FCC. BCC and HCP Metals

Introduction

The majority of common metals have either a Face Center Cubic Structure, fig la, a Body Centered Cubic Structure, fig.lb or an Hexagonal Close Packed structure fig.lc. These are usually abbreviated to FCC, BCC or HCP structures respectively. The major differences between these structures is the Unit Cell, the building block. These are shown in fig.l. The different cells leads to different physical properties of bulk metals. For example, FCC metals, Cu, Au, Ag, are usually soft and 'ductile', which means they can be bent and shaped easily. BCC metals are less ductile but stronger, eg iron, while HCP metals are usually brittle. Zinc is HCP and is difficult to bend without breaking, unlike copper. Many other features depend upon the crystal structure of metals, such as density, deformation processes, alloying behavior, and much more. Thus, it is important to understand metal structures.

Face Center Cubic Structure

Face Center Cubic Structure consists of an atom at each cube corner and an atom in the center of each cube face. A hard sphere concept can be used to describe atomic packing in unit cells. The FCC structure is shown in fig.la. The distance along unit cell edges is called the lattice parameter, OQ. For cubic crystals the lattice parameter is identical in all three

crystal axes. If a corner atom of the FCC unit cell is removed, six atoms are revealed in a hexagonal array. These atoms are closed packed, ie they cannot be packed any tighter, and each atom touches its neighbor in any direction.

Since a close packed plane such as this can be achieved by removing each of the eight corner atoms and because eight such planes form an octahedron, they are called the 'Octahedral' planes. Thus the FCC structure has four sets of two parallel planes.. As parallel planes with the same atomic arrangement are equivalent the FCC structure has four equivalent close packed planes. Using Miller indices from the previous crystallography experiment show them to be {111} planes. Thus the FCC structure has four {111} close packed planes. The atomic arrangement is shown in fig.2a. Three close packed directions are shown as well.

These correspond to (110) directions diagonally across cube faces. There are three of these for each {111} plane. Therefore, FCC structures have twelve possible combinations of {111} and (110).

Body Centered Cubic Structure

In this structure, atoms exist at each cube corner and one atom is at the center of the cube, fig lb. Comparison of figs, la and lb show that the BCC is much emptier than the FCC structure. In this case there are no close packed planes only close packed directions. Fig.2b shows the atomic arrangement of {110} planes in a BCC structure which are the planes of highest atomic density. There are 6 planes of this type, and each contains two close packed directions. Consideration of fig. 1b and 2b shows the closed packed direction

joins diagonally opposite corners of the BCC unit cell. It is therefore a (111) direction. As there are two (111) for each {110} plane there is a total of 12 possible combinations of {110} and (111).

Hexagonal Close Packed Structure

The hexagonal structure is shown in fig. lc. A close packed plane at the bottom and top of the unit cell is separated by 3 atoms in the cell center, which are also part of a closed packed plane. Closed packed planes are of the {001} family of which there is only 1 equivalent

type. Fig.2c shows the atomic arrangement and directions of close packing.
These are of the (2TTO) family and there are three for each {0001}. Thus, hexagonal structures have only three combinations of {0001} and (2TTO).

It should be noted that the lattice parameter differs with direction in HCP structures. Along a1,a2 and a3, the lattice parameter is identical, but along the c axis it is always

greater. This gives rise to the c/a ratio.

Stacking Sequence

FCC

An FCC structure has close packed octahedral planes, but these are tilted relative to the crystal axes. The FCC structure is made up of layers of octahedral,-type planes. These stack in a sequence ABC ABC as shown in fig.3a. A, B and C are atom center sites relative to a close packed layer. If atoms in the first-close packed layer sit in position A they form the arrangement shown in fig. 3a. The next row of atoms will sit in troughs between the hard sphere atoms, positions B or C. However both positions cannot be occupied. For FCC structures, the second layer of atoms chooses site B. Troughs left after the second layer are A or C, see fig.3a. Choice of C produces a stacking sequence of ABC, the FCC structure.

Stacking Faults in FCC Structures

The packing of ABC ABC can inadvertently be upset by a wrong stacking sequence. For example after AB, the atoms have choice of A or C positions. If it chooses A, the stacking sequence will be:

ABCABCAB ABCABC

The dashed line is where the stacking is out of the FCC sequence. A layer of C atoms is missed. This is called an 'instrinsic' fault as a layer is missed. An 'extrinsic' fault is from addition of a layer, eg.

