

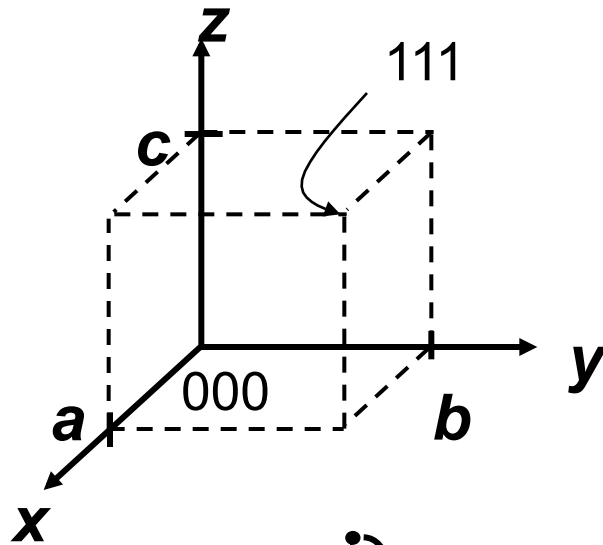
Crystallographic directions and planes

Outline

- Crystallographic directions
- Crystallographic planes
- Linear and planar atomic densities
- Close-packed crystal structures



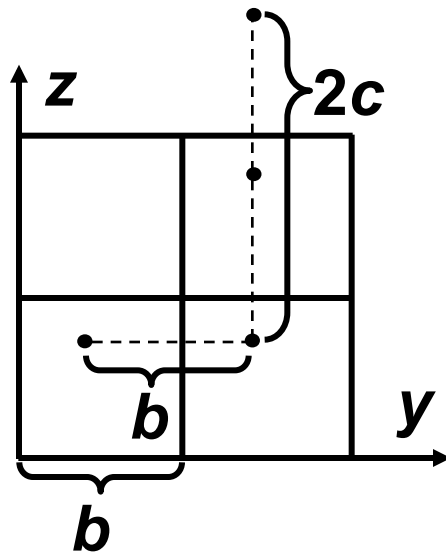
Point Coordinates



Point coordinates for unit cell center are

$$a/2, b/2, c/2 \quad \frac{1}{2} \frac{1}{2} \frac{1}{2}$$

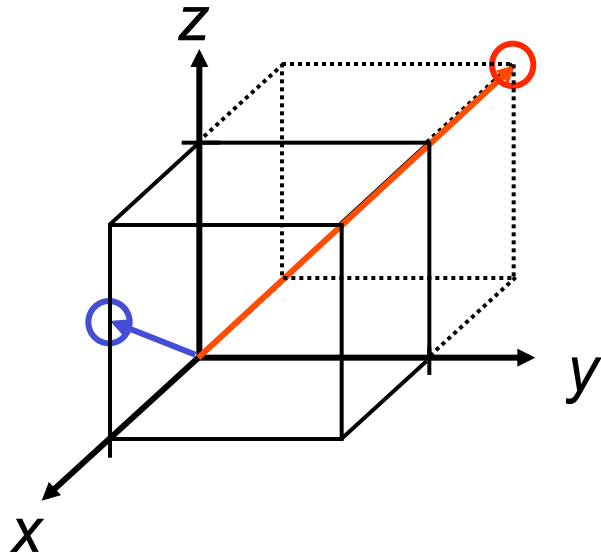
Point coordinates for unit cell corner are 111



Translation: integer multiple of lattice constants $\rightarrow$ identical position in another unit cell



