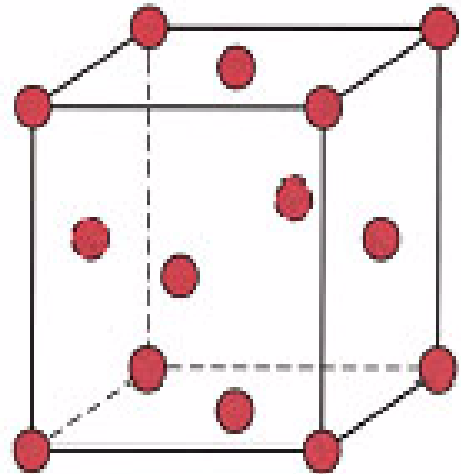
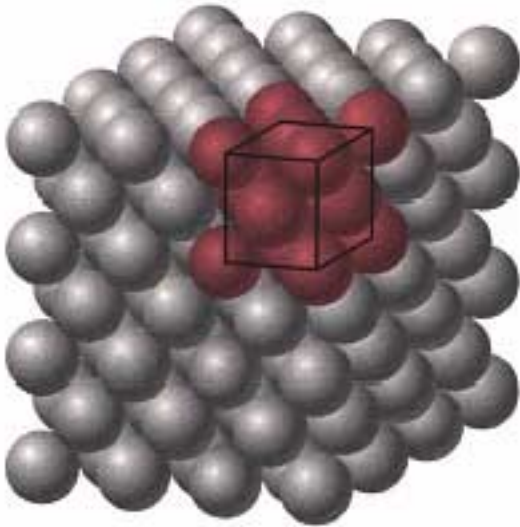


- **Fundamental concepts and language**
- **Unit cells**
- **Crystal structures**
  - **Face-centered cubic**
  - **Body-centered cubic**
  - **Hexagonal close-packed**
- **Close packed crystal structures**
- **Density computations''**

# Crystal structure

To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii. In this hard-sphere model, the shortest distance between two like atoms is one diameter.

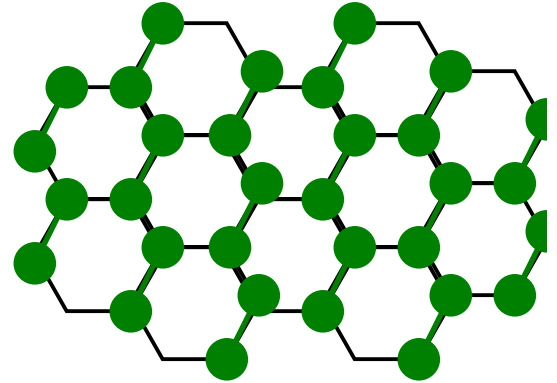
We can also consider crystalline structure as a lattice of points at atom/sphere centers.



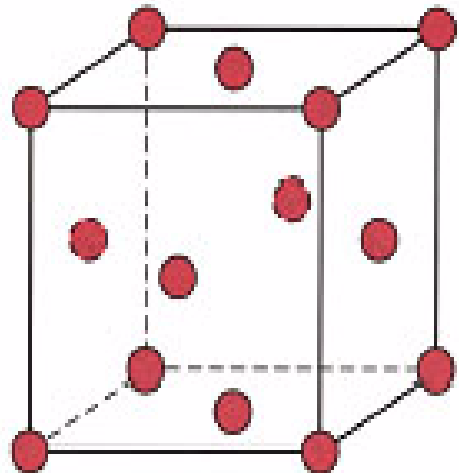
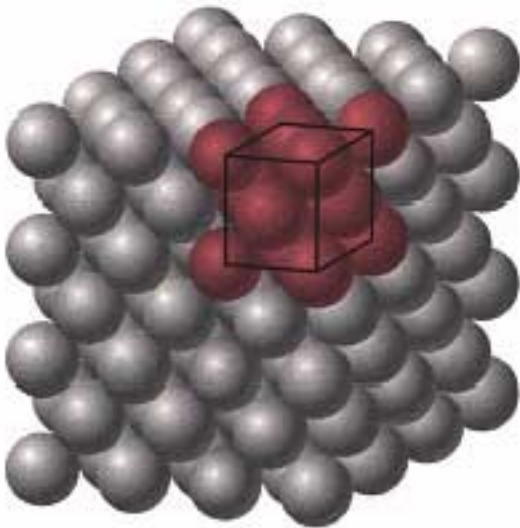
# Unit Cell

The **unit cell** is the smallest structural unit or building block that can describe the the crystal structure. Repetition of the unit cell generates the entire crystal.

Example: 2D honeycomb net can be represented by translation of two adjacent atoms that form a unit cell for this 2D crystalline structure



Example of 3D crystalline structure:



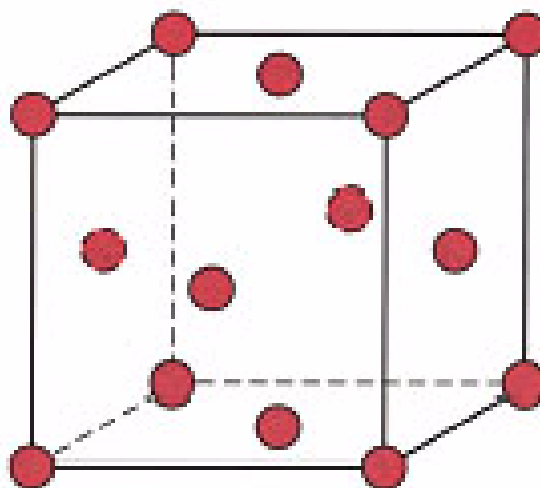
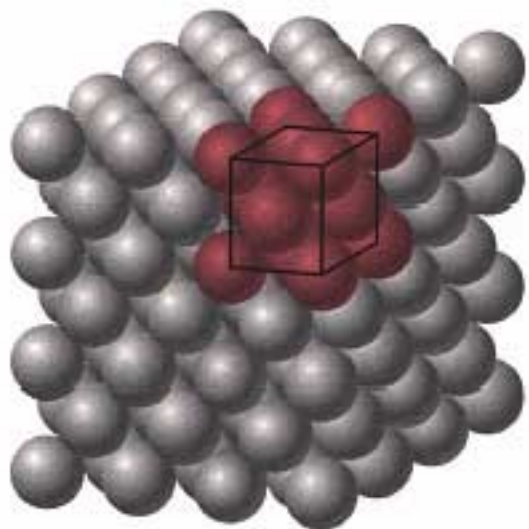
Different choices of unit cells possible, generally choose parallelepiped unit cell with highest level of symmetry