ABCAB A CAB

In thios case a layer of A atoms was added. Stacking faults are very important to dislocation dynamics in FCC metals.

BCC

BCC structure has no closed-packed planes and therefore does not have a stacking sequence. Neither does at have stacking faults.

HCP

HCP structures have closed packed planes. If the first layer at the bottom of the unit cell is the A position, the second layer of three atoms in the center of the unit cell has a choice of B or C. It chooses B. The third layer, ie the top plane of the unit cell, can choose A or C, but chooses A. So HCP has a stacking sequence of AB AB AB.

Atoms Per Unit Cell

When considering atoms per unit cell, remember some atoms are shared by other cells in the structure in planes above and below as well as the same plane as the unit cell being considered.

FCC

FCC has eight corner atoms shared by eight other cell and six face center atoms shared by two cells. Thus the # of atoms per cell is

$$8 \times 1/8 + 6 \times 1/2 = 4 \text{ atoms per cell for FCC}$$

BCC

Again eight corner atoms shared by eight cells and 1 center atom fully contained in the unit cell. So the # of atoms per cell for BCC is

$$8 \times 1/8 + 1 = 2 \text{ atoms per unit cell for BCC}$$

HCP

12 corner atoms shared by six unit cells each, two center face atoms shared by two cells and three atoms fully contained by the unit cell. Thus,

$$12 \times 1/6 + 2 \times 1/2 + 3 = 6 \text{ atoms per unit cell for HCP.}$$

Coordination Number

Coordination number relates the number of equidistant nearest neighbors an atom has, and is different for FCC, BCC, and HCP structures.

FCC

The atom in the center of a close packed plane, such as fig.3a, has six nearest neighbors in the octahedral plane above (ie B positions), and 3 below, (ie C positions). Therefore the coordination number of FCC structures is $6 + 3 + 3 = 12$.

BCC

BCC structures have no close packed planes. Its coordination number is just the number of equidistant neighbors from the atom in the center of the unit cell. BCC coordination number is therefore 8, as each cube corner atom is the nearest neighbor.

HCP

HCP is a closed-packed structure and therefore, by the same argument as that used for FCC, it has a coordination number of 12 (provided the c/a ratio shown in fig. lc is 1.633. A c/a = 1.633 is required for perfect packing of spheres. Magnesium is nearest to the perfect number with 1.62 c/a ratio.

Interstitial Sites

Consideration of the packing of spheres shows gaps will exist. These are called Interstitial Sites. Two types exist, octahedral and tetrahedral. The six atoms surrounding an octahedral interstitial site form a regular octahedron, and similarly the atoms around a tetrahedral site form a regular tetrahedron. These sites are shown in fig.4 the three most common metallic structures.

Experimental

Worksheet provided in lab.

