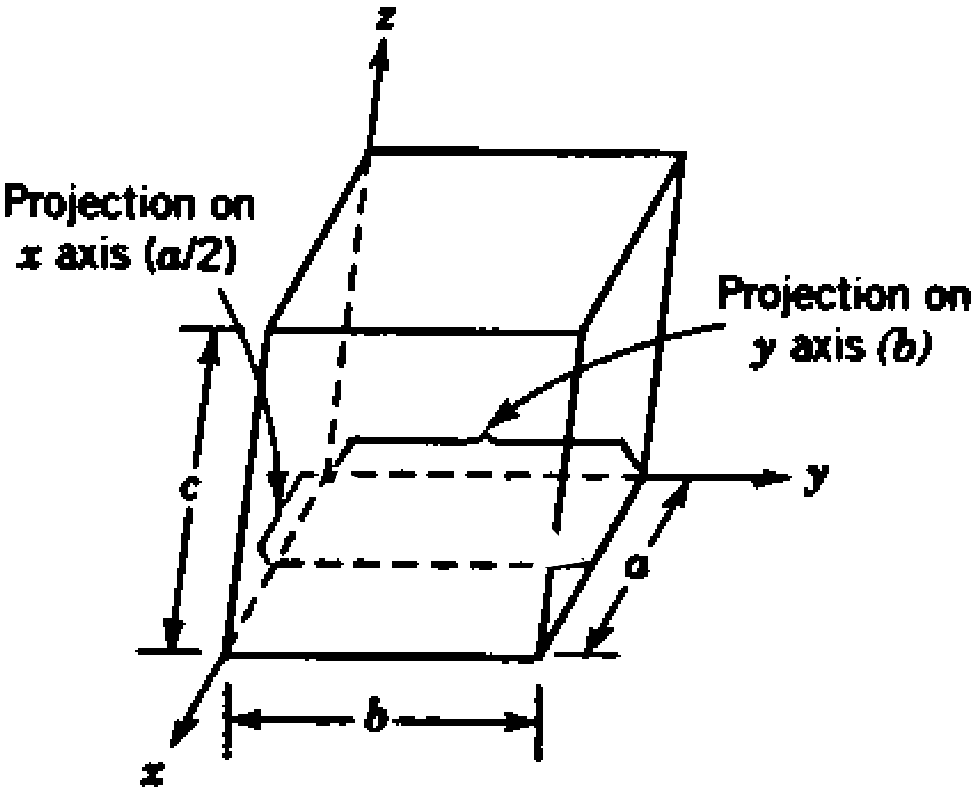
The "*q*" coordinate (which is a fraction) corresponds to the distance "*qa*" along the x-axis where "*a*" is the unit cell length along x-axis.

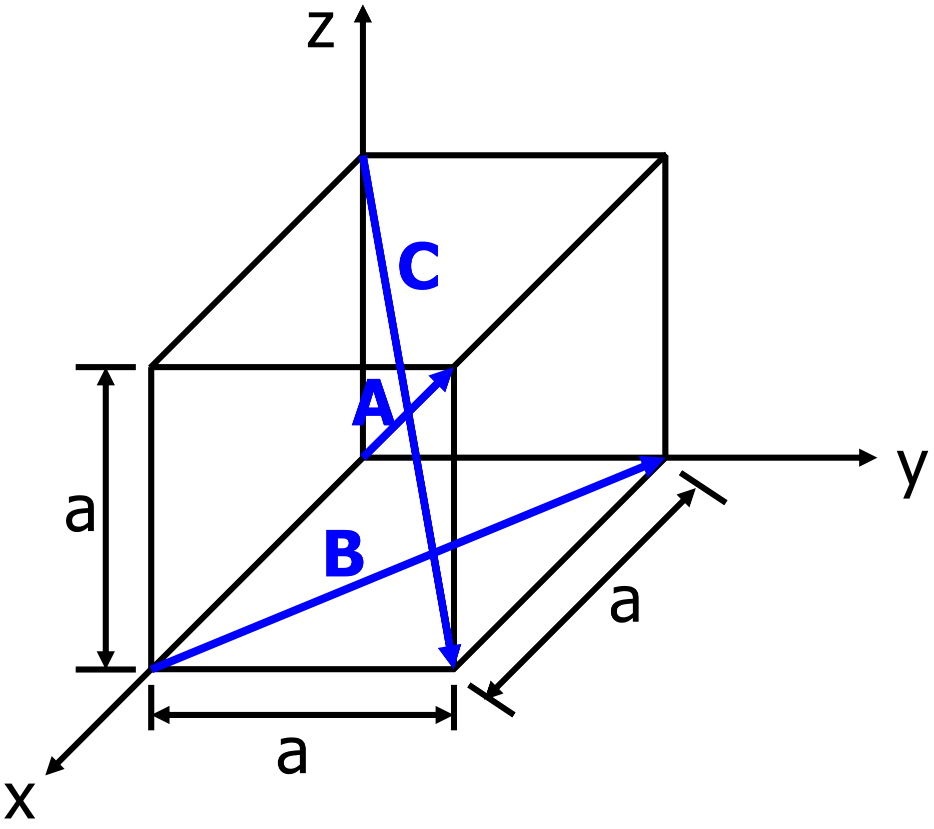
CRYSTALLOGRAPHIC DIRECTIONS

A crystallographic direction is defined as a line between two points (a vector).

1. A vector of convenient length is positioned such that it passes through the origin of the coordinate system. (Any vector can be translated throughout the crystal lattice, if parallelism is maintained).
2. The length of the vector projection on each of the three axes is determined in terms of the unit cell dimensions *a*, *b*, and *c*.
3. These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
4. The three indices are enclosed in brackets as [*uvw*]. The *u*, *v*, and *w* integers correspond to the reduced projections along x, y, and z-axes respectively.

1. The vector as drawn passes through the origin of the coordinate system, and therefore no translation is necessary.
2. Projections of this vector along x, y, and z axes are a/2, b, and 0c. In terms of unit cell dimensions ½, 1, 0.
3. Reduction of these numbers to the lowest set of integers could be done through multipliying these numbers by 2 to yield 1, 2, and 0
4. The crystallographic direction is then [120]





- Vector A → a, a, a 1/a, 1/a, 1/a [1 1 1]
- Vector B → [$\bar{1}$ 1 0]
- Vector C → [1 1 $\bar{1}$]

- For some crystal structures, several nonparallel directions with different indices are actually equivalent. (The spacing of atoms along each direction is the same)
- For example in **cubic crystals**, all the directions represented by the following indices are equivalent.

$$[100],[\bar{1}00],[010],[0\bar{1}0],[001],[00\bar{1}]$$

- **As a convenience, equivalent directions are grouped into a "family" which are grouped in angle brackets.**

$$\underbrace{[100],[\bar{1}00],[010],[0\bar{1}0],[001],[00\bar{1}]}_{\langle 100\rangle}$$

- ❑ Sometimes the angle between two directions may be necessary.

A $[h_1\ k_1\ l_1]$ and B $[h_2\ k_2\ l_2]$ → the angle between them is α.

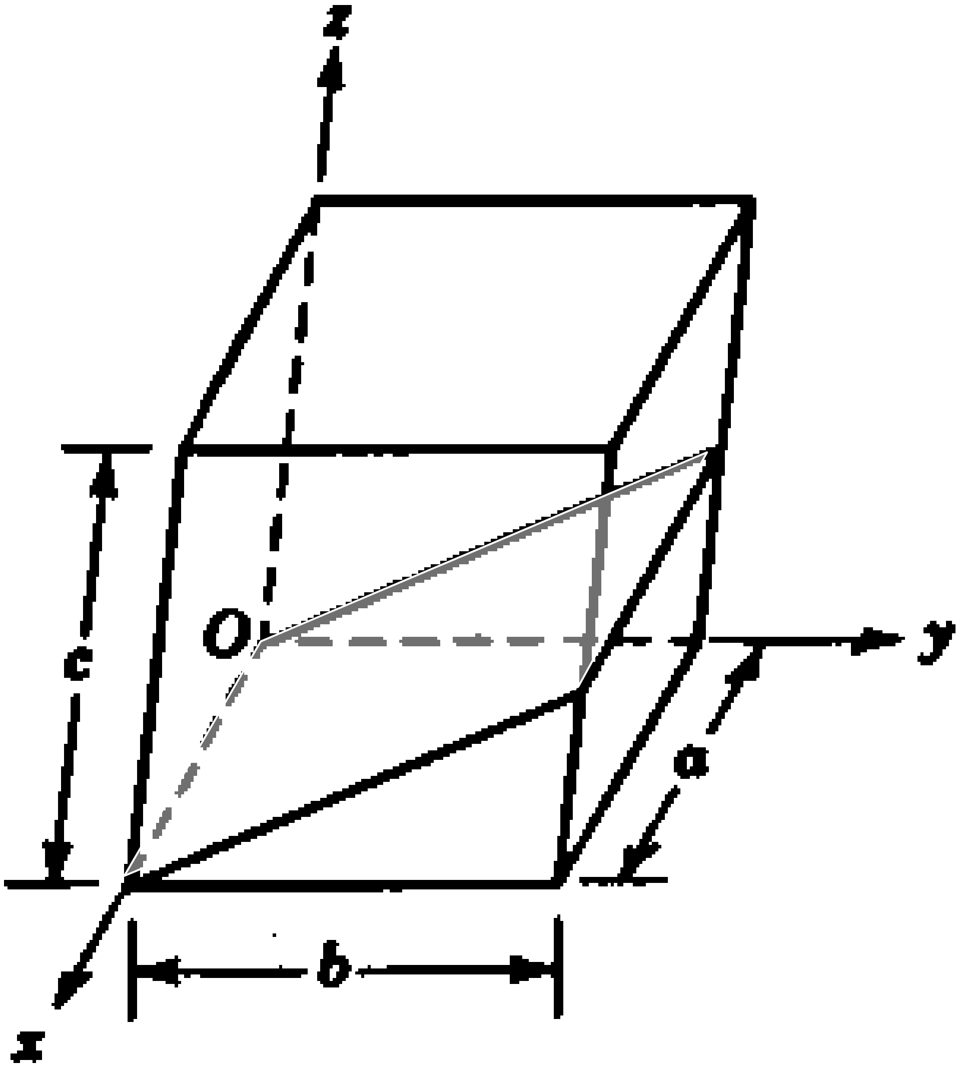
$$A \cdot B = |A|\ |B| \cos \alpha$$

$$\cos \alpha = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2+k_1^2+l_1^2)\ (h_2^2+k_2^2+l_2^2)}}$$