# Metallic Crystal Structures

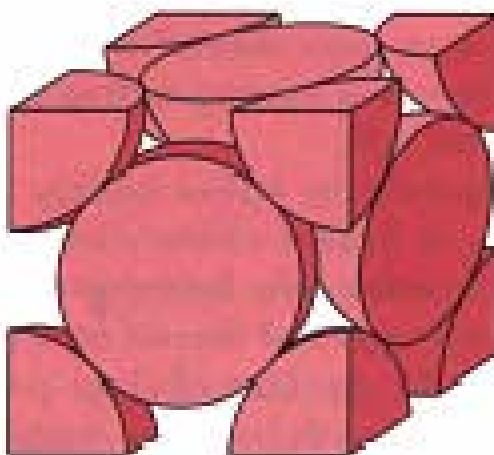
- Metals are usually (poly)crystalline; although formation of amorphous metals is possible by rapid cooling
- As we learned in Chapter 2, the atomic bonding in metals is non-directional  $\Rightarrow$  no restriction on numbers or positions of nearest-neighbor atoms  $\Rightarrow$  large number of nearest neighbors and dense atomic packing
- **Atom (hard sphere) radius,  $R$** , defined by ion core radius - typically 0.1 - 0.2 nm
- The most common types of unit cells are the face-centered cubic (FCC), the body-centered cubic (BCC) and the hexagonal close-packed (HCP).

# Face-Centered Cubic (FCC) Crystal Structure (I)

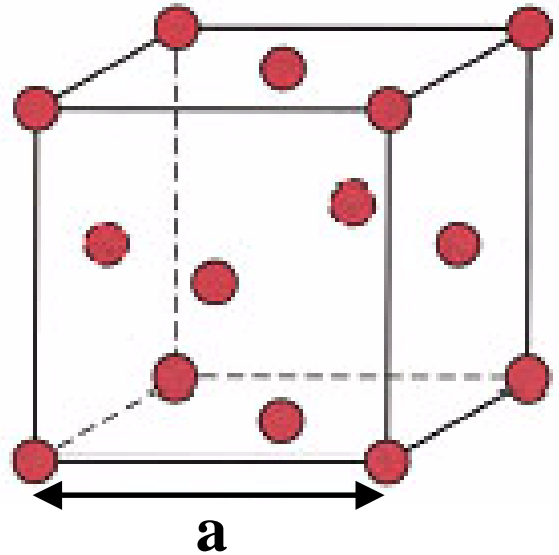
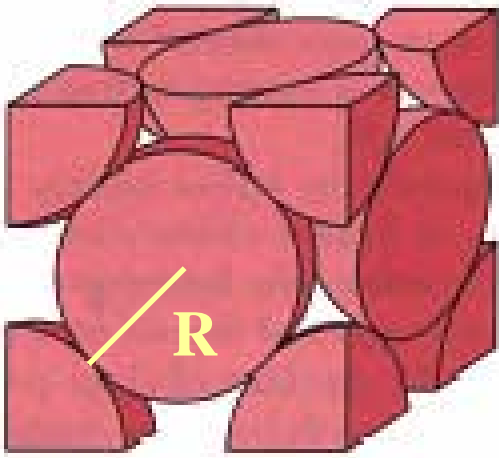
- Atoms are located at each of the corners and on the centers of all the faces of cubic unit cell
- Cu, Al, Ag, Au have this crystal structure