Reference

Engineering Materials and Their Applications, Rinn and Trojan.
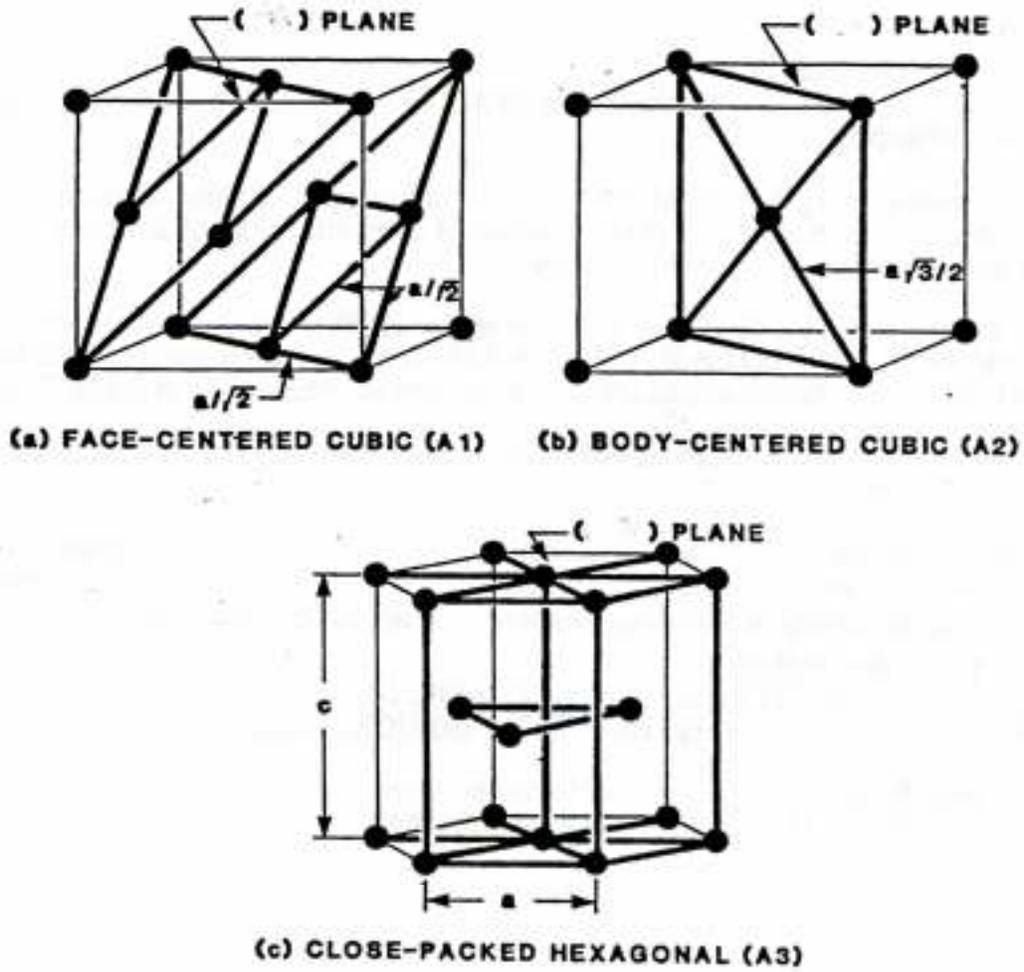Structure of Metals by C.S. Barrett and T.B. Masselki.

—( ) PLANE

—( ) PLANE

a/√2

a√3/2

a/√2

(a) FACE-CENTERED CUBIC (A1)   (b) BODY-CENTERED CUBIC (A2)

—( ) PLANE

c

a

(c) CLOSE-PACKED HEXAGONAL (A3)
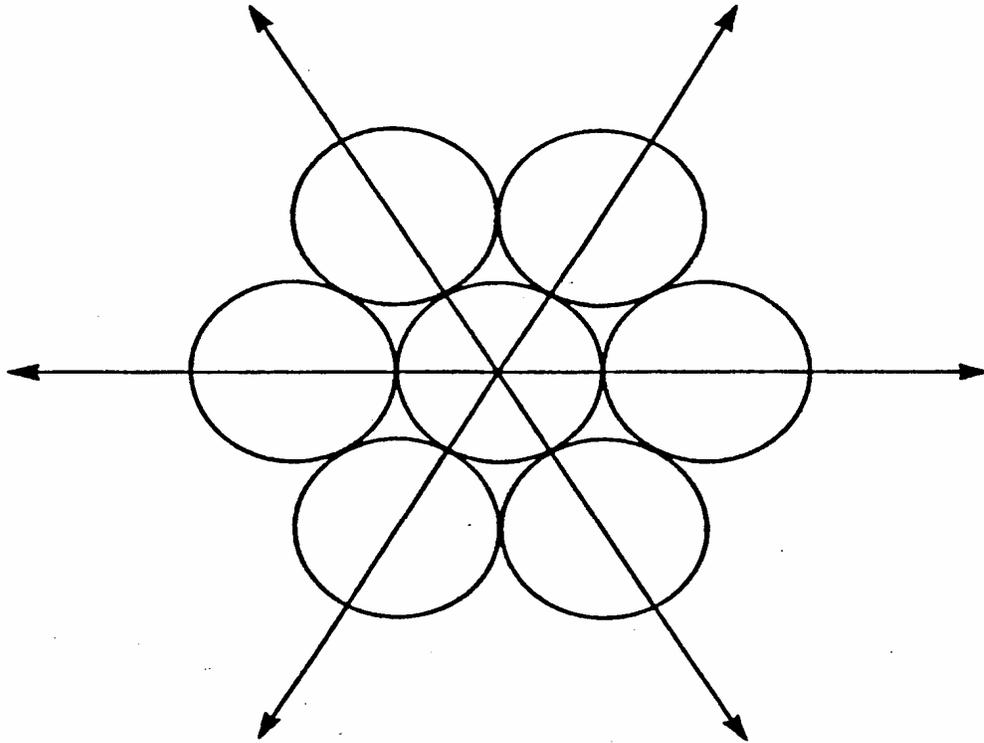
Fig.1   Atomic arrangement of the commonest metallic structures

