

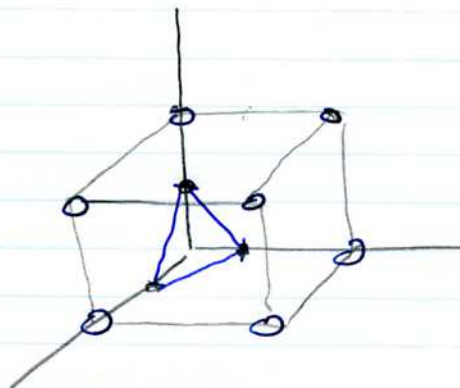
-6a²-

Do after top of High Index Planes

p 7

or $hkl \geq 2$

Equal high numbers; e.g. (222)

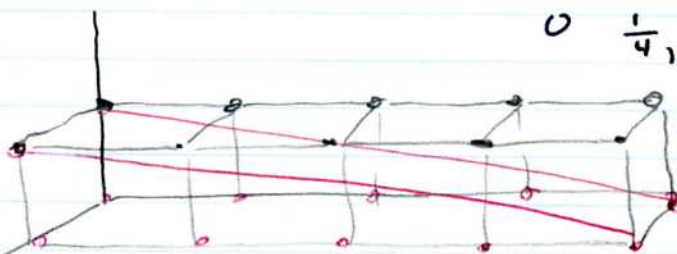


(intercepts: $\frac{1}{2} \frac{1}{2} \frac{1}{2}$)

|| to (111) but hits fewer bases

Unequal high numbers; e.g. $a = \infty, b = 4, c = 1$

$0 \frac{1}{4}, 1 \Rightarrow (014)$



mostly empty space

4 characteristics:

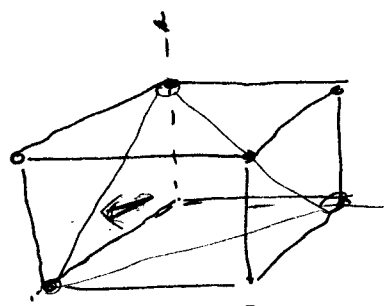
- (i) lower density of matter; if surface, open to inner layers ("rough")
- (ii) small angle with face of unequal indices
- (iii) encountered more with non-primitive lattices
- (iv) hard to cut \Rightarrow steps

Formulae: $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$ distance between hkl planes
(cubic systems)

angle between two sets $\cos \phi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}}$

$\phi = 14^\circ$ between $001 + 014$

Also:
 $\frac{1}{2}$ hexagonal mesh



(1 1 1) as in original example
 \perp vectors
 $[1 1 1]$ $[\bar{1} \bar{1} \bar{1}]$

What about vector in plane? $[1 \bar{1} 0]$

Spherical (Closest Packed) Representation

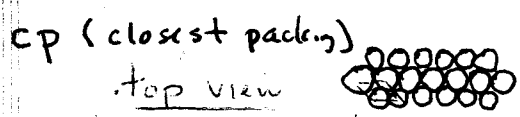
+ crystals

In representing surfaces; it is customary to use spheres for the basis and to crush them together as closely as they can go:



To get the surface right, we must consider the 3-D structures, which can lead to "~~cubic~~ closest packing". The spherical representation is perhaps more realistic for non-directional bonding and for $1/r^2$ distribution. The closest packing of spheres can represent metals well, and can do the same for "near spherical" models such as CH_4 . For simple systems, we can imagine that attractive long-range forces dominate. Remember that long-range forces are always attractive.

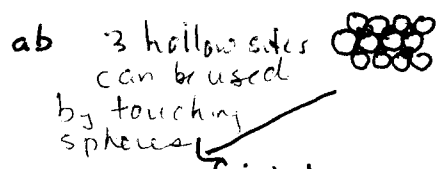
Cubic Lattices + Planes in Spherical Representation



note hexagonal mesh

1st layer (6 nearest neighbors)

2nd layer (spheres sit in hollow sites above 1st layer)



same as first layer
 ababab...