Two representations  
of the FCC unit cell



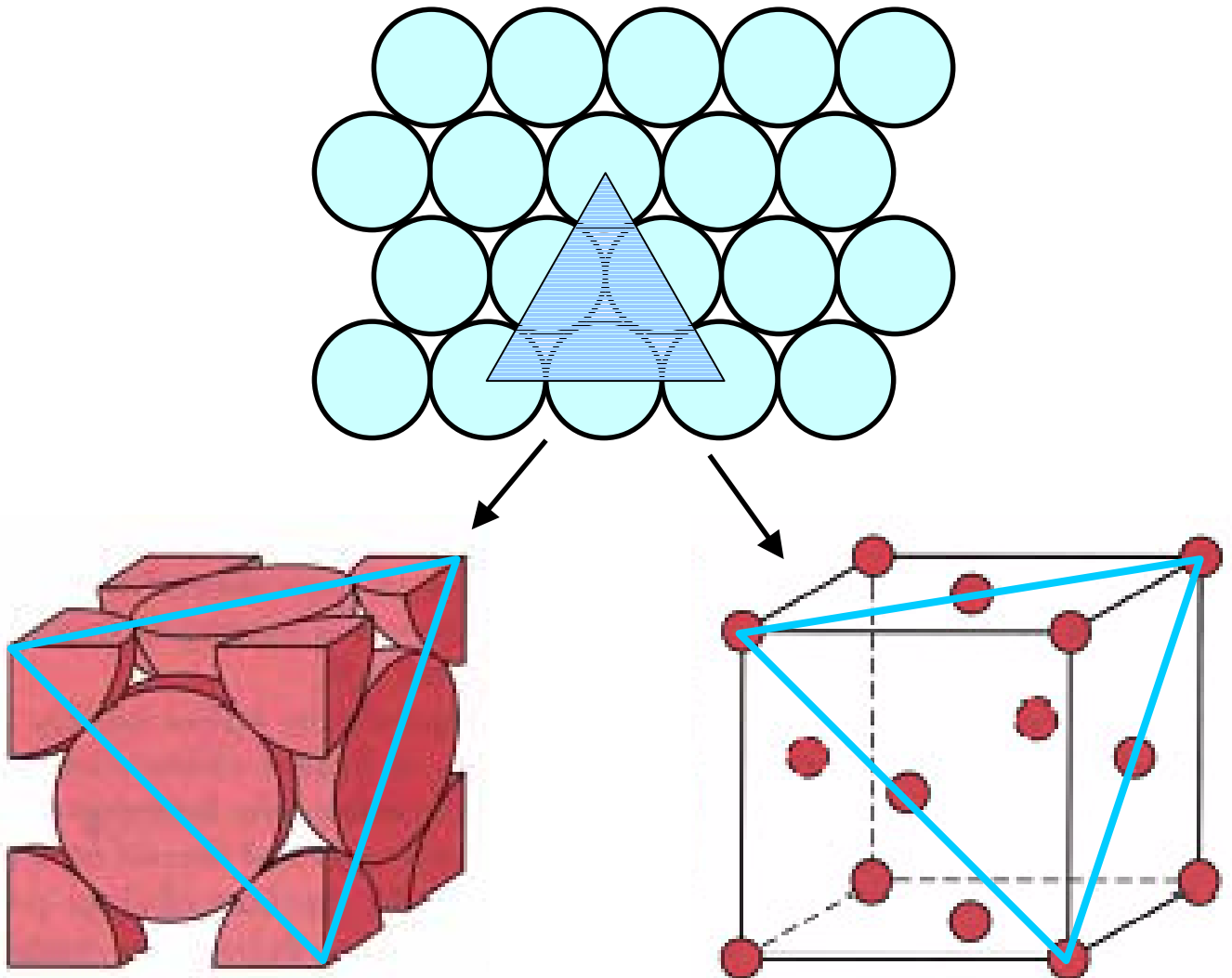
# Face-Centered Cubic Crystal Structure (II)



- The hard spheres or ion cores touch one another across a face diagonal  $\Rightarrow$  the cube edge length,  $a = 2R\sqrt{2}$
- **The coordination number, CN** = the number of closest neighbors to which an atom is bonded = number of touching atoms, **CN = 12**
- **Number of atoms per unit cell, n = 4.** (For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, 1/m). In FCC unit cell we have:
  - 6 face atoms shared by two cells:  $6 \times 1/2 = 3$
  - 8 corner atoms shared by eight cells:  $8 \times 1/8 = 1$
- **Atomic packing factor, APF** = fraction of volume occupied by hard spheres = (Sum of atomic volumes)/(Volume of cell) = **0.74** (maximum possible)

# Face-Centered Cubic Crystal Structure (III)

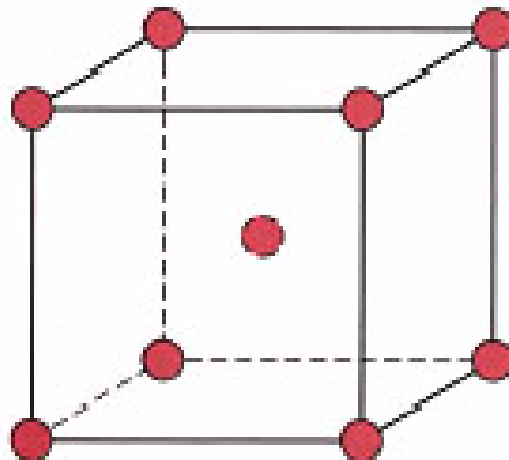
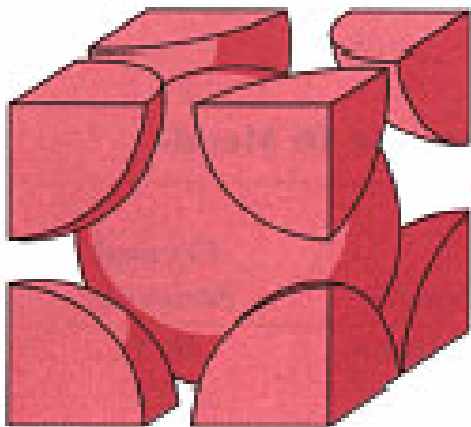
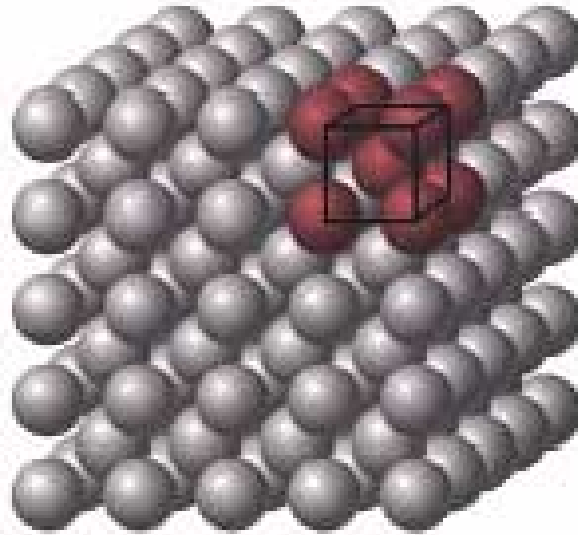
- Corner and face atoms in the unit cell are equivalent
- FCC crystal has APF of 0.74, the maximum packing for a system equal-sized spheres  $\Rightarrow$  FCC is a **close-packed structure**
- FCC can be represented by a stack of **close-packed planes** (planes with highest density of atoms)