Fig.2a Atomic arrangement of the (111) close packed planes in the FCC structure. The arrows indicate three different ⟨110⟩ directions.
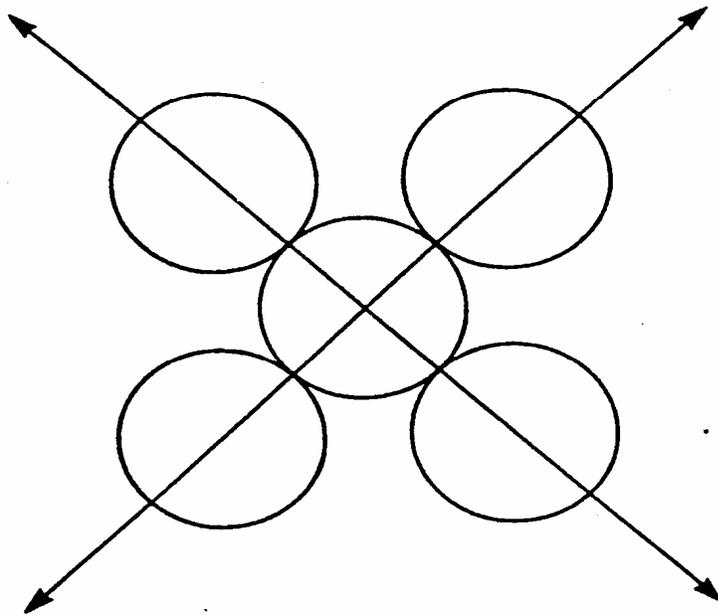

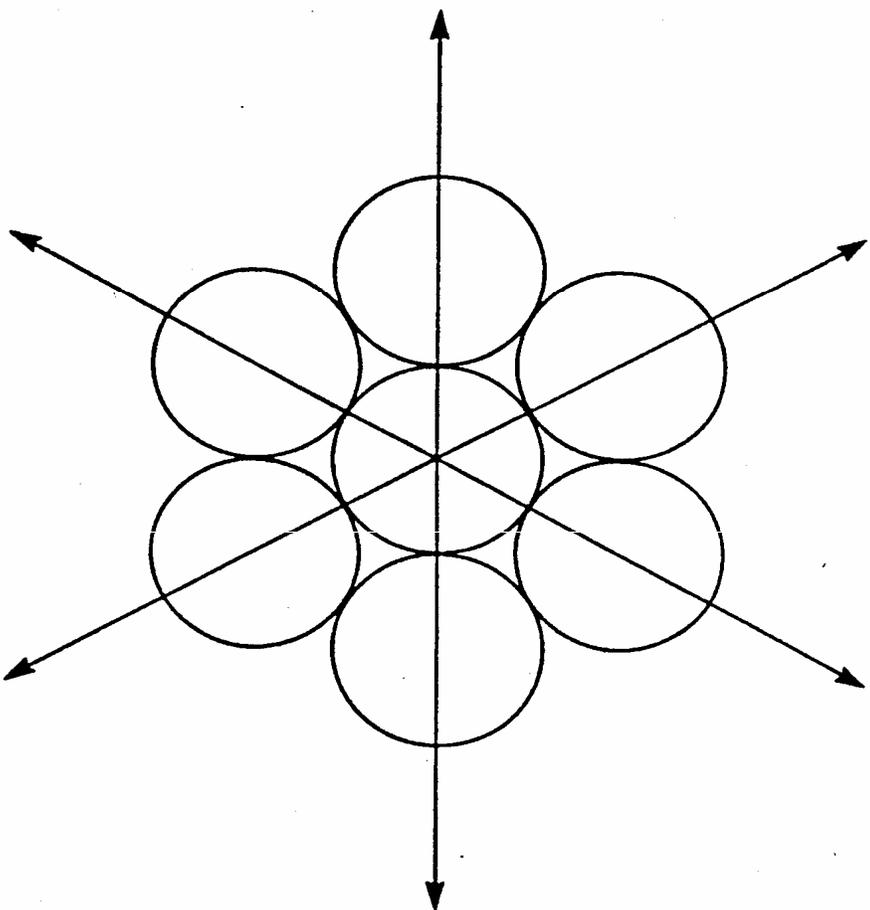Fig.2b Atomic arrangement of the (110) plane in the BCC structure. Arrows indicate two ⟨111⟩ directions.