3rd layer
 another set of holes
 abc abc abc

leads to hexagonal unit cell
 "hcp"

leads to face centered cubic cell
 fcc = ccp

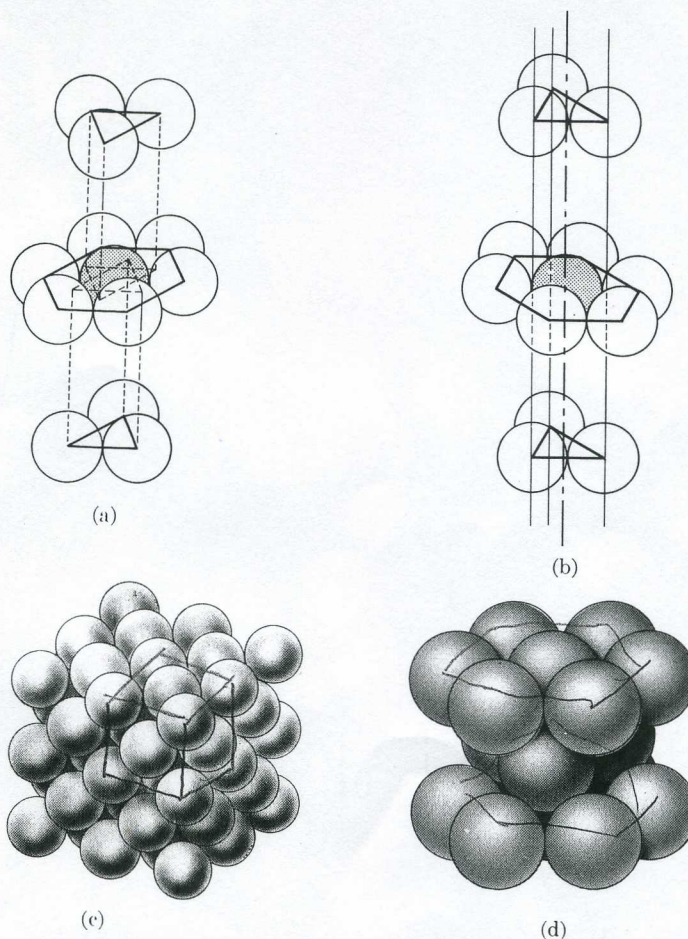


Fig. 26-3 Close-packed structures. (a) and (c) fcc. (b) and (d) hcp.

and fcc structures are the typical structures encountered in metals. The high coordination number (twelve), in these structures results in a crystal of comparatively high density.

Another common arrangement of spheres which occurs in a few metals is the body-centered cubic (bcc), which is built up of layers having the arrangement shown in Fig. 26-4. The second layer fits in the notches of the first and the pattern of layers repeats, $xyxy \dots$. In these layers the number of nearest neighbors around any sphere is four, as compared with six in the close-packed layers. In the body-centered structure the overall coordination number is eight; there are four nearest neighbors within the most closely packed layer, two in the layer above, and two in that below. As a result of the less efficient packing, the bcc structure has an inherently lower density than the hcp or the fcc structures.

The view in
 tion of
 center
 specific
 layer, &
 rigid s
 are not
 fied sep
 Table 2
 values



Metal
Al
Cu
Au
Pb

(Show 4/15 IntroSurfChem_16)

hcp, ccp(fcc) Coordination Number C.N. = no. nearest neighbors
 C.N. = 3 + 6 + 3 = 12
 Volume occupied by spheres = 74%

For body-centered cubic (not as closely packed):
 C.N. = 8 V = 68%

(trig problems: hw)

Metallc Crystals:	FCC	BCC	HCP
	Al	Cr	Co
	Cu	Fe	Mg
	Au	W	Ti
	Pb	Na	Zn
	Pd		
	Pt		
	Ag		
	Ni		

Important Planes: Ideal Surfaces & 2D cells

Show (7/15 Intro)

(low index surfaces)