# Body-Centered Cubic (BCC) Crystal Structure (I)

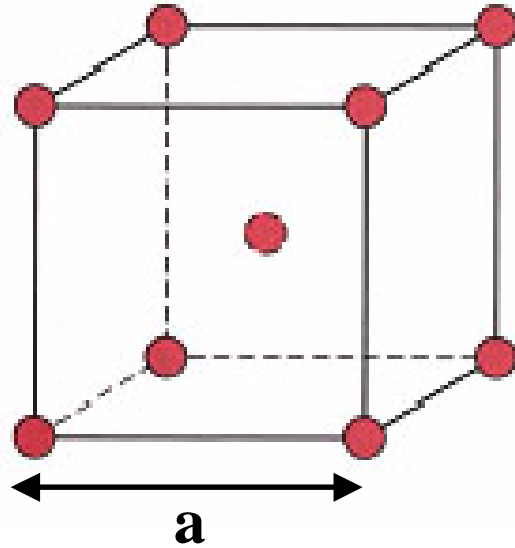
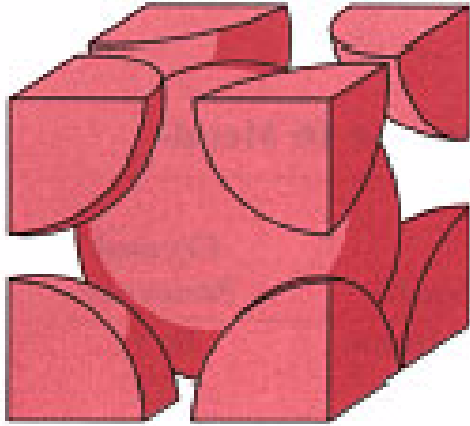
Atom at each corner and at center of cubic unit cell

Cr,  $\alpha$ -Fe, Mo have this crystal structure





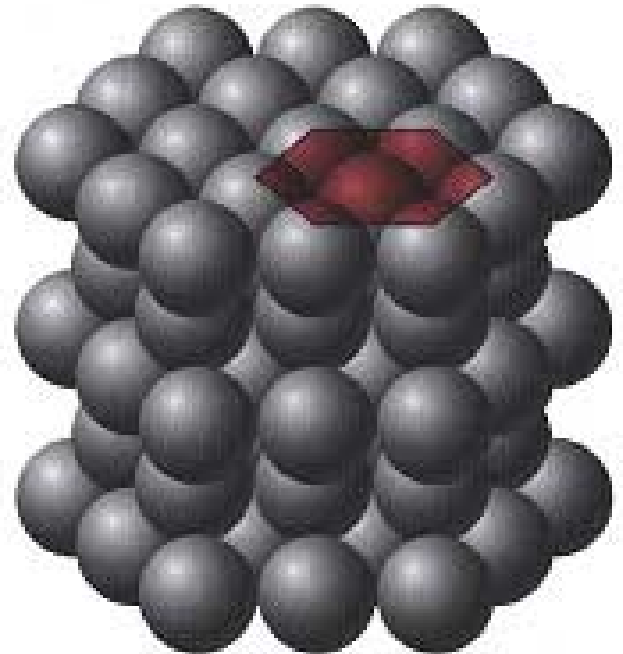
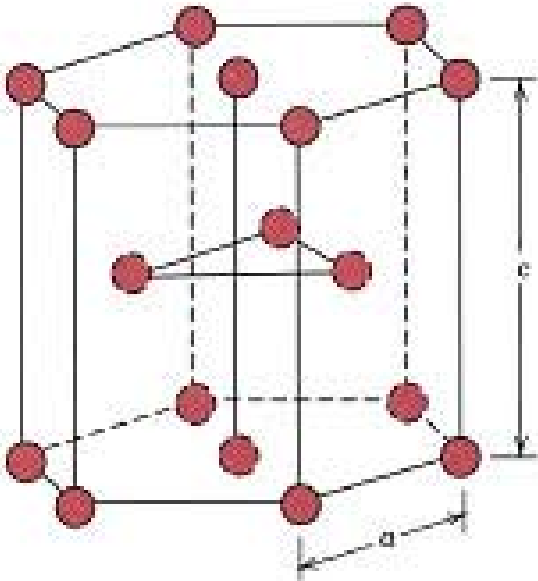
# Body-Centered Cubic Crystal Structure (II)



- The hard spheres touch one another along cube diagonal  
⇒ the cube edge length,  **$a = 4R/\sqrt{3}$**
- **The coordination number,  $CN = 8$**
- **Number of atoms per unit cell,  $n = 2$** 
  - Center atom (1) shared by no other cells:  $1 \times 1 = 1$
  - 8 corner atoms shared by eight cells:  $8 \times 1/8 = 1$
- **Atomic packing factor,  $APF = 0.68$**
- Corner and center atoms are equivalent

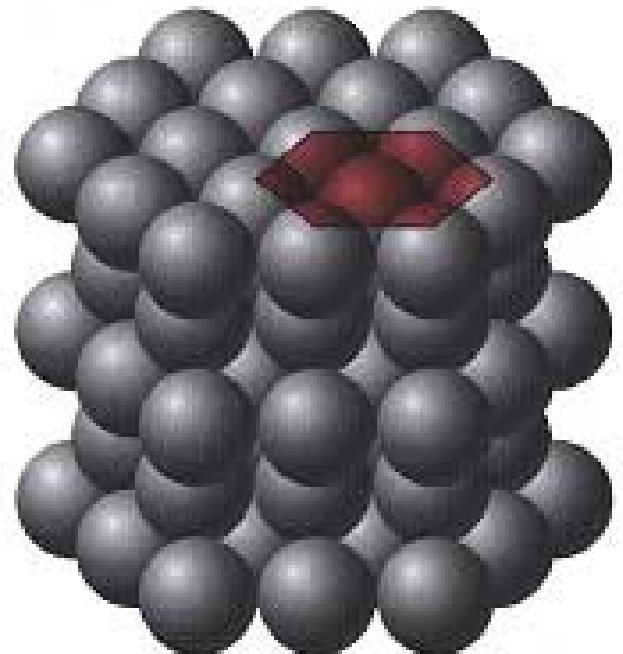
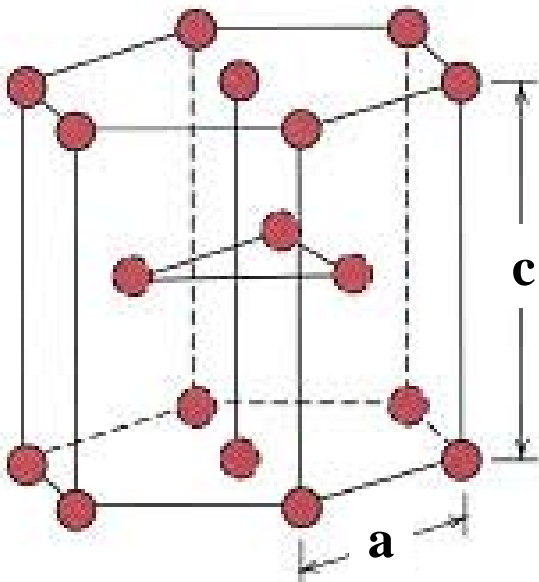
# Hexagonal Close-Packed Crystal Structure (I)