Crystallographic Directions



Algorithm

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

$[uvw]$

ex: $1, 0, \frac{1}{2} \Rightarrow 2, 0, 1 \Rightarrow [201]$

$-1, 1, 1 \Rightarrow [\bar{1}11]$ where overbar represents a negative index

families of directions $\langle uvw \rangle$

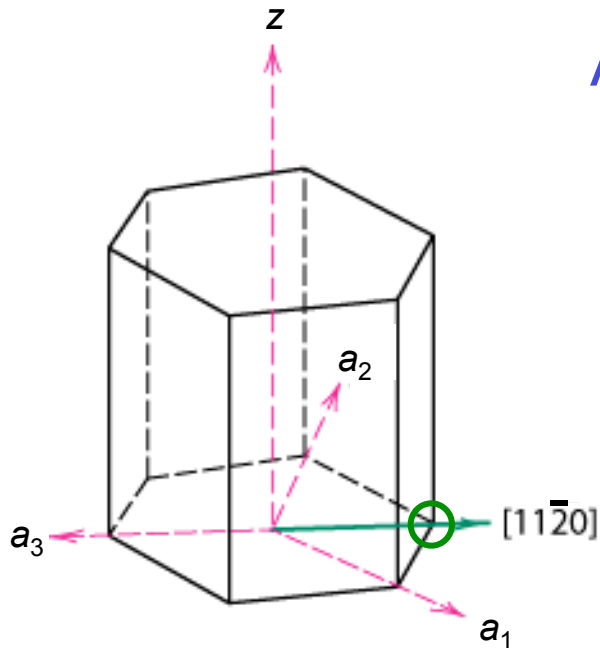


Examples

Sketch the following directions : $[110]$, $[-1-21]$, $[-1\ 0\ 2]$



HCP Crystallographic Directions

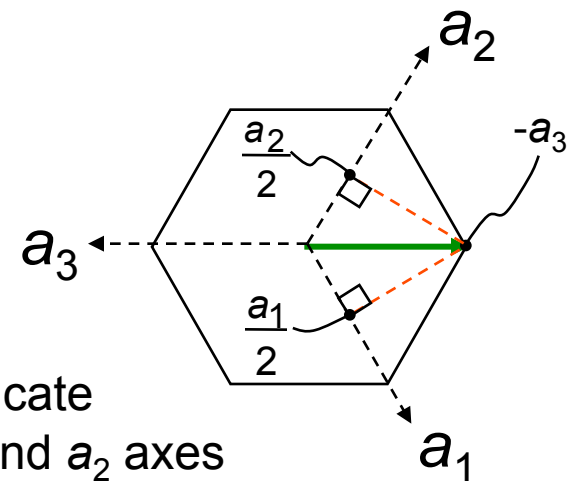


Adapted from Fig. 3.8(a), Callister 7e.

ex: $\frac{1}{2}, \frac{1}{2}, -1, 0$

$\Rightarrow [11\bar{2}0]$

dashed red lines indicate
projections onto a_1 and a_2 axes



HCP Crystallographic Directions

- Hexagonal Crystals
 - 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $u'v'w'$) as follows.

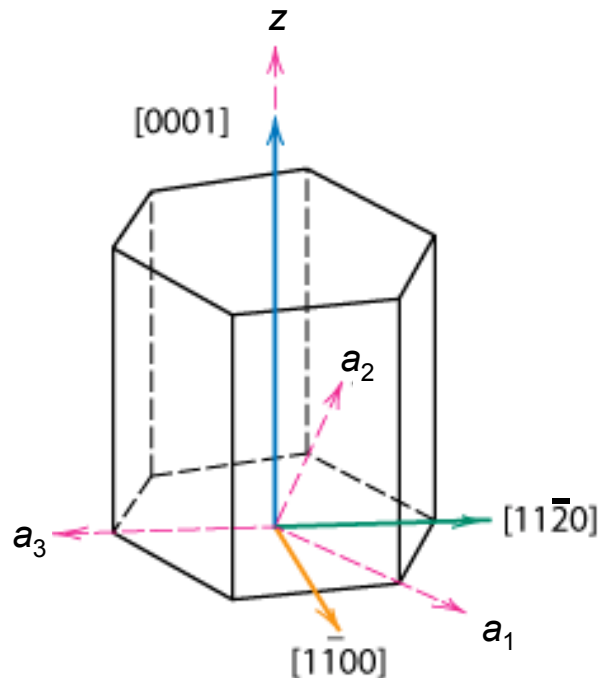


Fig. 3.8(a), Callister 7e.