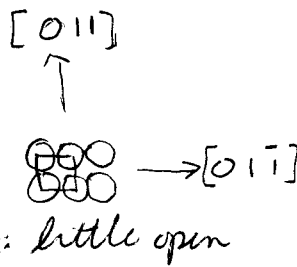
FCC



primitive
 → 100
 → 010
 → 001
 2r x 2r



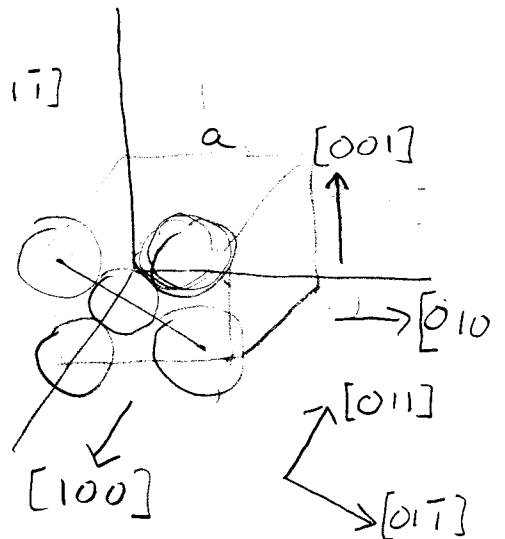
or (rotating)



$$4r = \sqrt{2} a$$

$$a = 4r / \sqrt{2}$$

Side of primitive cell ∴ $2r = \frac{\sqrt{2} a}{2}$
 90°



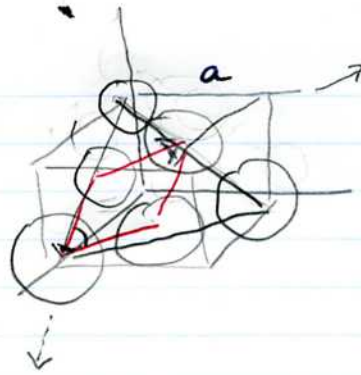
can check \perp
 (dot product)

can remove spheres to get directions



b) 111

equilateral triangle $\Rightarrow 60^\circ$

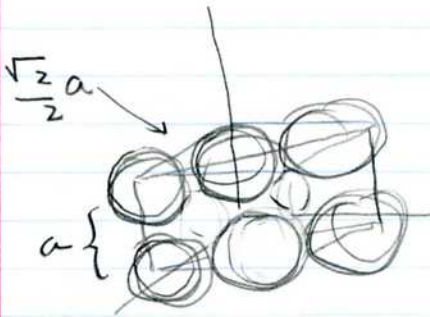


$[10\bar{1}]$
 $[\bar{1}10]$

$2r = \frac{\sqrt{2}a}{2}$ $\angle = 120^\circ, 60^\circ$

primitive cell rhombus (hexagonal)

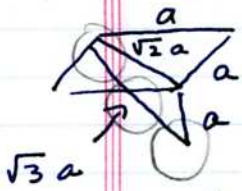
c) 110 (homework)