CRYSTALLOGRAPHIC PLANES

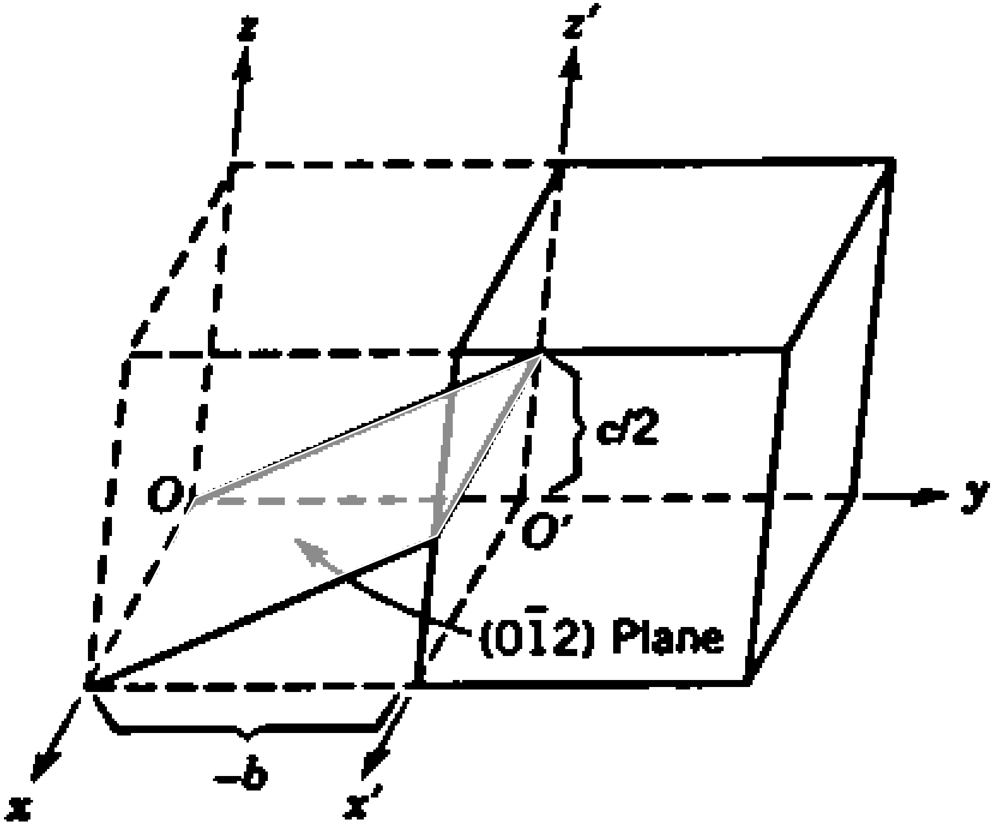
- The orientations of planes for a crystal structure are represented in a similar manner.
- In all except for the hexagonal crystal system, crystallographic planes are specified by three Miller Indices as (*hkl*).
- Any two parallel planes are equivalent and have identical indices.
- The following procedure is employed in determining the *h*, *k*, and *l* index numbers of a plane:

1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
2. At this point the crystallographic plane either intersects or parallels each of the three axes; the length of the planar intercept for each axis is determined in terms of the lattice parameters *a*, *b*, and *c*.
3. The reciprocals of these numbers are taken.
4. If necessary, these three numbers are changed to the set of smallest integers by multiplication or division by a common factor.
5. The integer indices are enclosed within parantheses as (hkl).

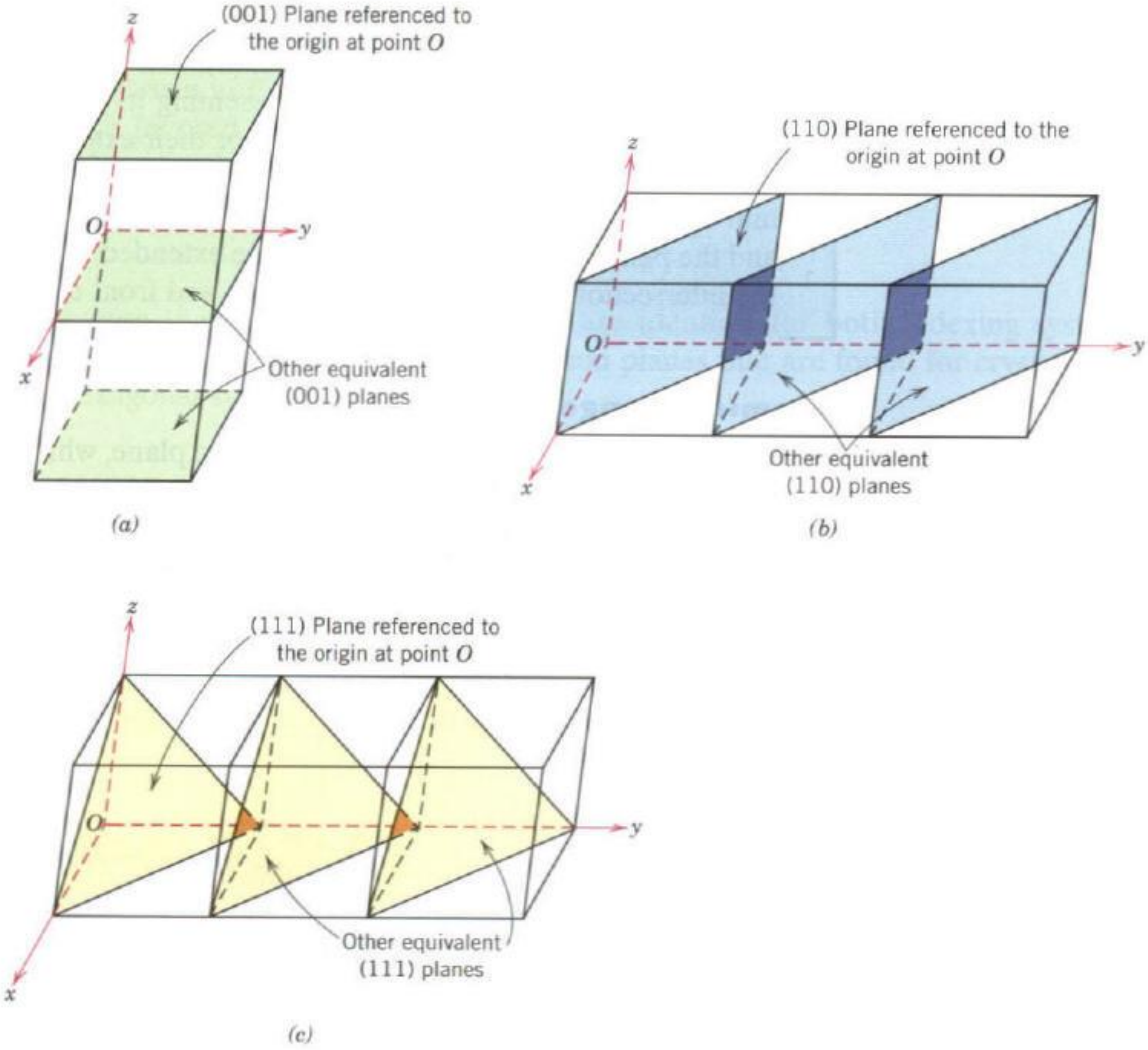


1. The plane passes through the selected origin O. Therefore, a new origin must be selected at the corner of an adjacent unit cell.

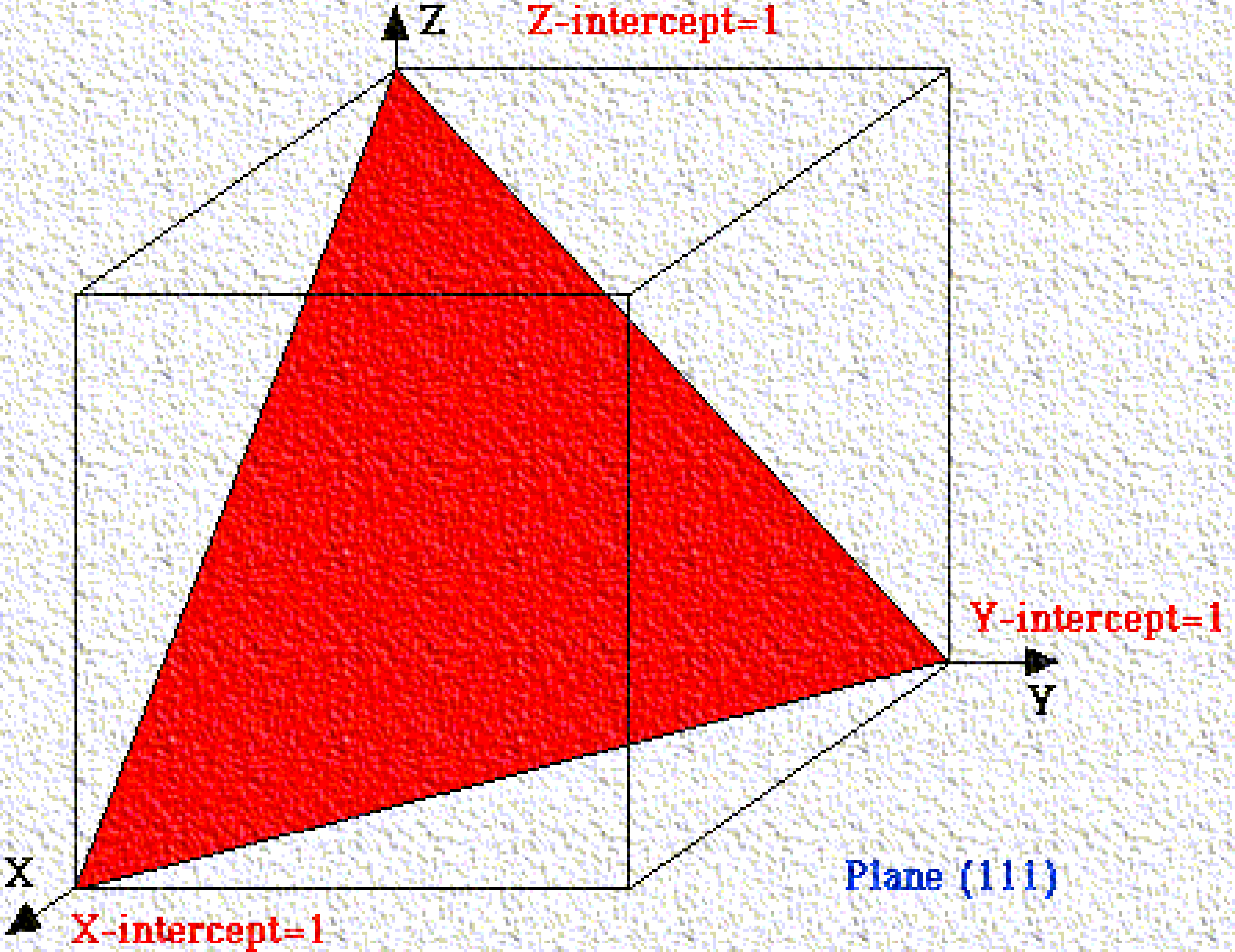
2. The plane is parallel to the x’-axis and the intercept can be taken as ∞a. The y’ and z’ intersections are –b anc c/2. Lattice parameters are ∞, -1, and 1/2.
3. Reciprocals are 0, -1, 2.