$$[u'v'w'] \rightarrow [uvtw]$$

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

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

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

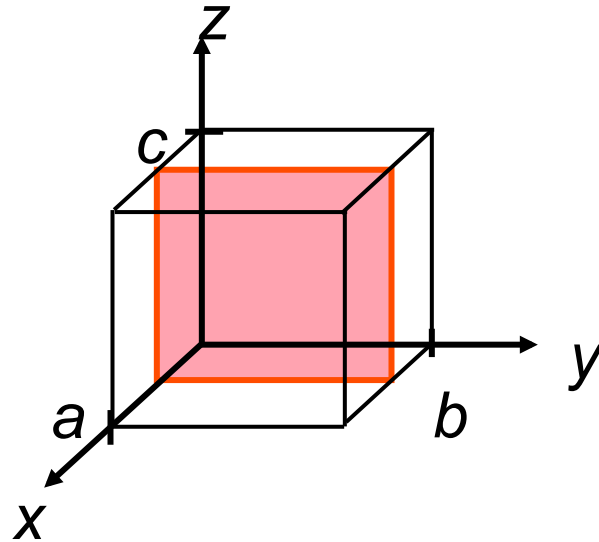
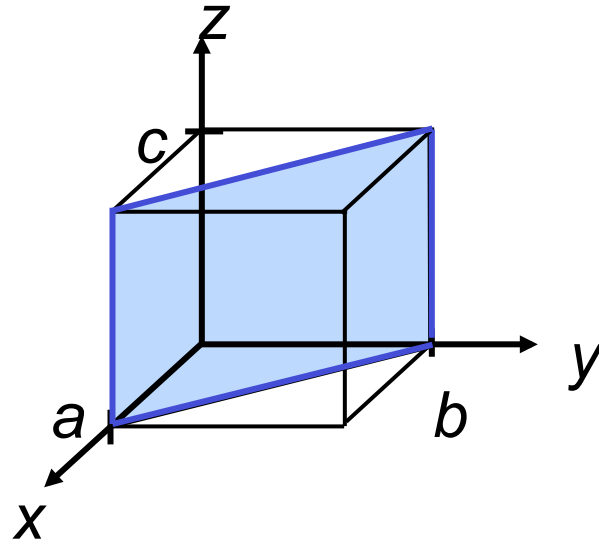
$$w = w'$$

Crystallographic Planes

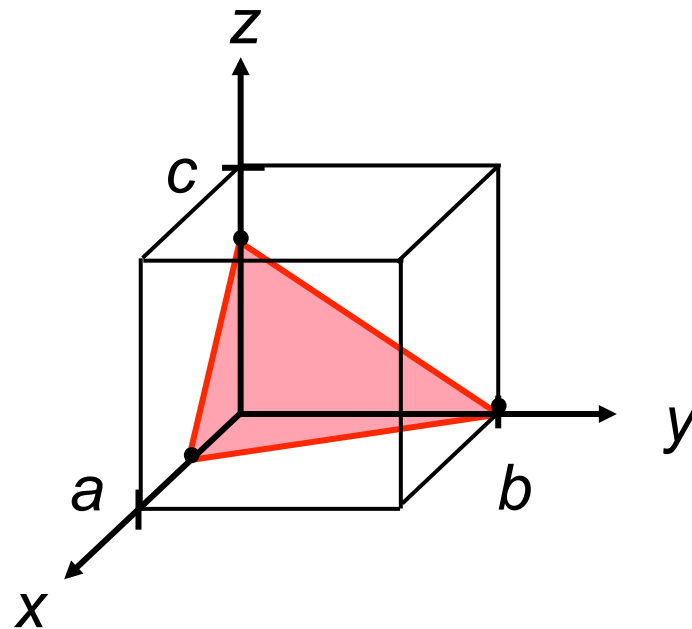
- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.
- Algorithm
 1. Read off intercepts of plane with axes in terms of a , b , c
 2. Take reciprocals of intercepts
 3. Reduce to smallest integer values
 4. Enclose in parentheses, no commas i.e., (hkl)



Crystallographic Planes



Crystallographic Planes



Crystallographic planes (*continued*)

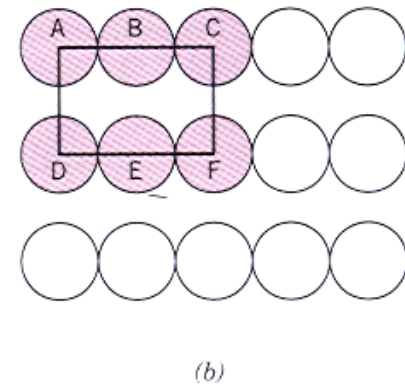
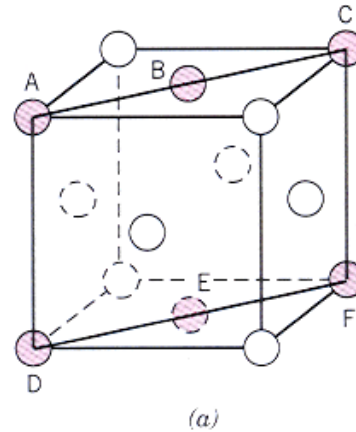
- Construct planes by Miller indices of planes $(0 \ -1 \ -1)$ and $(1 \ 1 \ -2)$