- HCP is one more common structure of metallic crystals
- Six atoms form regular hexagon, surrounding one atom in center. Another plane is situated halfway up unit cell (c-axis), with 3 additional atoms situated at interstices of hexagonal (close-packed) planes
- Cd, Mg, Zn, Ti have this crystal structure



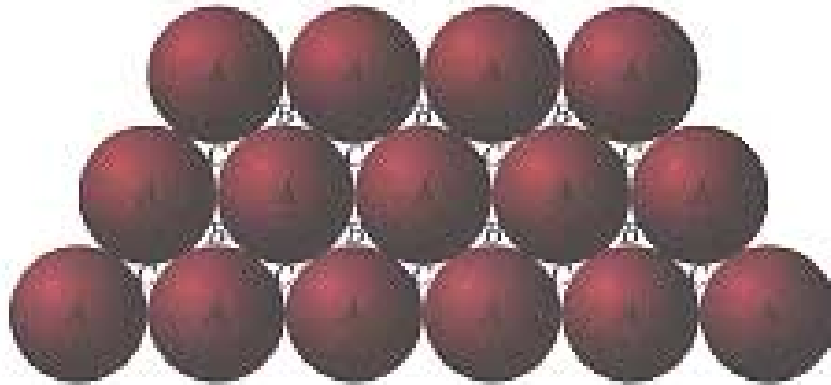
# Hexagonal Close-Packed Crystal Structure (II)

- Unit cell has two lattice parameters  $a$  and  $c$ . Ideal ratio  $c/a = 1.633$
- **The coordination number,  $CN = 12$  (same as in FCC)**
- **Number of atoms per unit cell,  $n = 6$ .**
  - 3 mid-plane atoms shared by no other cells:  $3 \times 1 = 3$
  - 12 hexagonal corner atoms shared by 6 cells:  $12 \times 1/6 = 2$
  - 2 top/bottom plane center atoms shared by 2 cells:  $2 \times 1/2 = 1$
- **Atomic packing factor,  $APF = 0.74$  (same as in FCC)**
- All atoms are equivalent



# Close-packed Structures (FCC and HCP)

- Both FCC and HCP crystal structures have atomic packing factors of 0.74 (maximum possible value)
- Both FCC and HCP crystal structures may be generated by the stacking of close-packed planes
- **The difference between the two structures is in the stacking sequence**



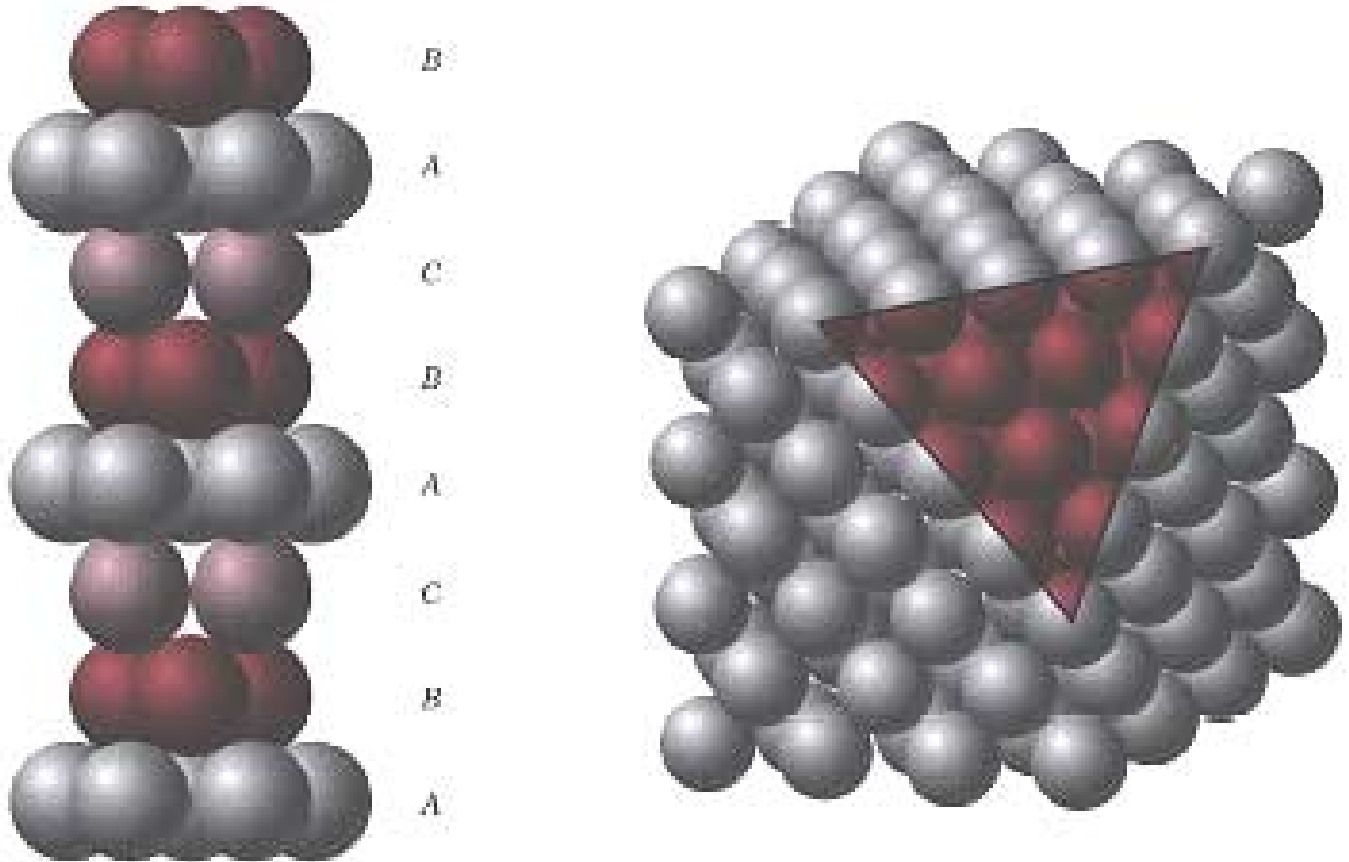
(a)