4. All are integers no reduction is necessary.
5. The crystallographic plane is $(0\bar{1}2)$

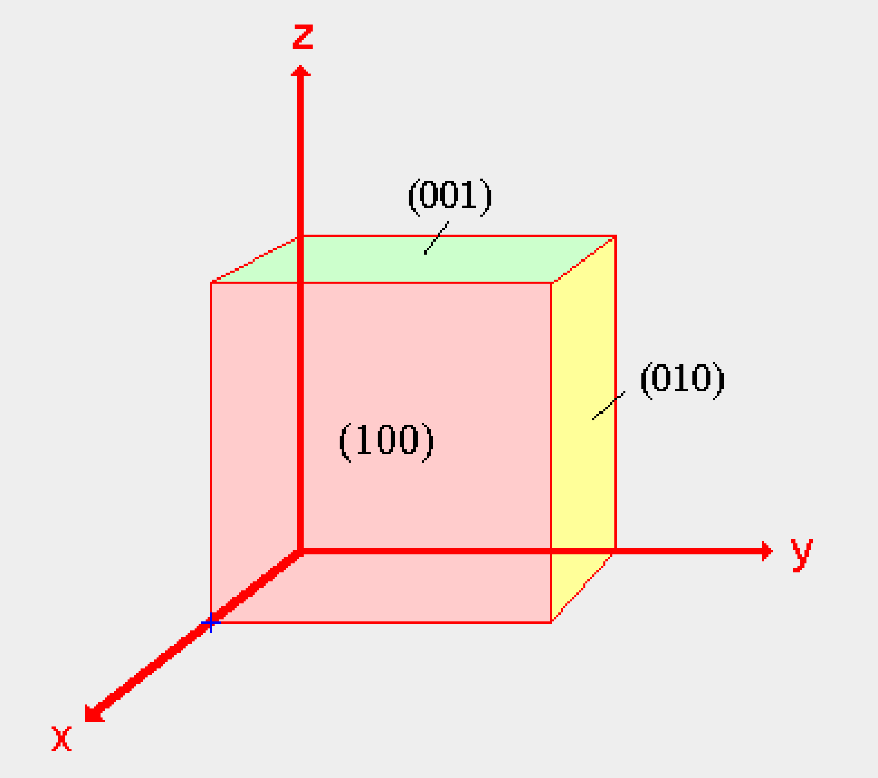


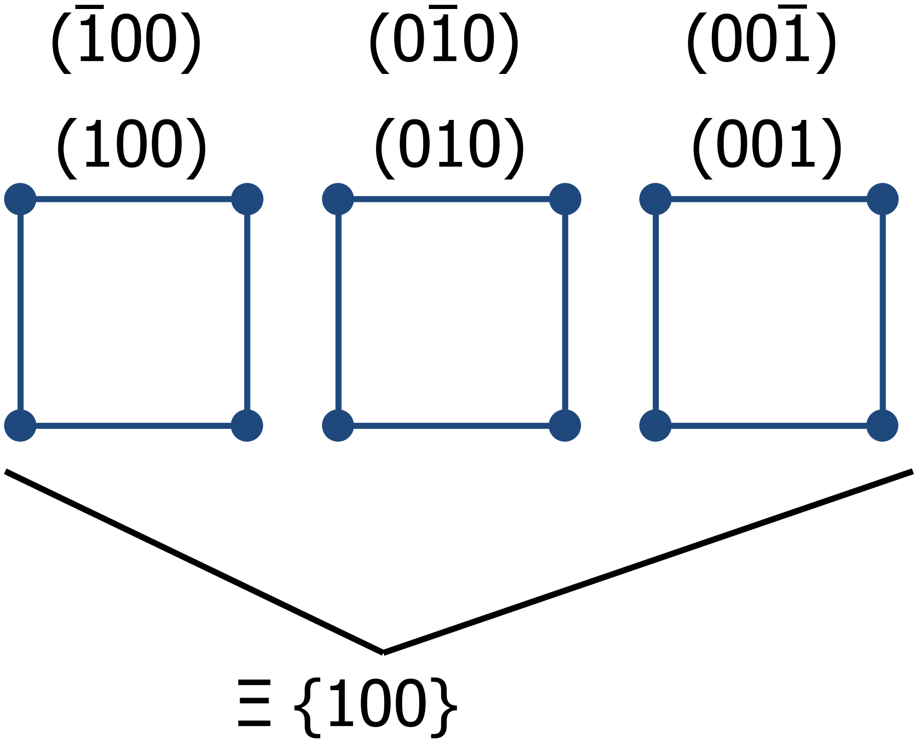
(001) Plane referenced to the origin at point O
Other equivalent (001) planes
z
y
x
O
(a)
(110) Plane referenced to the origin at point O
Other equivalent (110) planes
z
y
x
O
(b)
(111) Plane referenced to the origin at point O
Other equivalent (111) planes
z
y
x
O
(c)


Z
Z-intercept=1
Y-intercept=1
Y
X
X-intercept=1
Plane (111)

- Various non-parallel planes may have similarities (crystallographically equivalent). Such planes are referred to as “family of planes” and are designated as {h k l}

Example: Faces of a cubic unit cell.





PLANAR DENSITY

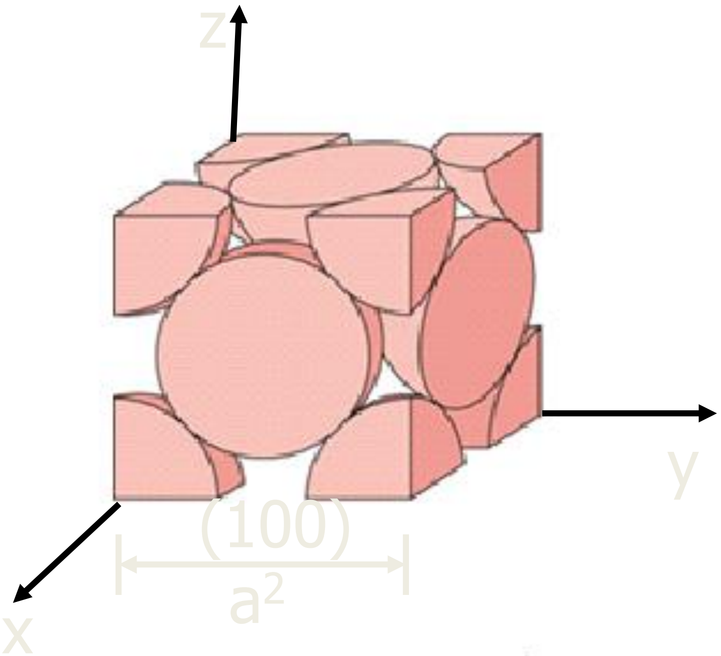
- **When slip occurs under stress, it takes place on the planes on which the atoms are most densely packed.**

$$\delta_{(hkl)} = \frac{\#\ \text{of atoms in a plane}}{\text{area}}$$

Example: FCC unit cell

$$\delta_{(100)} = \frac{4*1/4+1}{a^2} = \frac{2}{a^2}$$

$$a = \frac{4}{\sqrt{2}}\,r \Longrightarrow \delta_{(100)} = \frac{1}{4r^2}$$



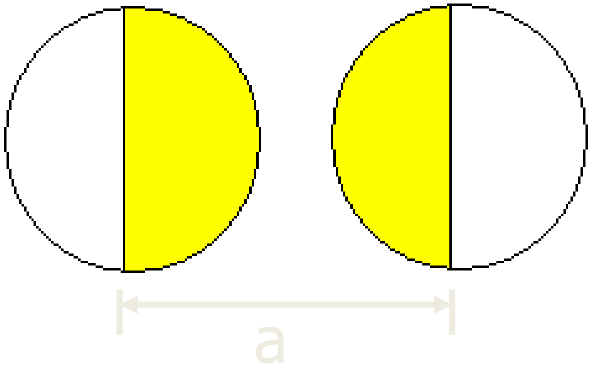
LINEAR DENSITY

- **When planes slip over each other, slip takes place in the direction of closest packing of atoms on the planes.**

The linear density of a crystal direction [h k l] is determined as:

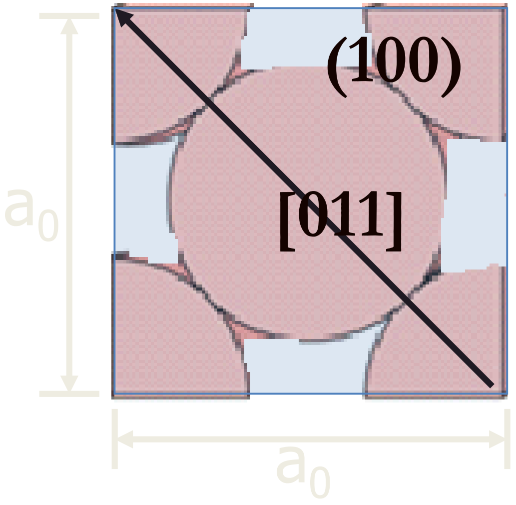
$$\delta_{[h\ k\ l]} = \frac{\#\ \text{of atoms}}{\text{Length of direction}}$$

- ☐ Example: [100] of cubic unit cell



$\delta_{[100]} = 1/a$

- ☐ Example: Calculate planar density of the face plane (100) and linear density on the face diagonal [011] of an FCC structure.



$$\delta_{(100)} = \frac{2}{a_0^2}$$

$$\delta_{[011]} = \frac{2}{a_0\sqrt{2}}$$

QUESTIONS

2.15 For an $Na^+ - Cl^-$ ion pair, attractive and repulsive energies E_A and E_R, respectively, depend on the distance between the ions r, according to

$$E_A = -\frac{1.436}{r}$$

$$E_R = \frac{7.32 \times 10^{-6}}{r^8}$$

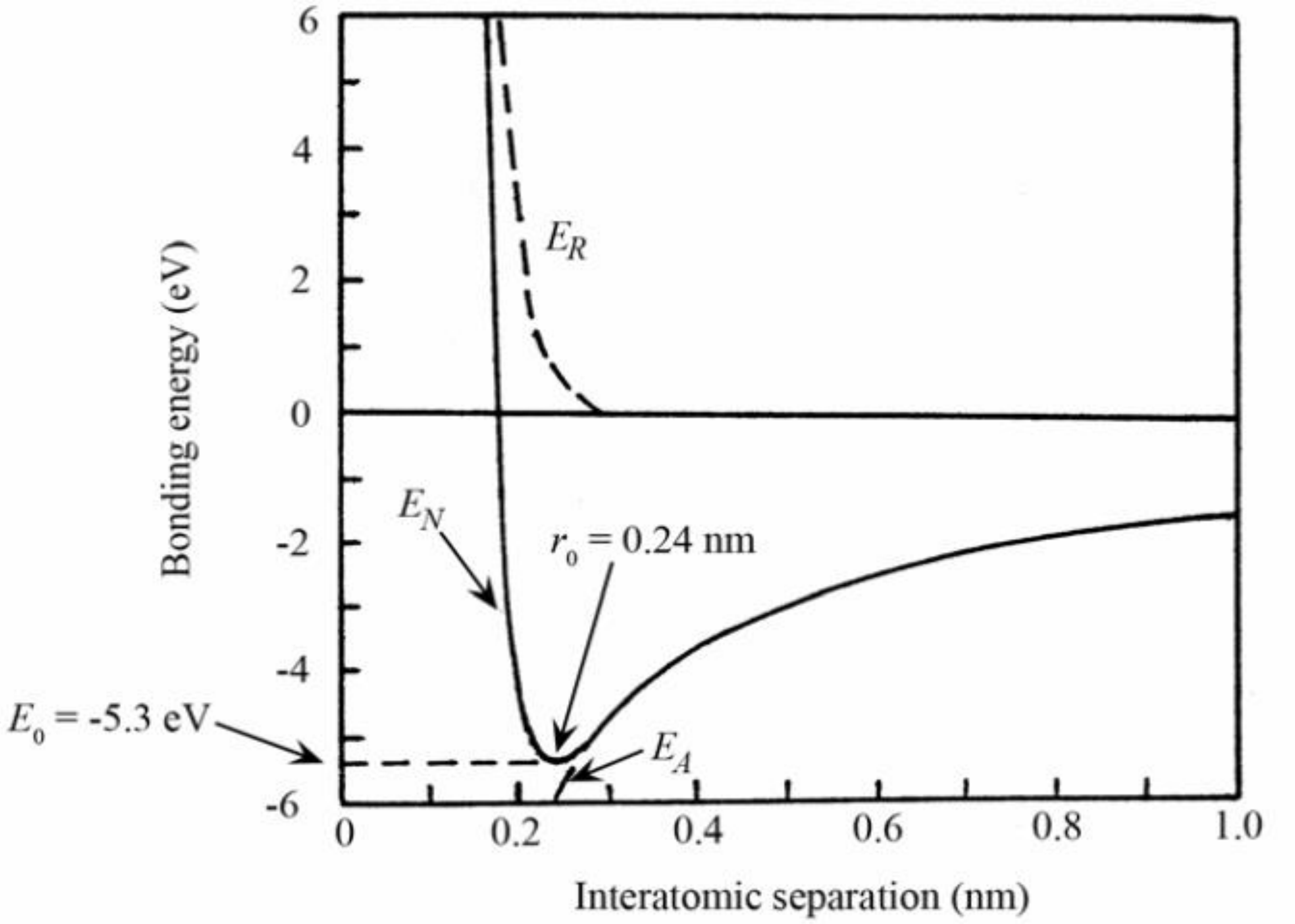
For these expressions, energies are expressed in electron volts per $Na^+ - Cl^-$ pair, and r is the distance in nanometers. The net energy E_N is just the sum of the two expressions above.

(a) Superimpose on a single plot E_N, E_R, and E_A versus r up to 1.0 nm.

(b) On the basis of this plot, determine (i) the equilibrium spacing r_0 between the Na^+ and Cl^- ions, and (ii) the magnitude of the bonding energy E_0 between the two ions.

(c) Mathematically determine the r_0 and E_0 values using the solutions to Problem 2.14 and compare these with the graphical results from part (b).

2.15 (a) Curves of E_A, E_R, and E_N are shown on the plot below.