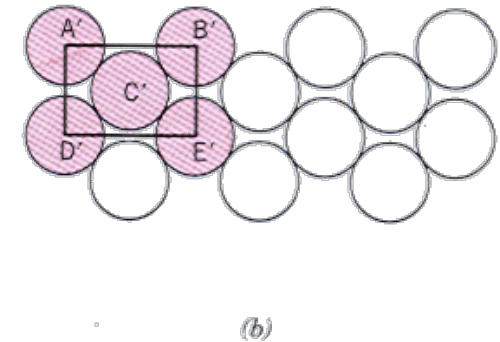
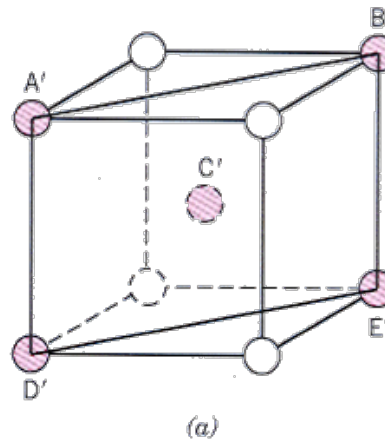
Atomic arrangements

- The atomic arrangement for a crystallographic plane depends on the crystal structure

FCC: (a) reduced sphere
(b) atomic packing of an FCC (110) plane



BCC: (a) reduced sphere
(b) atomic packing of an BCC (110) plane



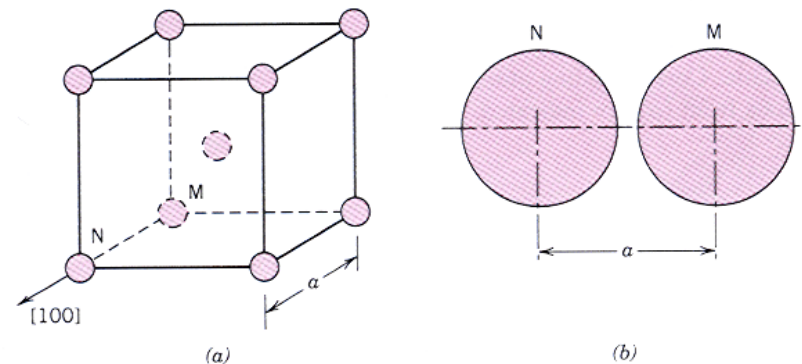
Atomic arrangements

- A family of planes contains all the planes that are crystallographically equivalent.
- In cubic system, planes with same indices, irrespective of order and sign, are equivalent
 - (111) , $(\bar{1}\bar{1}\bar{1})$, $(11\bar{1})$... belong to $\{111\}$ family
 - $(\bar{1}00)$, (100) , (010) , and (001) belong to $\{100\}$ family
 - (123) , $(1\bar{2}\bar{3})$, (312) in cubic crystals belong to $\{123\}$ family
- In tetragonal, (001) $(00\bar{1})$ are not as same family as (100) , $(\bar{1}00)$



Linear and planar atomic density

- Linear Density of Atoms $\equiv LD = \frac{\text{Number of atoms}}{\text{Unit length of direction vector}}$



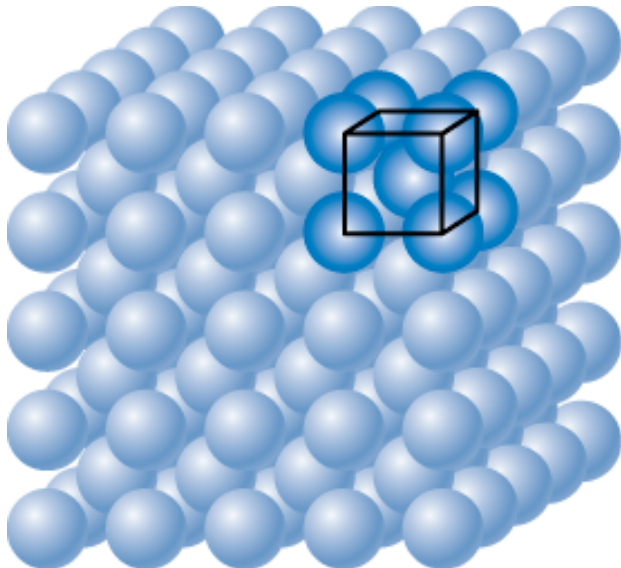
- Atomic planar density: number of atoms centered on a plane/area of plane**