**HCP: ABABAB...**

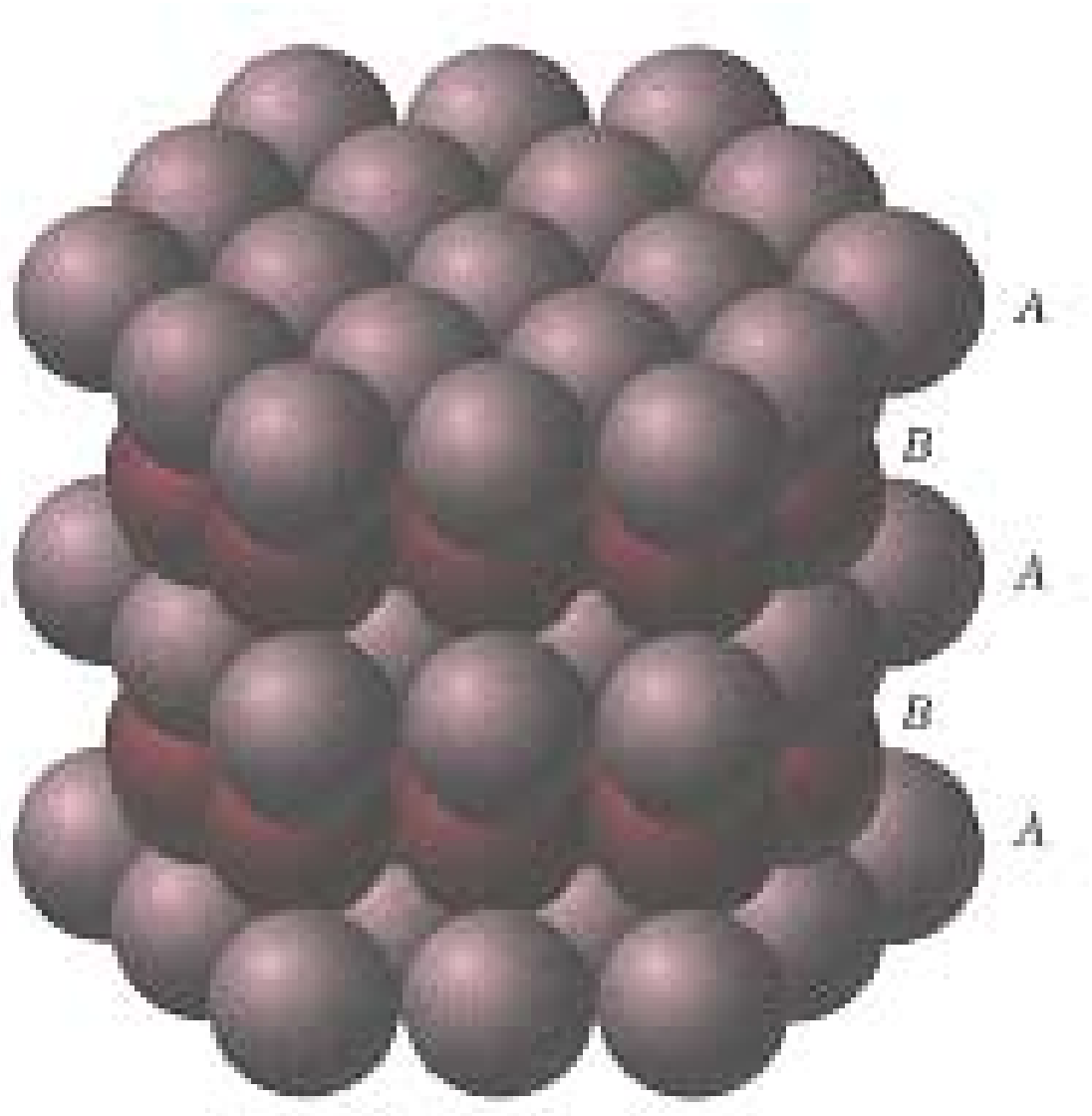
**FCC: ABCABCABC...**

# FCC: Stacking Sequence ABCABCABC...



Third plane is placed above the “holes” of the first plane not covered by the second plane

# HCP: Stacking Sequence ABABAB...



Third plane is placed directly above the first plane of atoms

# Density Computations

Since the entire crystal can be generated by the repetition of the unit cell, **the density of a crystalline material,  $\rho$  = the density of the unit cell = (atoms in the unit cell,  $n$ )  $\times$  (mass of an atom,  $M$ ) / (the volume of the cell,  $V_c$ )**

**Atoms in the unit cell,  $n$  = 2 (BCC); 4 (FCC); 6 (HCP)**

**Mass of an atom,  $M$  = Atomic weight,  $A$ , in amu (or g/mol)** is given in the periodic table. To translate mass from amu to grams we have to divide the atomic weight in amu by the Avogadro number  $N_A = 6.023 \times 10^{23}$  atoms/mol

**The volume of the cell,  $V_c = a^3$  (FCC and BCC)**

$$a = 2R\sqrt{2} \text{ (FCC); } a = 4R/\sqrt{3} \text{ (BCC)}$$

where  $R$  is the atomic radius

Thus, the formula for the density is:

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

Atomic weight and atomic radius of many elements you can find in the table at the back of the textbook front cover.