(b) From this plot

$$r_0 = 0.24 \text{ nm}$$

$$E_0 = -5.3 \text{ eV}$$

(c) From Equation 2.11 for E_N $\quad E_N = -\frac{A}{r} + \frac{B}{r^n}$

$$\frac{dE_N}{dr} = \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0$$

Now, solving for **r** (= **r**$_\mathbf{o}$)

$$\frac{A}{r_o^{\,2}} = \frac{nB}{r_o^{(n+1)}}$$

$$r_o = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

$$A = 1.436$$

$$B = 7.32 \text{ x } 10^{-6}$$

$$n = 8$$

Thus,

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1 - n)}$$

$$\left[\frac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{1/(1 - 8)} = 0.236 \text{ nm}$$

and

$$E_0 = -\frac{1.436}{\left[\dfrac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{1/(1-8)}} + \frac{7.32 \times 10^{-6}}{\left[\dfrac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{8/(1-8)}}$$

$$= -5.32 \text{ eV}$$

2.19 Compute the percentage ionic character of the interatomic bond for each of the following compounds: MgO, GaP, CsF, CdS, and FeO.

Solution:

$$\%\text{ ionic character} = \{1 - \exp[-(0.25)(X_A - X_B)^2]\} \times 100 \qquad (2.10)$$

where X_A and X_B are the electronegativities for the respective elements.

2.19 The percent ionic character is a function of the electron negativities of the ions $\mathbf{X_A}$ and $\mathbf{X_B}$ according to Equation (2.10). The electronegativities of the elements are found in Figure 2.7.

For MgO, $\mathbf{X_{Mg}}$ = 1.2 and $\mathbf{X_O}$ = 3.5, and therefore,

$$\%IC = \left[1 - \mathbf{e}^{(-0.25)(3.5-1.2)^2}\right] \text{x } 100 = 73.4\%$$

For GaP, $\mathbf{X_{Ga}}$ = 1.6 and $\mathbf{X_{P}}$ = 2.1, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(2.1-1.6)^2}\right] \text{x } 100 = 6.1\%$$

For CsF, $\mathbf{X_{Cs}}$ = 0.7 and $\mathbf{X_{F}}$ = 4.0, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(4.0-0.7)^2}\right] \text{x } 100 = 93.4\%$$

For CdS, $\mathbf{X_{Cd}}$ = 1.7 and $\mathbf{X_{S}}$ = 2.5, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(2.5-1.7)^2}\right] \text{x } 100 = 14.8\%$$

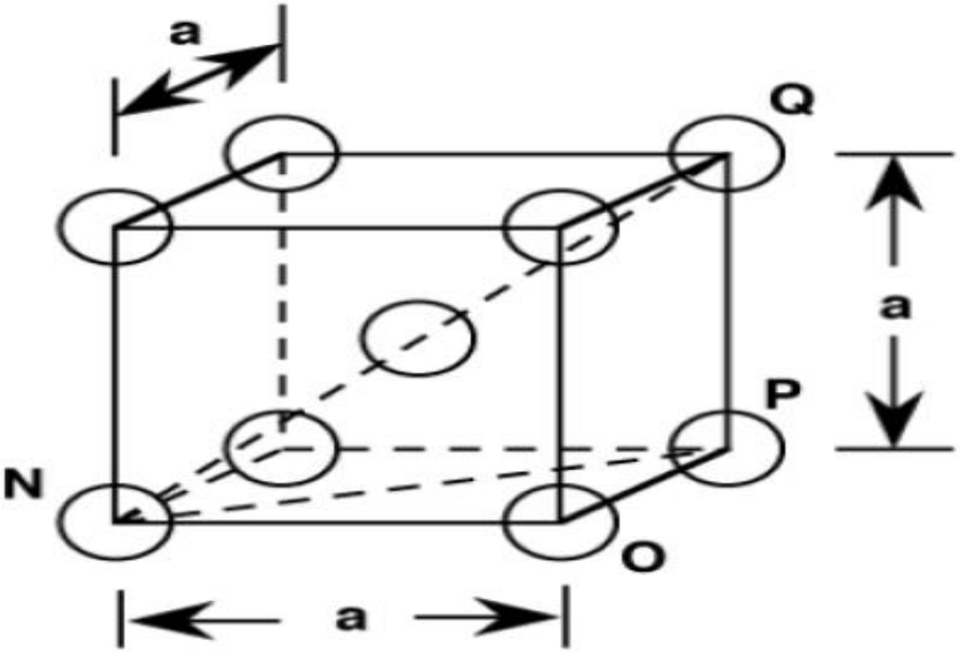
For FeO, $\mathbf{X_{Fe}}$ = 1.8 and $\mathbf{X_O}$ = 3.5, and therefore,

$$\%IC = \left[1 - e^{(-0.25)(3.5-1.8)^2}\right] \times 100 = 51.4\%$$

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 $a = 4R/\sqrt{3}$.

Solution:

3.4 This problem calls for a demonstration of the relationship $\mathbf{a} = \mathbf{4R}\sqrt{3}$ for BCC. Consider the BCC unit cell shown below



Using the triangle **NOP**

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle **NPQ**,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4\mathbf{R}$, **R** being the atomic radius. Also, $\overline{QP} = \mathbf{a}$. Therefore,

$$(4R)^2 = a^2 + 2a^2 \text{, or}$$

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

3.5 Show that the atomic packing factor for BCC is 0.68.

Solution:

We are asked to show that the atomic packing factor for BCC is 0.68. The atomic packing factor is defined as the ratio of sphere volume to the total unit cell volume, or

$$\mathrm{APF} = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $\mathbf{V_C} = a^3$. But a depends on **R** according to Equation (3.3), and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Thus,

$$\mathrm{APF} = \frac{8\pi R^3 / 3}{64R^3 / 3\sqrt{3}} = 0.68$$

3.8 *Calculate the radius of an iridium atom, given that Ir has an FCC crystal structure, a density of 22.4 g/cm*^{3}*, and an atomic weight of 192.2 g/mol.*

Solution

We are asked to determine the radius of an iridium atom, given that Ir has an FCC crystal structure. For FCC, $n = 4$ atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Now,

$$\rho = \frac{nA_{\mathrm{Ir}}}{V_C N_{\mathrm{A}}}$$

$$= \frac{nA_{\mathrm{Ir}}}{(16R^3\sqrt{2})N_{\mathrm{A}}}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{\text{Ir}}}{16\rho N_{\text{A}}\sqrt{2}} \right)^{1/3}$$

$$= \left[\frac{(4\text{ atoms/unit cell})(192.2\text{ g/mol})}{(16)(22.4\text{ g/cm}^3)(6.022 \times 10^{23}\text{ atoms/mol})(\sqrt{2})} \right]^{1/3}$$

$$= 1.36 \times 10^{-8}\text{ cm} = 0.136\text{ nm}$$

3.13 Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm^3. Determine whether it has an FCC or BCC crystal structure.

Solution

In order to determine whether Rh has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, $n = 4$, and $a = 2R\sqrt{2}$ (Equation 3.1). Also, from Figure 2.6, its atomic weight is 102.91 g/mol. Thus, for FCC (employing Equation 3.5)

$$\rho = \frac{nA_{\mathrm{Rh}}}{a^3 N_{\mathrm{A}}} = \frac{nA_{\mathrm{Rh}}}{(2R\sqrt{2})^3 N_{\mathrm{A}}}$$

$$= \frac{(4\ \text{atoms/unit cell})(102.91\ \text{g/mol})}{\left\{\left[(2)(1.345 \times 10^{-8}\ \text{cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23}\ \text{atoms/mol})}$$

$$= 12.41\ \text{g/cm}^3$$

which is the value provided in the problem statement. Therefore, Rh has the FCC crystal structure.

3.16 *Iodine has an orthorhombic unit cell for which the a, b, and c lattice parameters are 0.479, 0.725, and 0.978 nm, respectively.*

(a) If the atomic packing factor and atomic radius are 0.547 and 0.177 nm, respectively, determine the number of atoms in each unit cell.

(b) The atomic weight of iodine is 126.91 g/mol; compute its theoretical density.

Solution

(a) For indium, and from the definition of the APF

$$\text{APF} = \frac{V_S}{V_C} = \frac{n\left(\frac{4}{3}\pi R^3\right)}{abc}$$

we may solve for the number of atoms per unit cell, n, as

$$n = \frac{(\text{APF})\,abc}{\frac{4}{3}\pi R^3}$$

Incorporating values of the above parameters provided in the problem state leads to

$$= \frac{(0.547)(4.79 \times 10^{-8}\ \text{cm})(7.25 \times 10^{-8}\ \text{cm})(9.78 \times 10^{-8}\ \text{cm})}{\frac{4}{3}\pi(1.77 \times 10^{-8}\ \text{cm})^3}$$

= 8.0 atoms/unit cell

(b) In order to compute the density, we just employ Equation 3.5 as

$$\rho = \frac{nA_{\text{I}}}{abc\,N_{\text{A}}}$$

$$= \frac{(8\text{ atoms/unit cell})(126.91\text{ g/mol})}{\left\{\left[(4.79 \times 10^{-8}\text{ cm})(7.25 \times 10^{-8}\text{ cm})(9.78 \times 10^{-8}\text{ cm})\right]/\text{unit cell}\right\}(6.022 \times 10^{23}\text{ atoms/mol})}$$

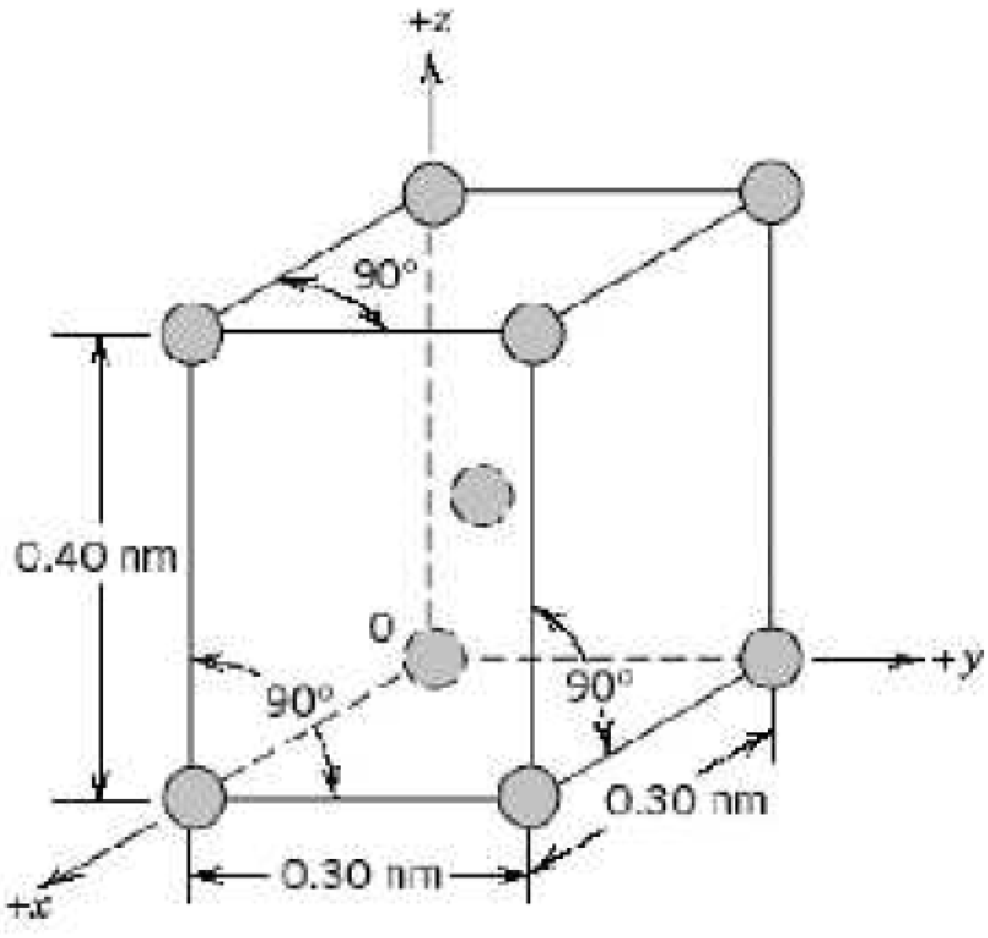
$$= 4.96\text{ g/cm}^3$$

3.20 *Below is a unit cell for a hypothetical metal.*

(a) To which crystal system does this unit cell belong?