Fig.2c Atomic arrangement of the (0001) close packed plane in the HCP structure. Arrows indicate three $\langle 2\bar{1}\bar{1}0 \rangle$ directions.
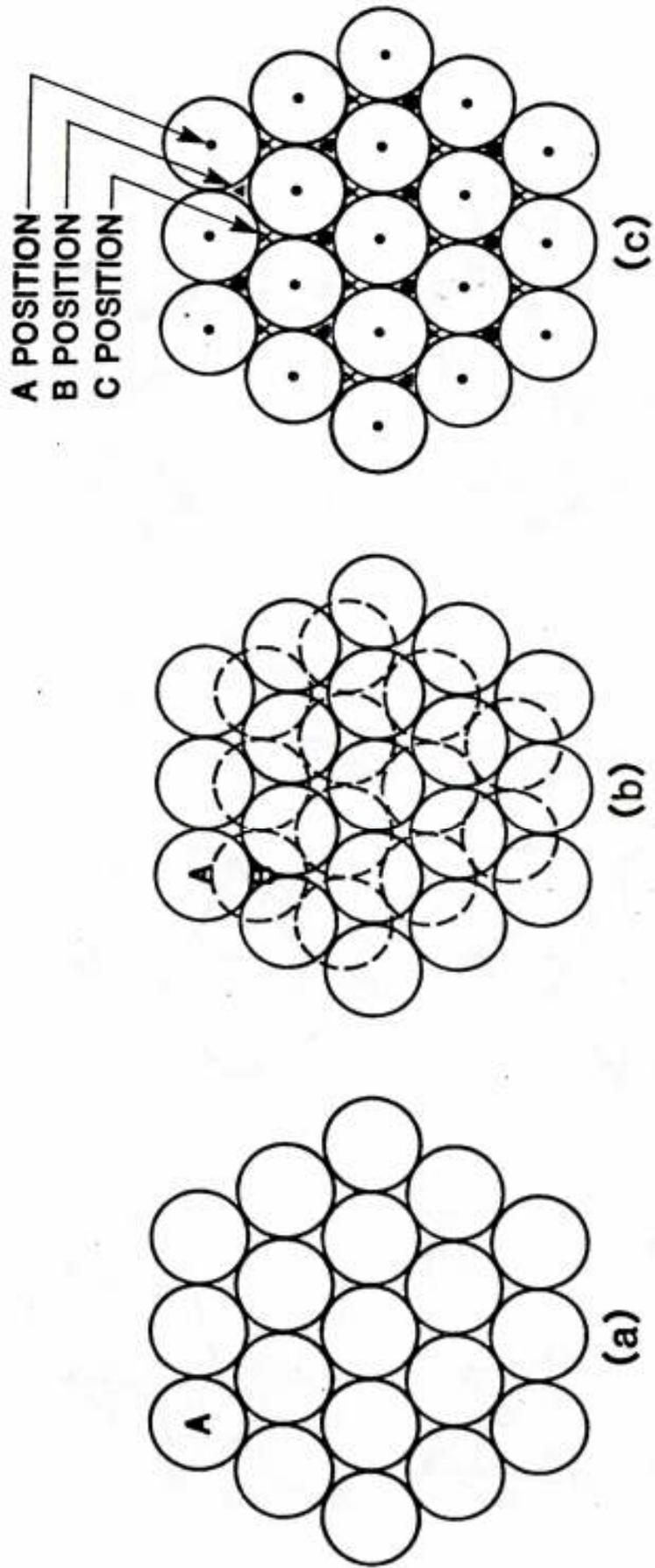
A POSITION
B POSITION
C POSITION

(a)

(b)

(c)

Fig.3   Atomic stacking sequence for the FCC close packed structure.