# Anisotropy

Different directions in a crystal have a different packing. For instance, atoms along the edge of FCC unit cell are more separated than along the face diagonal. This causes **anisotropy** in the properties of crystals, for instance, the deformation depends on the direction in which a stress is applied.

In some polycrystalline materials, grain orientations are random, so bulk material properties are **isotropic**

Some polycrystalline materials have grains with preferred orientations (**texture**), so properties are dominated by those relevant to the texture orientation and the material exhibits anisotropic properties



# Metal Structure-Unit cell Direct Tutorial

M.A.E. Saleh

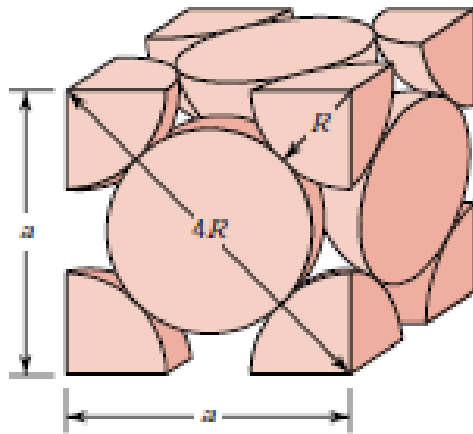
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### EXAMPLE PROBLEM 3.1

Calculate the volume of an FCC unit cell in terms of the atomic radius  $R$ .

#### **SOLUTION**

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is  $4R$ . Since the unit cell is a cube, its volume is  $a^3$ , where  $a$  is the cell edge length. From the right triangle on the face,

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

or, solving for  $a$ ,

$$a = 2R\sqrt{2} \quad (3.1)$$

The FCC unit cell volume  $V_C$  may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \quad (3.4)$$

### EXAMPLE PROBLEM 3.2

Show that the atomic packing factor for the FCC crystal structure is 0.74.

#### *SOLUTION*

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{total sphere volume}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total sphere and unit cell volumes may be calculated in terms of the atomic radius  $R$ . The volume for a sphere is  $\frac{4}{3}\pi R^3$ , and since there are four atoms per FCC unit cell, the total FCC sphere volume is

$$V_S = (4) \frac{4}{3} \pi R^3 = \frac{16}{3} \pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3 \sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{\left(\frac{16}{3}\right) \pi R^3}{16R^3 \sqrt{2}} = 0.74$$

### EXAMPLE PROBLEM 3.3

Copper has an atomic radius of 0.128 nm (1.28 Å), an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

#### *SOLUTION*

Equation 3.5 is employed in the solution of this problem. Since the crystal structure is FCC,  $n$ , the number of atoms per unit cell, is 4. Furthermore, the atomic weight  $A_{\text{Cu}}$  is given as 63.5 g/mol. The unit cell volume  $V_C$  for FCC was determined in Example Problem 3.1 as  $16R^3\sqrt{2}$ , where  $R$ , the atomic radius, is 0.128 nm.

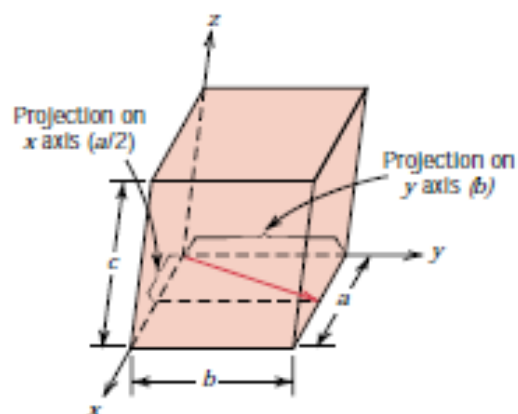
Substitution for the various parameters into Equation 3.5 yields

$$\begin{aligned}\rho &= \frac{nA_{\text{Cu}}}{V_C N_A} = \frac{nA_{\text{Cu}}}{(16R^3\sqrt{2})N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 8.89 \text{ g/cm}^3\end{aligned}$$

The literature value for the density of copper is 8.94 g/cm<sup>3</sup>, which is in very close agreement with the foregoing result.

### EXAMPLE PROBLEM 3.7

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



#### SOLUTION

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

This procedure may be summarized as follows:

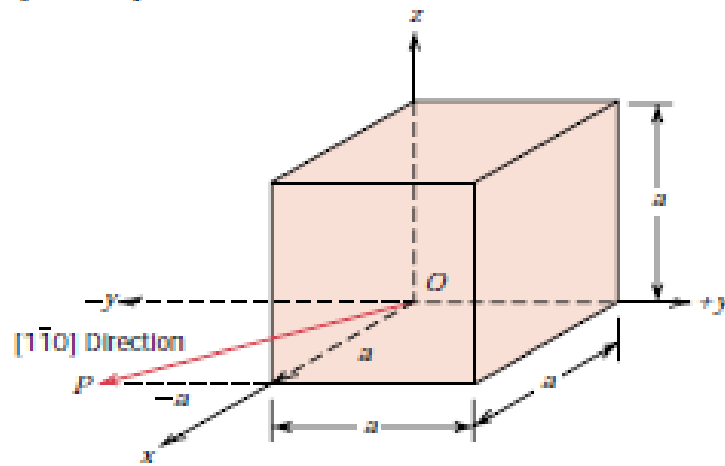
	$x$	$y$	$z$
Projections	$a/2$	$b$	$0c$
Projections (in terms of $a$ , $b$ , and $c$ )	$\frac{1}{2}$	1	0
Reduction	1	2	0
Enclosure		$[120]$	