(b) What would this crystal structure be called?

(c) Calculate the density of the material, given that its atomic weight is 141 g/mol.



(a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since $a = b = 0.30$ nm, $c = 0.40$ nm, and $\alpha = \beta = \gamma = 90°$.

(b) The crystal structure would be called *body-centered tetragonal*.

(c) As with BCC, $n = 2$ atoms/unit cell. Also, for this unit cell

$$V_C = (3.0 \times 10^{-8}\ \text{cm})^2(4.0 \times 10^{-8}\ \text{cm})$$

$$= 3.60 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

Thus, using Equation 3.5, the density is equal to

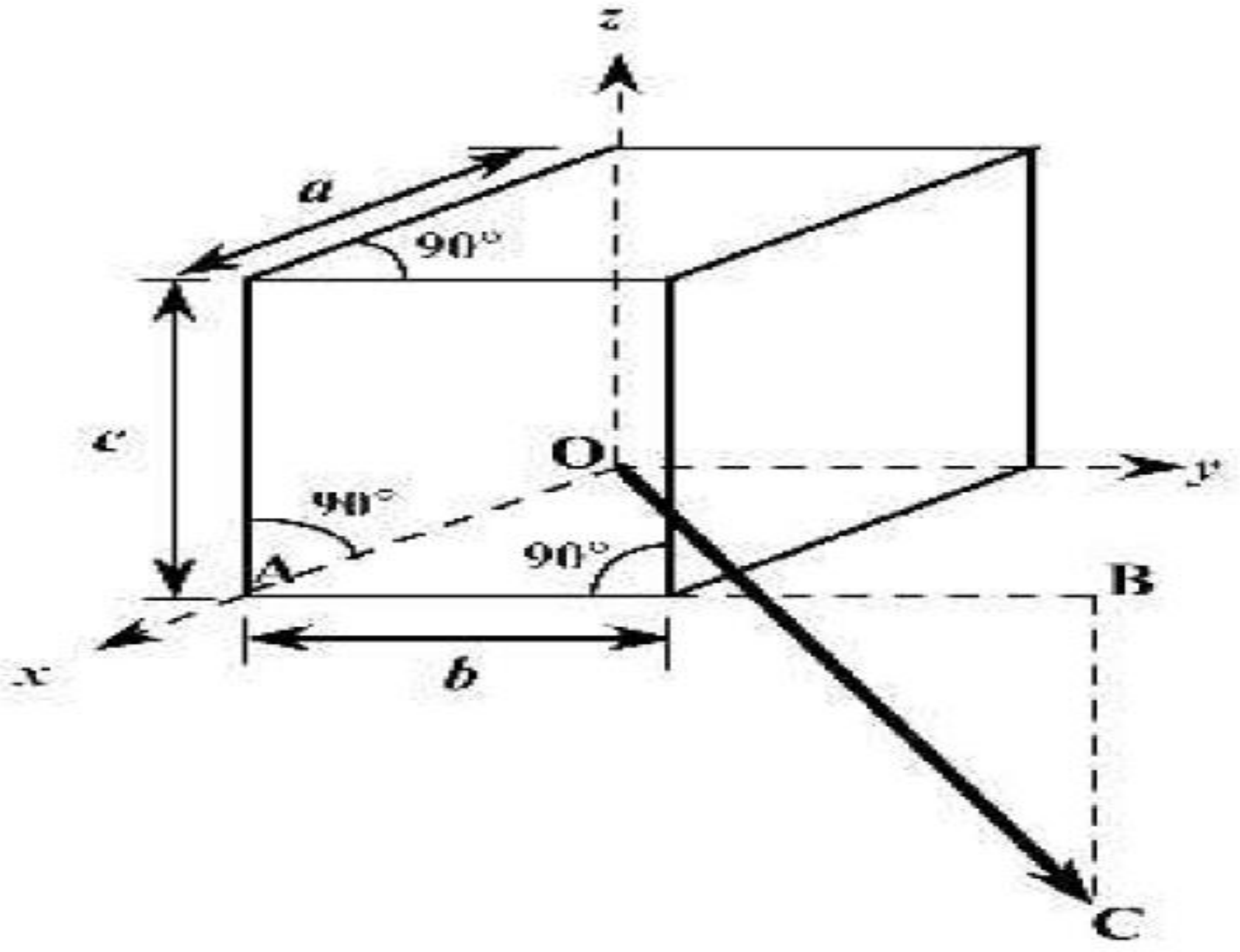
$$\rho = \frac{nA}{V_C N_A}$$

$$= \frac{(2\ \text{atoms/unit cell})(141\ \text{g/mol})}{\left(3.60 \times 10^{-23}\ \text{cm}^3\text{/unit cell}\right)\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}$$

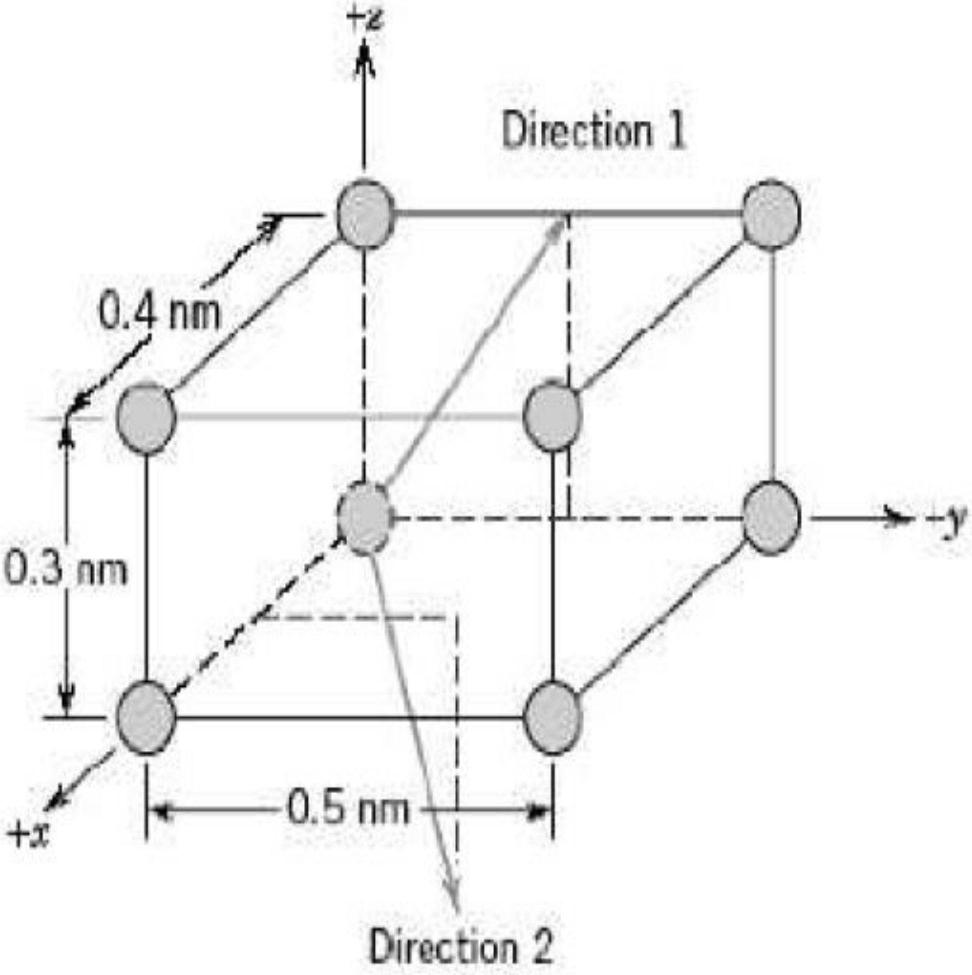
$$= 13.0\ \text{g/cm}^3$$

3.27 *Draw an orthorhombic unit cell, and within that cell a* $[12\bar{1}]$ *direction.*

This problem calls for us to draw a $[12\bar{1}]$ direction within an orthorhombic unit cell ($a \neq b \neq c$, $\alpha = \beta = \gamma =$ 90°). Such a unit cell with its origin positioned at point O is shown below. We first move along the +*x*-axis *a* units (from point O to point A), then parallel to the +*y*-axis 2*b* units (from point A to point B). Finally, we proceed parallel to the *z*-axis -*c* units (from point B to point C). The $[12\bar{1}]$ direction is the vector from the origin (point O) to point C as shown.


z
a
90°
c
O
y
90°
90°
A
B
x
b
C

3.29 *What are the indices for the directions indicated by the two vectors in the sketch below?*



For direction 1, the projection on the *x*-axis is zero (since it lies in the *y*-*z* plane), while projections on the *y*- and *z*-axes, *b*/2 and *c*, respectively. This is a [012] direction as indicated in the summary below.

	x	*y*	*z*
Projections	0*a*	*b*/2	*c*
Projections in terms of *a*, *b*, and *c*	0	1/2	1
Reduction to integers	0	1	2
Enclosure		[012]	

Direction 2 is $[11\bar{2}]$ as summarized below.

	x	y	z
Projections	$a/2$	$b/2$	$-c$
Projections in terms of *a*, *b*, and *c*	1/2	1/2	-1
Reduction to integers	1	1	-2
Enclosure		$[11\bar{2}]$	