METAL ATOMS
○ OCTAHEDRAL INTERSTICES

METAL ATOMS
○ TETRAHEDRAL INTERSTICES

Metal atoms
○ Octahedral interstices
(a)

Metal atoms
○ Tetrahedral interstices
(b)

Metal atoms
○ Octahedral interstices
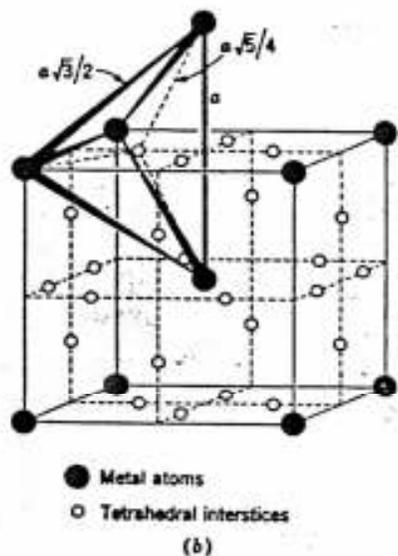(a)
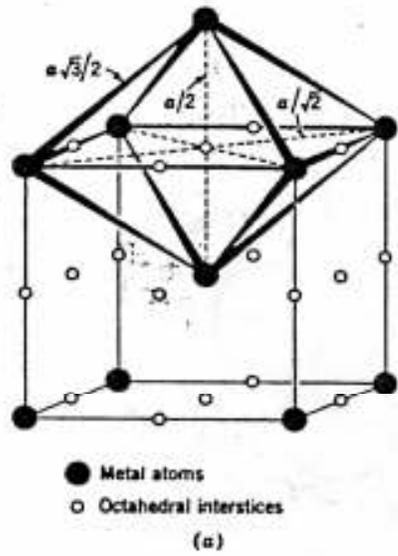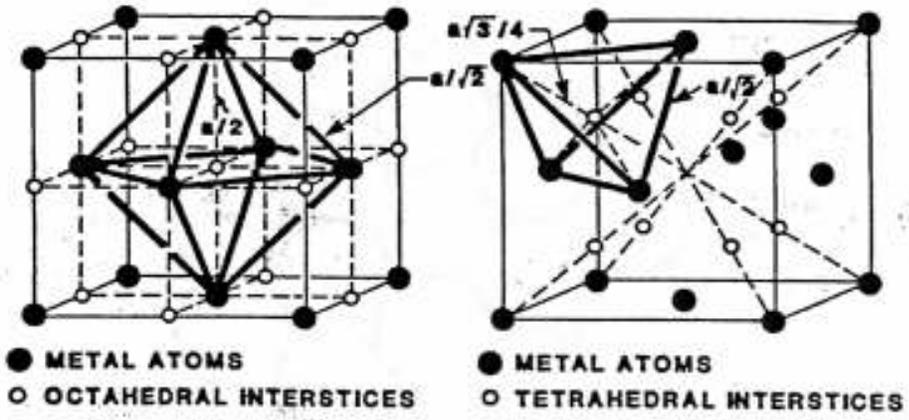
Metal atoms
○ Tetrahedral interstices
(b)
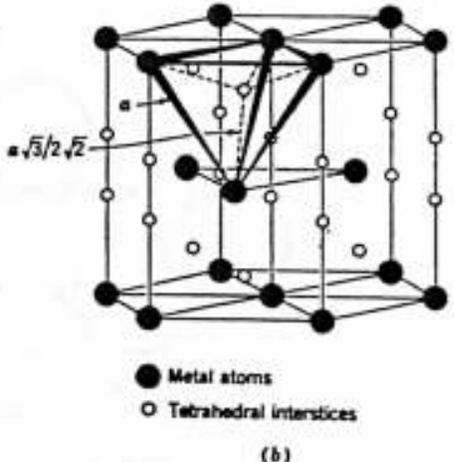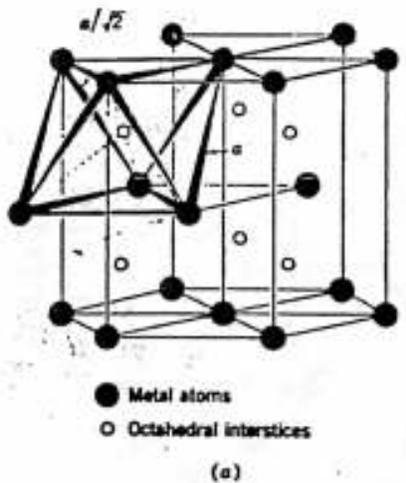
Fig.4   Interstitial sites for the three commonest metallic structures
(a) FCC, (b) BCC, (c) HCP.