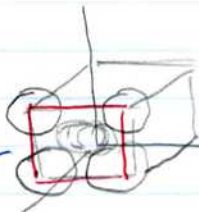
← 2nd layer salient

BCC

Major diagonal = $\sqrt{3}a = 4r$ $r = \frac{\sqrt{3}a}{4}$
4 radii fit in



a) 100



square cell $a \times a$ $a = \frac{4r}{\sqrt{3}} = 2.31r$

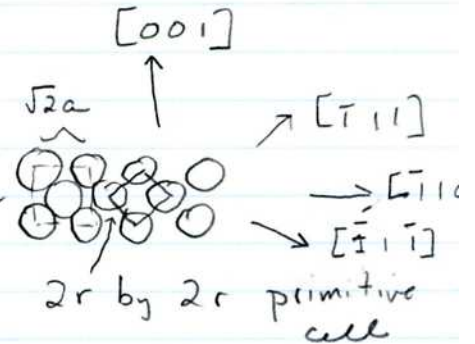
2nd layer

$[00\bar{1}]$ $\rightarrow [010]$

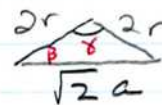
b) 110



Kolashinski
all 1st layer



$2r = \frac{\sqrt{3}a}{2}$



$c^2 = a^2 + b^2 - 2ab \cos \gamma$

$2a^2 = \frac{3}{2}a^2 - \frac{3}{2}a^2 \cos \gamma$

$\gamma = 109.47^\circ$

$2\beta = 70.53^\circ$

McCash

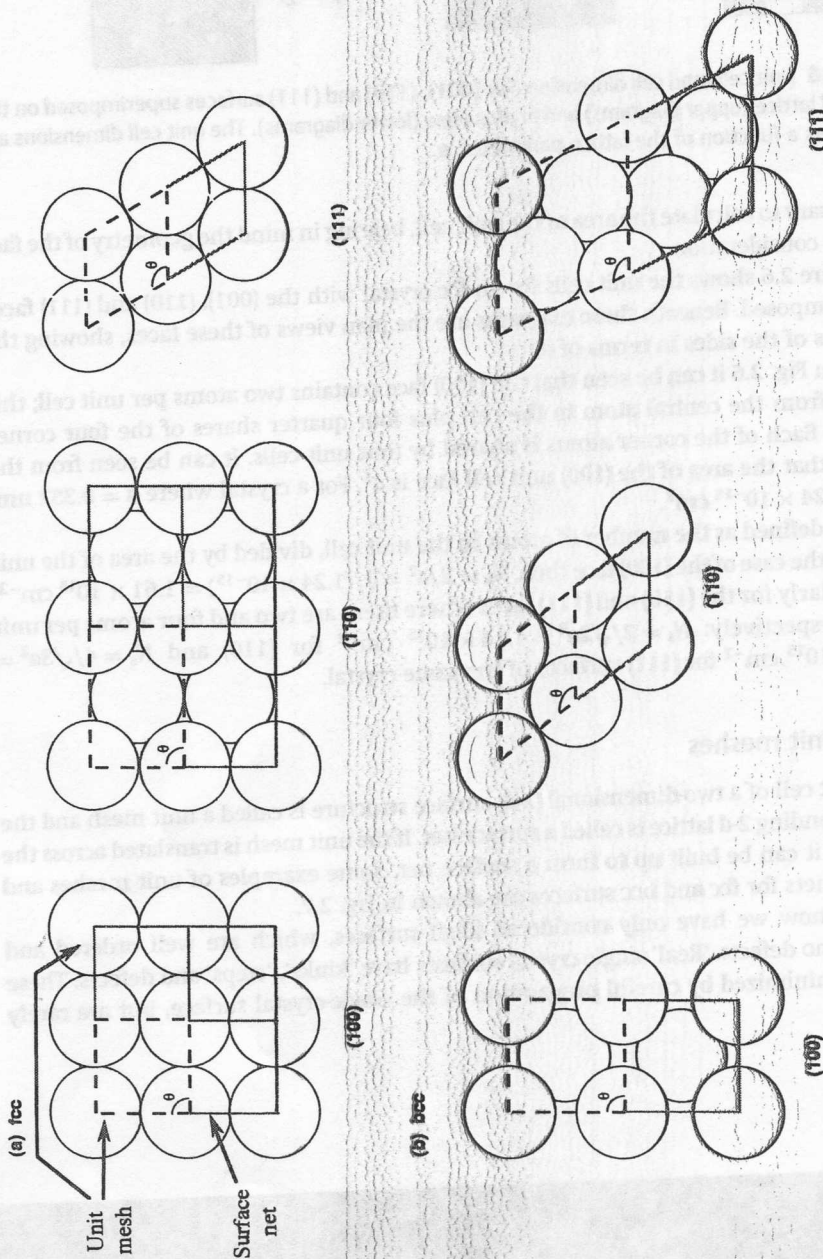
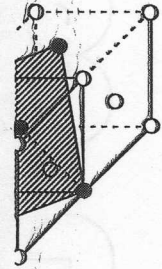


Fig. 2.7 Unit meshes for (a) fcc and (b) bcc surfaces shown as dashed lines. The associated surface nets are also illustrated and are built up by translating the unit mesh across the surface, as indicated by pale solid lines.