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

(a) $[101]$,

(b) $[211]$,

(c) $[10\bar{2}]$,

(d) $[3\bar{1}3]$,

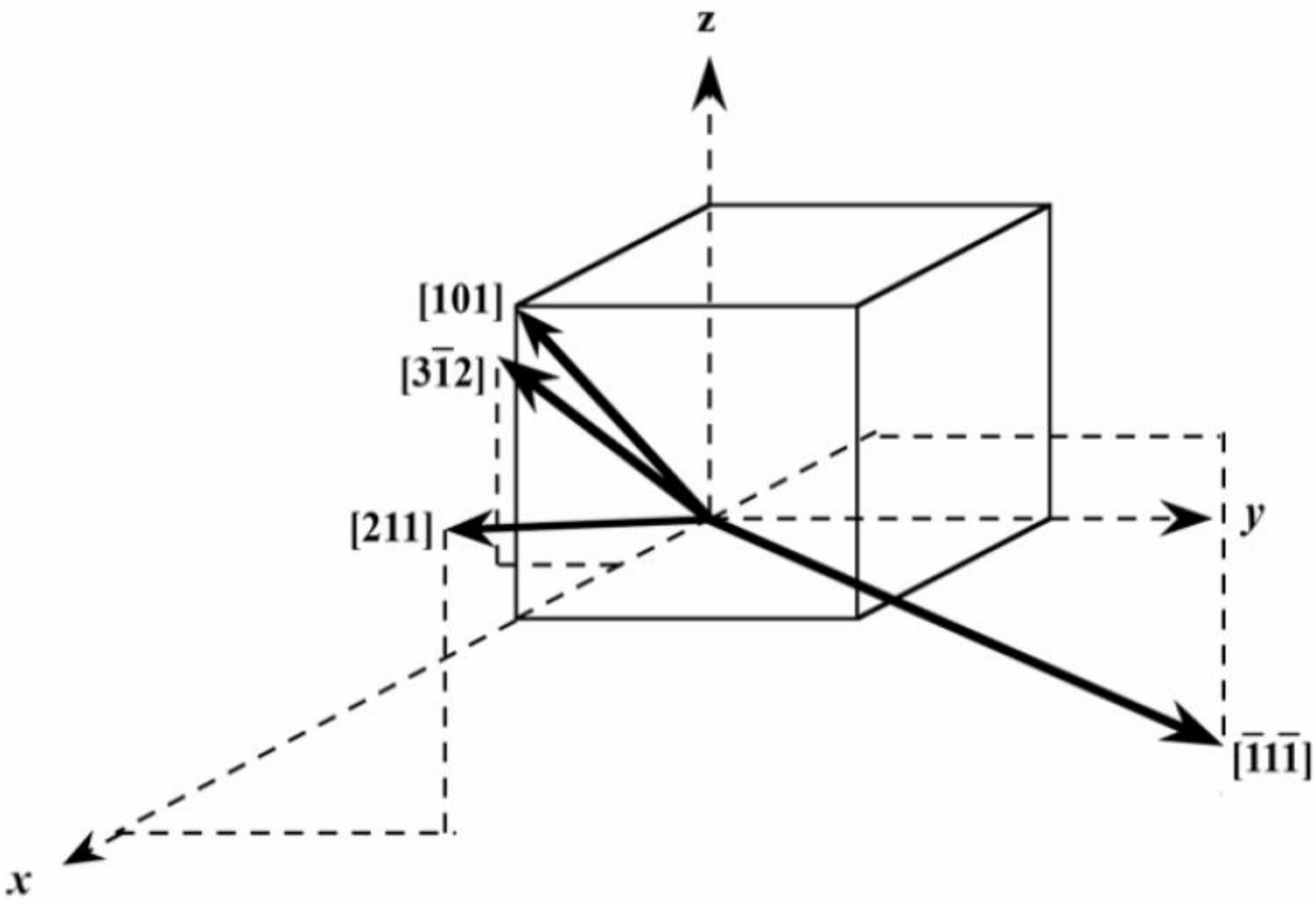
(e) $[\bar{1}1\bar{1}]$,

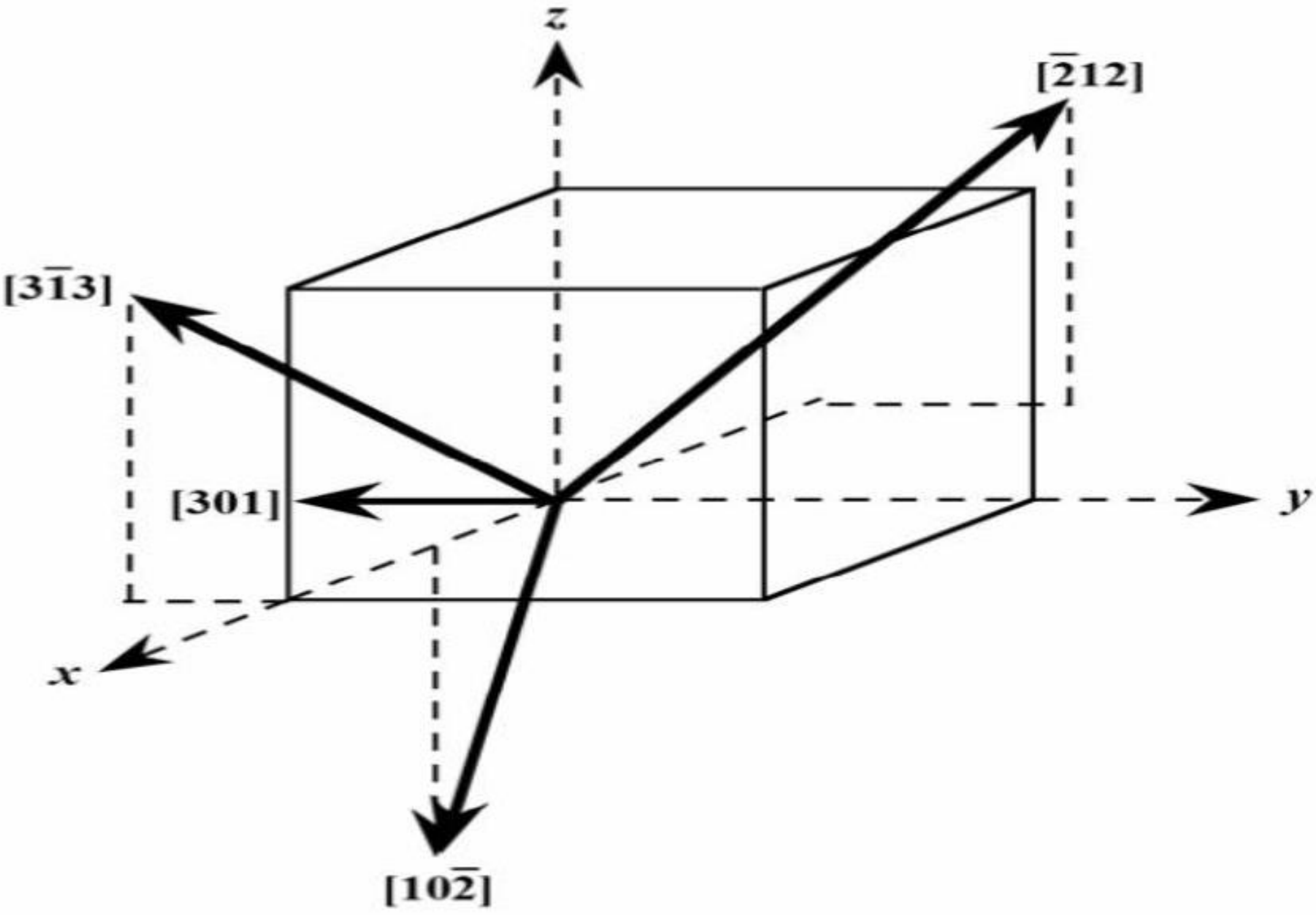
(f) $[\bar{2}12]$,

(g) $[3\bar{1}2]$,

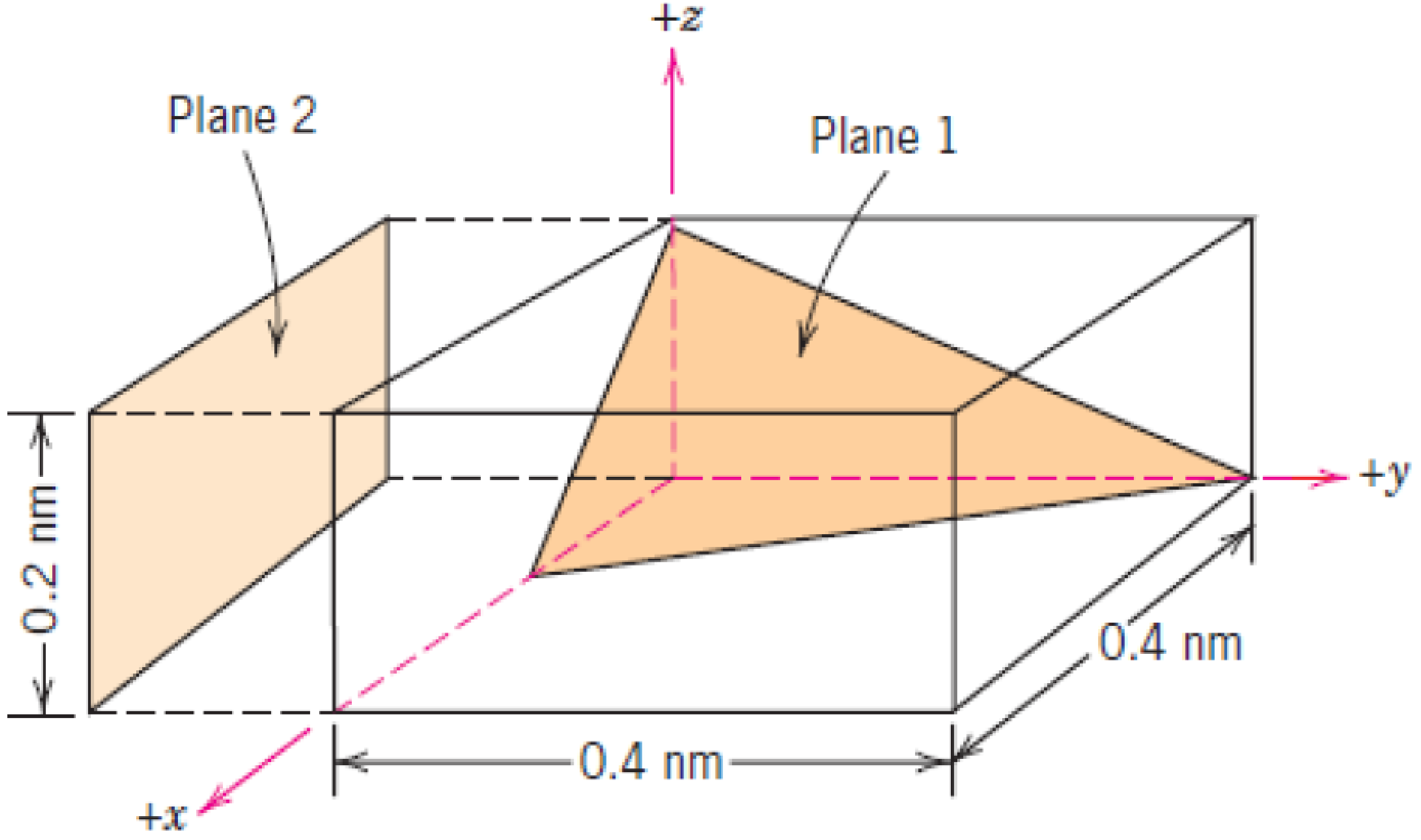
(h) $[301]$.

3.30 The directions asked for are indicated in the cubic unit cells shown below.




z
[$\bar{2}$12]
[3$\bar{1}$3]
[301]
y
x
[10$\bar{2}$]

3.38 What are the indices for the two planes drawn in the sketch below?



Solution:

3.38 This problem calls for specification of the indices for the two planes that are drawn in the sketch.

Plane 1 is a (211) plane. The determination of its indices is summarized below.

	<u>*x*</u>	<u>*y*</u>	<u>*z*</u>
Intercepts	$a/2$	b	c
Intercepts in terms of a, b, and c	1/2	1	1
Reciprocals of intercepts	2	1	1
Enclosure		(211)	

Plane 2 is a $(0\bar{2}0)$ plane, as summarized below.

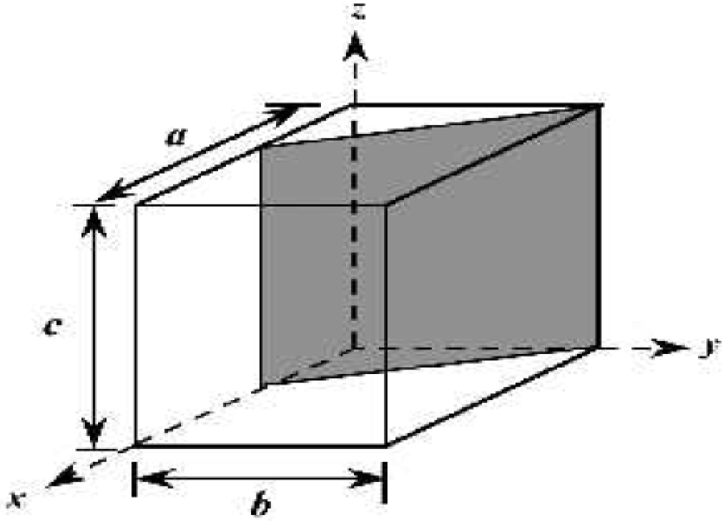
	$\underline{x}$	$\underline{y}$	$\underline{z}$
Intercepts	∞a	$-b/2$	∞c
Intercepts in terms of *a*, *b*, and *c*	∞	-1/2	∞
Reciprocals of intercepts	0	-2	0
Enclosure		$(0\bar{2}0)$	