### EXAMPLE PROBLEM 3.8

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

#### **SOLUTION**

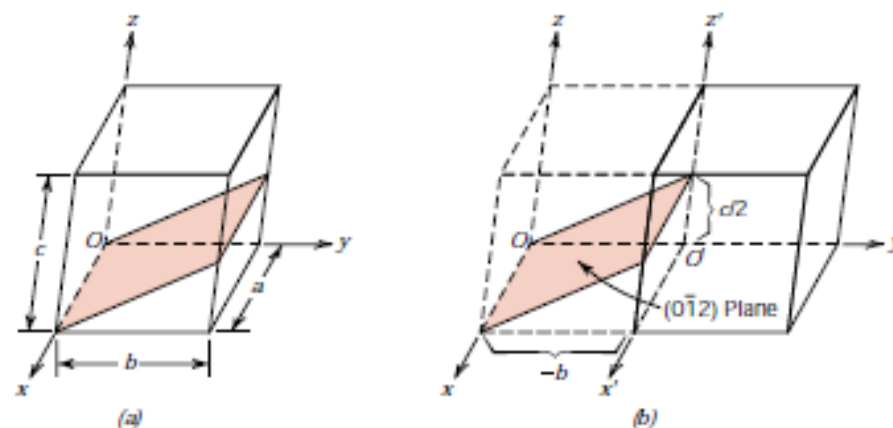
First construct an appropriate unit cell and coordinate axes system. In the accompanying figure the unit cell is cubic, and the origin of the coordinate system, point  $O$ , is located at one of the cube corners.



This problem is solved by reversing the procedure of the preceding example. For this  $[1\bar{1}0]$  direction, the projections along the  $x$ ,  $y$ ,  $z$  axes are  $a$ ,  $-a$ , and  $0a$ , respectively. This direction is defined by a vector passing from the origin to point  $P$ , which is located by first moving along the  $x$  axis  $a$  units, and from this position, parallel to the  $y$  axis  $-a$  units, as indicated in the figure. There is no  $z$  component to the vector, since the  $z$  projection is zero.

### EXAMPLE PROBLEM 3.9

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



#### SOLUTION

Since the plane passes through the selected origin  $O$ , a new origin must be chosen at the corner of an adjacent unit cell, taken as  $O'$  and shown in sketch (b). This plane is parallel to the  $x$  axis, and the intercept may be taken as  $\infty a$ . The  $y$  and  $z$  axes intersections, referenced to the new origin  $O'$ , are  $-b$  and  $c/2$ , respectively. Thus, in terms of the lattice parameters  $a$ ,  $b$ , and  $c$ , these intersections are  $\infty$ ,  $-1$ , and  $\frac{1}{2}$ . The reciprocals of these numbers are  $0$ ,  $-1$ , and  $2$ ; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields  $(0\bar{1}2)$ .

These steps are briefly summarized below:

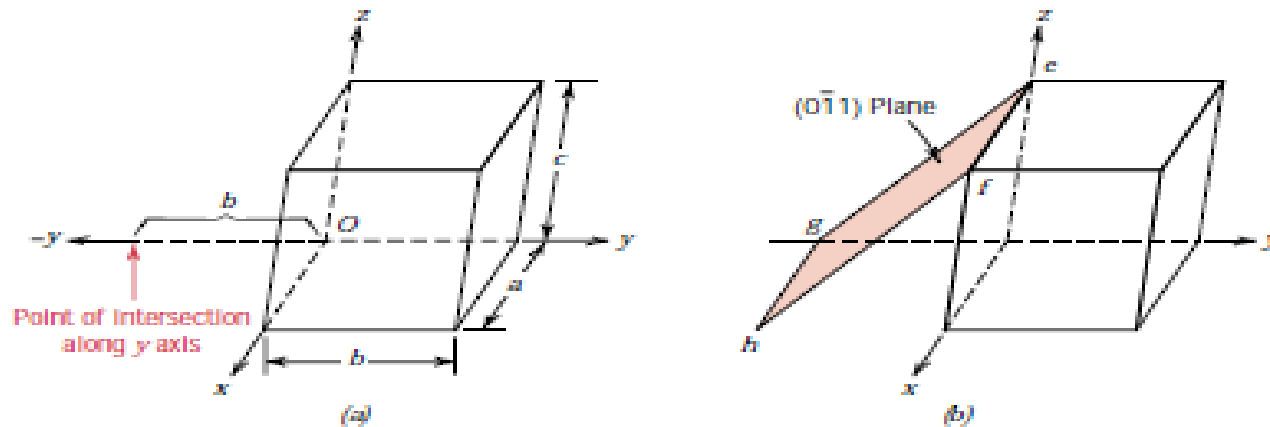
	$x$	$y$	$z$
Intercepts	$\infty a$	$-b$	$c/2$
Intercepts (in terms of lattice parameters)	$\infty$	$-1$	$\frac{1}{2}$
Reciprocals	$0$	$-1$	$2$
Reductions (unnecessary)			
Enclosure		$(0\bar{1}2)$	

### EXAMPLE PROBLEM 3.10

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

#### SOLUTION

To solve this problem, carry out the procedure used in the preceding example in reverse order. To begin, the indices are removed from the parentheses, and reciprocals are taken, which yields  $\infty$ ,  $-1$ , and  $1$ . This means that the particular plane parallels the  $x$  axis while intersecting the  $y$  and  $z$  axes at  $-b$  and  $c$ , respectively, as indicated in the accompanying sketch (a). This plane has been drawn in sketch (b). A plane is indicated by lines representing its intersections with the planes that constitute the faces of the unit cell or their extensions. For example, in this figure, line  $ef$  is the intersection between the  $(0\bar{1}1)$  plane and



the top face of the unit cell; also, line  $gh$  represents the intersection between this same  $(0\bar{1}1)$  plane and the plane of the bottom unit cell face extended. Similarly, lines  $eg$  and  $fh$  are the intersections between  $(0\bar{1}1)$  and back and front cell faces, respectively.