imposed on the dimensions are

metry of the face

and (111) faces, showing the

r unit cell; this is the four corner atoms seen from the $a = 0.352 \text{ nm}$,

area of the unit cell is $1 \times 10^{15} \text{ cm}^{-2}$. atoms per unit cell $N_s = 4/\sqrt{3}a^2 =$

t mesh and the lattice is extended across the unit meshes and

ll ordered and defects. These defects are rarely

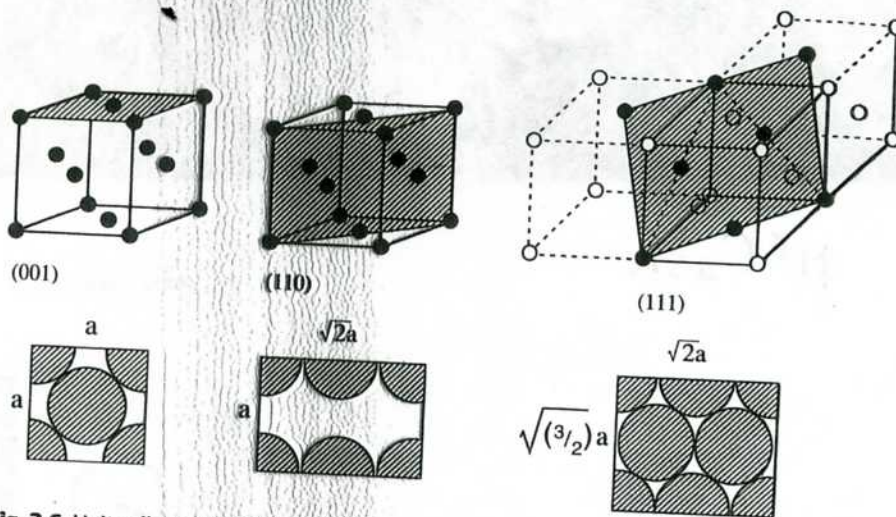


Fig. 2.6 Unit cells and cell dimensions for (001), (110) and (111) surfaces superimposed on the crystal lattice (upper diagrams) and in plan view (lower diagrams). The unit cell dimensions are given as a function of the lattice parameter, a .

necessary to calculate the area of the unit cell, bearing in mind the geometry of the face under consideration.

Figure 2.6 shows the unit cells for an fcc crystal with the (001), (110) and (111) faces superimposed. Beneath these diagrams are the plan views of these faces, showing the lengths of the sides in terms of a .

From Fig. 2.6 it can be seen that the (100) face contains two atoms per unit cell; this arises from the central atom in the cell plus four quarter shares of the four corner atoms. Each of the corner atoms is shared by four unit cells. It can be seen from the figure that the area of the (100) unit cell face is a^2 . For a crystal where $a = 0.352$ nm, $a^2 = 1.24 \times 10^{-15}$ cm².

N_s is defined as the number of atoms in the unit cell, divided by the area of the unit cell. In the case of the (100) face then, $N_s = 2/a^2 = 2/(1.24 \times 10^{-15}) = 1.61 \times 10^{15}$ cm⁻².

Similarly for the (110) and (111) faces where there are two and four atoms per unit cell, respectively: $N_s = 2/\sqrt{2}a^2 = 1.41 \times 10^{15}$ cm⁻² for (110) and $N_s = 4/\sqrt{3}a^2 = 1.86 \times 10^{15}$ cm⁻² for (111) surfaces of the same crystal.

2.1.4 Unit meshes

The unit cell of a two-dimensional (2-d) surface structure is called a unit mesh and the corresponding 2-d lattice is called a surface net. If the unit mesh is translated across the surface, it can be built up to form a surface net. Some examples of unit meshes and surface nets for fcc and bcc surfaces are shown in Fig. 2.7.

Until now we have only considered ideal surfaces, which are well ordered and contain no defects. 'Real' single crystal surfaces have 'kinks', 'steps' and defects. These can be minimized by careful preparation of the single-crystal surface, but are rarely