3.38 *(a) Draw an orthorhombic unit cell, and within that cell a (210) plane.*

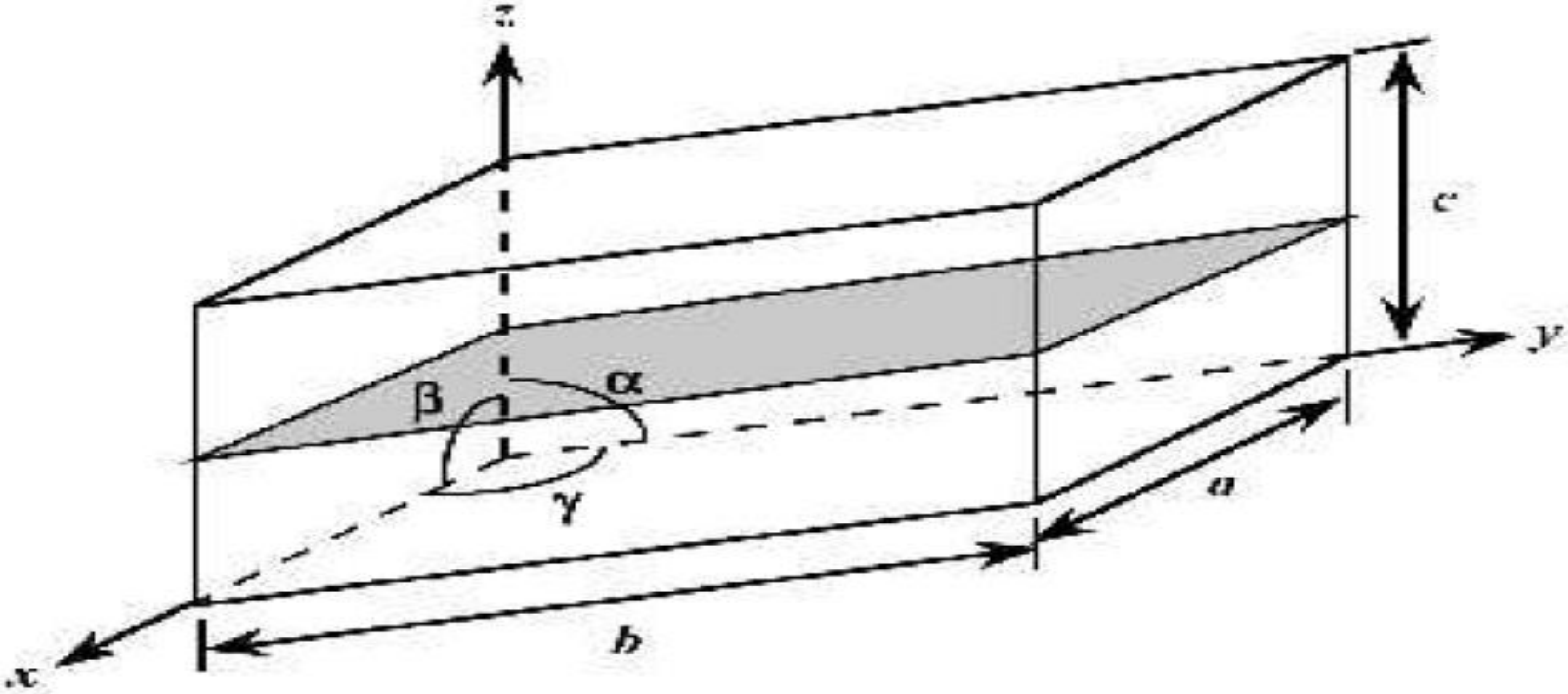
(b) Draw a monoclinic unit cell, and within that cell a (002) plane.

Solution

(a) We are asked to draw a (210) plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals--i.e., 1/2, 1, and ∞. This means that the plane intercepts the x-axis at $a/2$, the y-axis at b, and parallels the z-axis. The plane that satisfies these requirements has been drawn within the orthorhombic unit cell below. (For orthorhombic, $a \neq b \neq c$, and $\alpha = \beta = \gamma = 90°$.)



(b) A (002) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives ∞, ∞, and 1/2. Thus, the (002) plane parallels both *x*- and *y*-axes, and intercepts the *z*-axis at *a*/2, as indicated in the drawing. (For monoclinic, $a \neq b \neq c$, and $\alpha = \gamma = 90° \neq \beta$.)

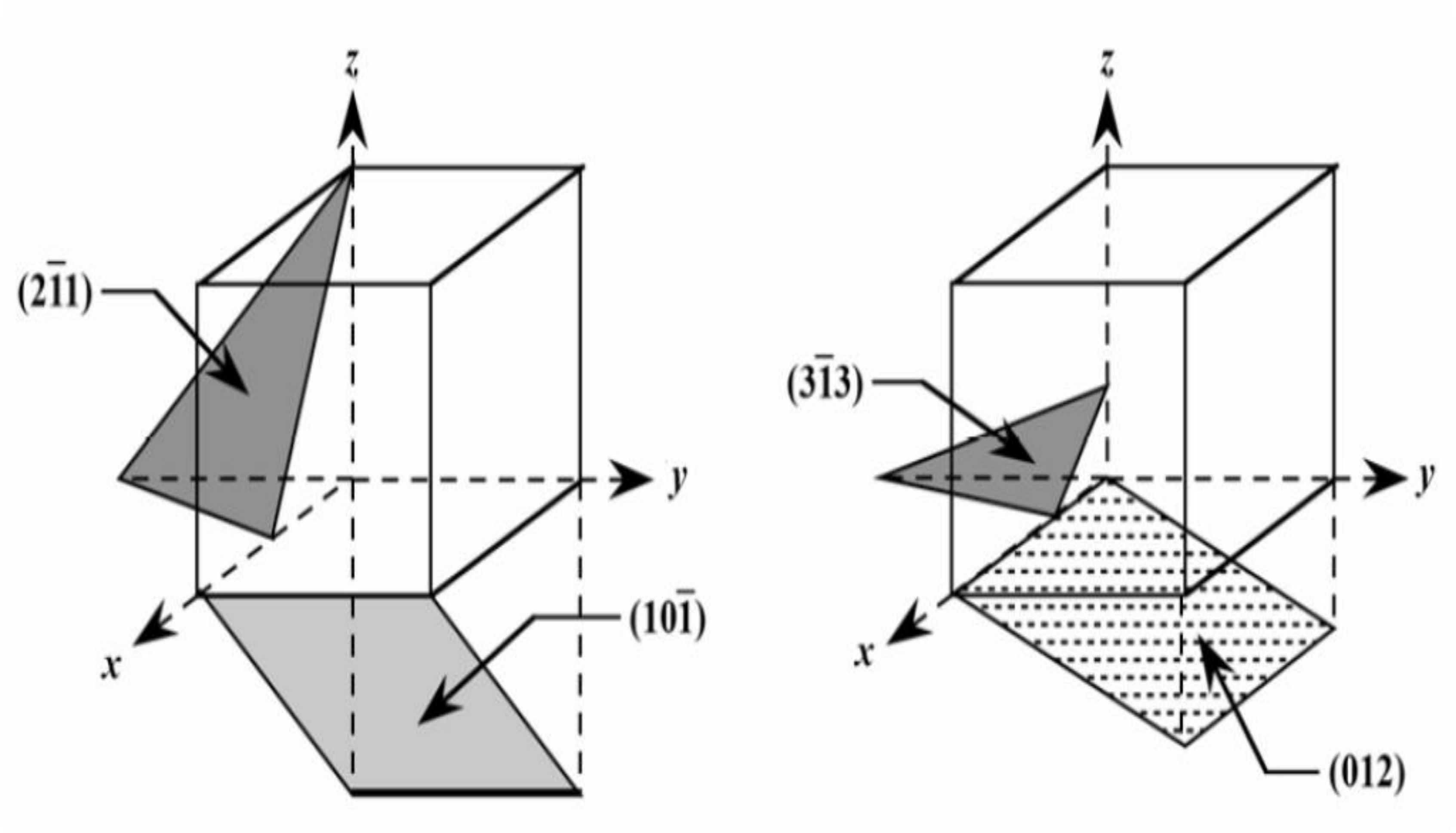


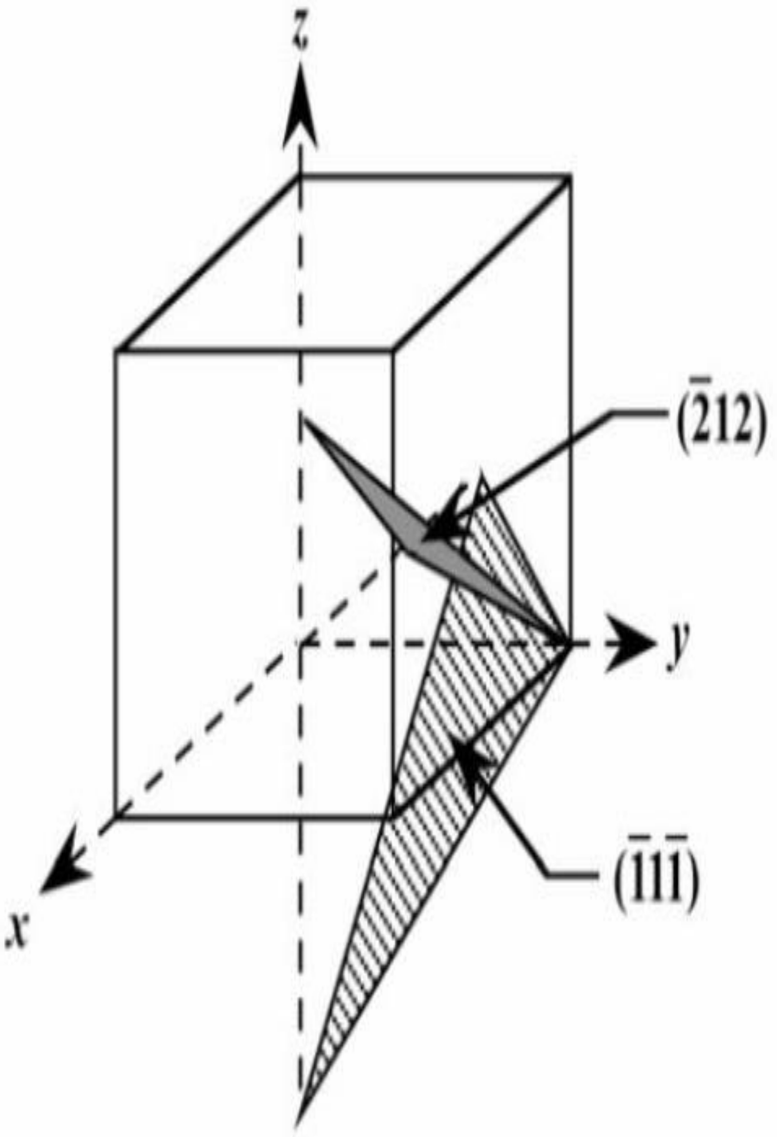
3.39 Sketch within a cubic unit cell the following planes:

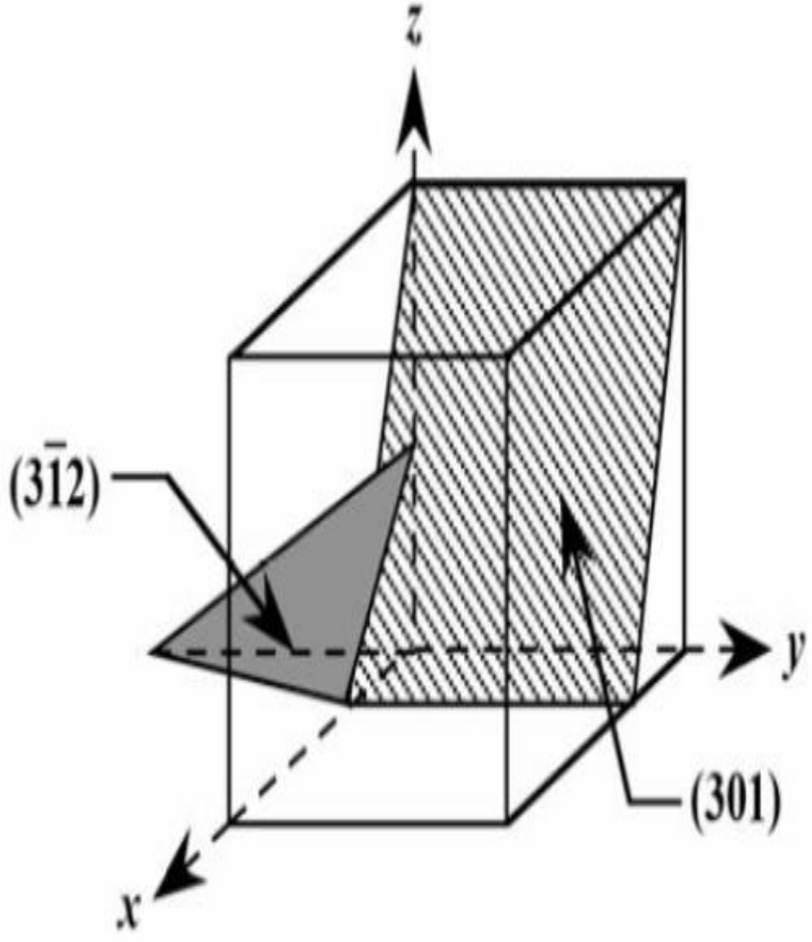
- **(a)** $(10\bar{1})$,
- **(b)** $(2\bar{1}1)$,
- **(c)** (012),
- **(d)** $(3\bar{1}3)$,
- **(e)** $(\bar{1}1\bar{1})$,
- **(f)** $(\bar{2}12)$,
- **(g)** $(3\bar{1}2)$,
- **(h)** (301).