$$\text{Planar Density} = \frac{\text{\#atoms}}{\text{Area(2D repeat unit)}}$$

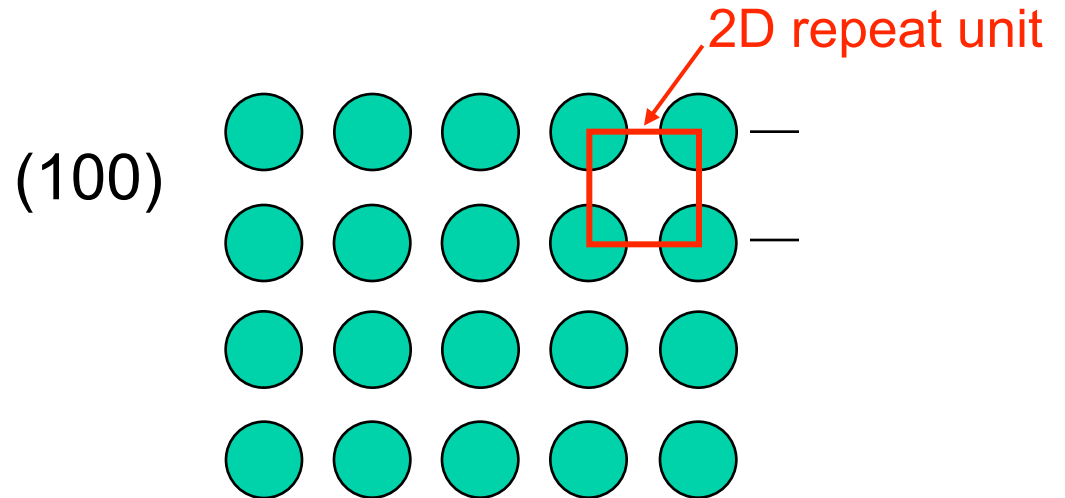


Planar Density of (100) Iron

Solution: At $T < 912^{\circ}\text{C}$ iron has the BCC structure.

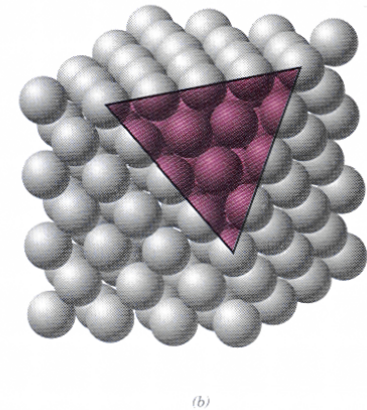
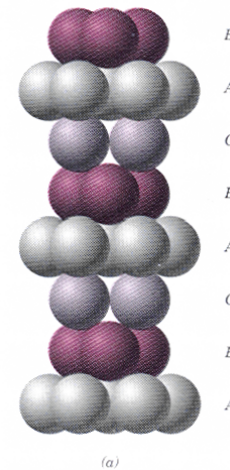
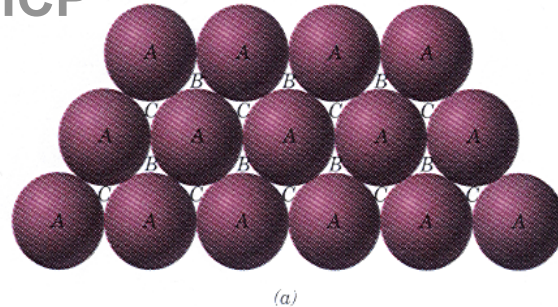


Adapted from Fig. 3.2(c), *Callister 7e*.



Close-packed crystal structures

Close-packed plane stacking sequence for HCP



Close-packed plane stacking sequence for HCP