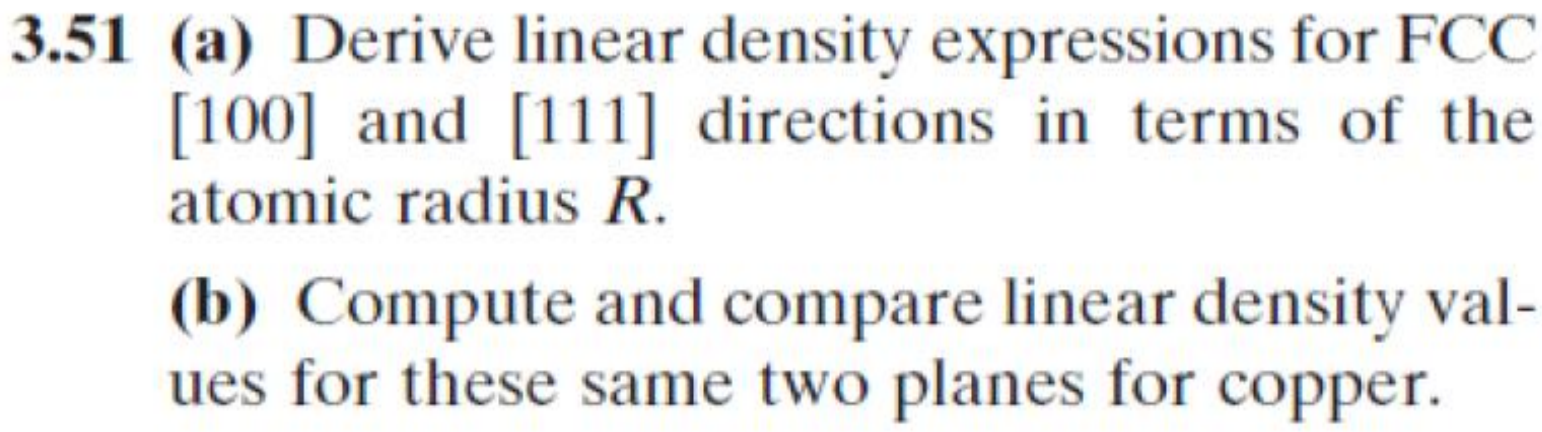
Solution:

3.39 The planes called for are plotted in the cubic unit cells shown below.




z
$(\bar{2}12)$
y
x
$(\bar{1}1\bar{1})$


z
$(3\bar{1}2)$
y
x
(301)

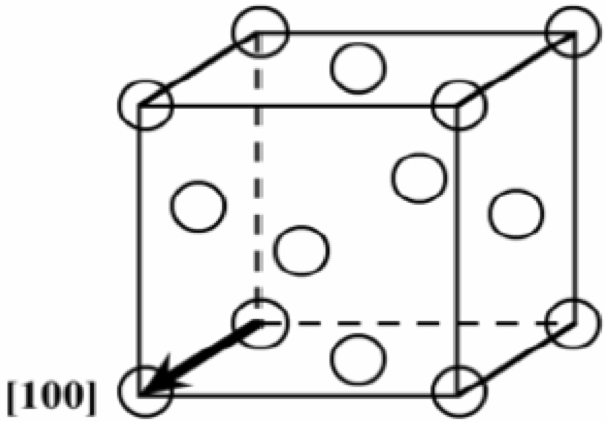


3.51 **(a)** Derive linear density expressions for FCC [100] and [111] directions in terms of the atomic radius *R*.

(b) Compute and compare linear density values for these same two planes for copper.

Solution:

3.51 (a) In the figure below is shown a [100] direction within an FCC unit cell.

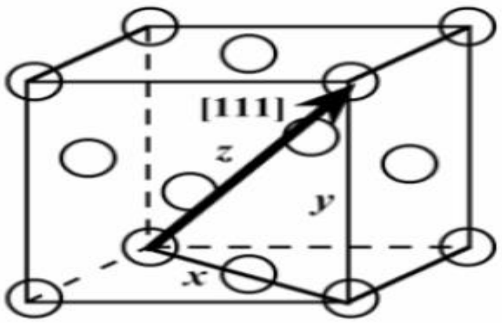


For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the linear density of this plane is

$$\mathrm{LD}_{100} = \frac{\text{number of atoms centered on [100] direction vector}}{\text{length of [100] direction vector}}$$

$$= \frac{1 \text{ atom}}{2R\sqrt{2}} = \frac{1}{2R\sqrt{2}}$$

An FCC unit cell within which is drawn a [111] direction is shown below.



For this [111] direction, the vector shown passes through only the centers of the single atom at each of its ends, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by z in this figure, which is equal to

$$z = \sqrt{x^2 + y^2}$$

where x is the length of the bottom face diagonal, which is equal to $4R$. Furthermore, y is the unit cell edge length, which is equal to $2R\sqrt{2}$ (Equation 3.1). Thus, using the above equation, the length z may be calculated as follows:

$$z = \sqrt{(4R)^2 + (2R\sqrt{2})^2} = \sqrt{24R^2} = 2R\sqrt{6}$$

Therefore, the expression for the linear density of this direction is

$$\mathrm{LD}_{111} = \frac{\text{number of atoms centered on [111] direction vector}}{\text{length of [111] direction vector}}$$

$$= \frac{1\ \text{atom}}{2R\sqrt{6}} = \frac{1}{2R\sqrt{6}}$$

(b) From the table inside the front cover, the atomic radius for copper is 0.128 nm. Therefore, the linear density for the [100] direction is

$$\mathrm{LD}_{100}(\mathrm{Cu}) = \frac{1}{2R\sqrt{2}} = \frac{1}{(2)(0.128\ \mathrm{nm})\sqrt{2}} = 2.76\ \mathrm{nm}^{-1} = 2.76 \times 10^{9}\ \mathrm{m}^{-1}$$

While for the [111] direction

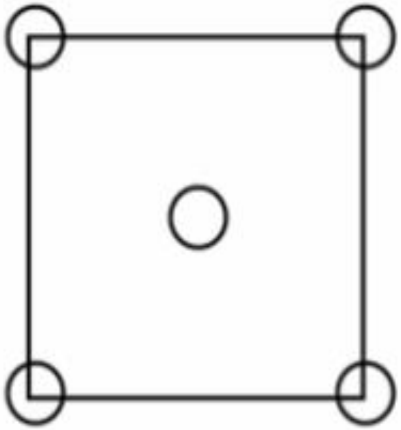
$$\mathrm{LD}_{111}(\mathrm{Cu}) = \frac{1}{2R\sqrt{6}} = \frac{1}{(2)(0.128\ \mathrm{nm})\sqrt{6}} = 1.59\ \mathrm{nm}^{-1} = 1.59 \times 10^{9}\ \mathrm{m}^{-1}$$

3.53 (a) Derive planar density expressions for FCC (100) and (111) planes in terms of the atomic radius *R*.

(b) Compute and compare planar density values for these same two planes for aluminum.

Solution:

3.53 (a) In the figure below is shown a (100) plane for an FCC unit cell.

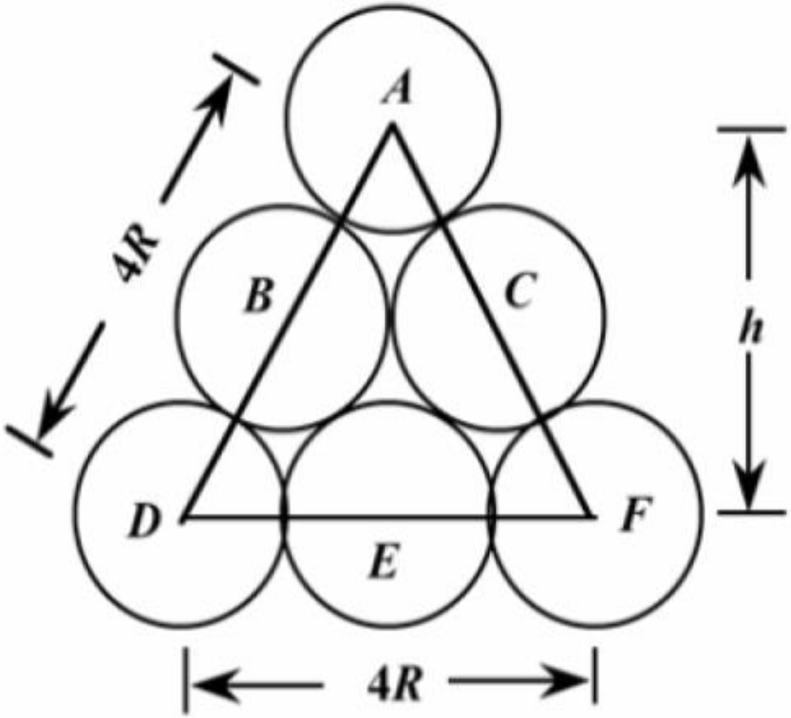


For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this FCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1); and, thus, the area of this square is just $(2R\sqrt{2})^2 = 8R^2$. Hence, the planar density for this (100) plane is just

$$\mathrm{PD}_{100} = \frac{\text{number of atoms centered on (100) plane}}{\text{area of (100) plane}}$$

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

That portion of an FCC (111) plane contained within a unit cell is shown below.



There are six atoms whose centers lie on this plane, which are labeled *A* through *F*. One-sixth of each of atoms *A*, *D*, and *F* are associated with this plane (yielding an equivalence of one-half atom), with one-half of each of atoms *B*, *C*, and *E* (or an equivalence of one and one-half atoms) for a total equivalence of two atoms. Now, the area of the triangle shown in the above figure is equal to one-half of the product of the base length and the height, h. If we consider half of the triangle, then

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

which leads to $h = 2R\sqrt{3}$. Thus, the area is equal to

$$\text{Area} = \frac{4R(h)}{2} = \frac{(4R)\left(2R\sqrt{3}\right)}{2} = 4R^2\sqrt{3}$$

And, thus, the planar density is

$$\text{PD}_{111} = \frac{\text{number of atoms centered on (111) plane}}{\text{area of (111) plane}}$$

$$= \frac{2 \text{ atoms}}{4R^2\sqrt{3}} = \frac{1}{2R^2\sqrt{3}}$$

(b) From the table inside the front cover, the atomic radius for aluminum is 0.143 nm. Therefore, the planar density for the (100) plane is

$$\mathrm{PD}_{100}(\mathrm{Al}) = \frac{1}{4R^2} = \frac{1}{4(0.143\ \mathrm{nm})^2} = 12.23\ \mathrm{nm}^{-2} = 1.223 \times 10^{19}\ \mathrm{m}^{-2}$$

While for the (111) plane

$$\mathrm{PD}_{111}(\mathrm{Al}) = \frac{1}{2R^2\sqrt{3}} = \frac{1}{2\sqrt{3}\,(0.143\ \mathrm{nm})^2} = 14.12\ \mathrm{nm}^{-2} = 1.412 \times 10^{19}\ \mathrm{m}^{-2}$$