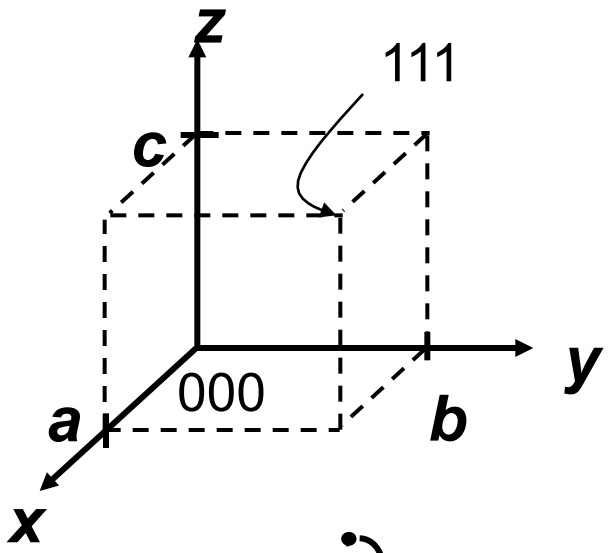
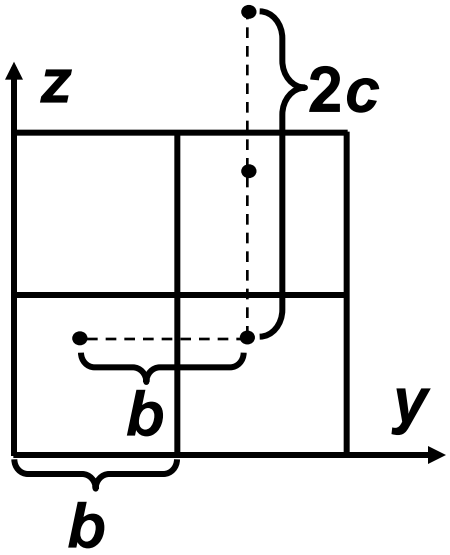
Crystallographic directions and planes

Outline

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

Point Coordinates





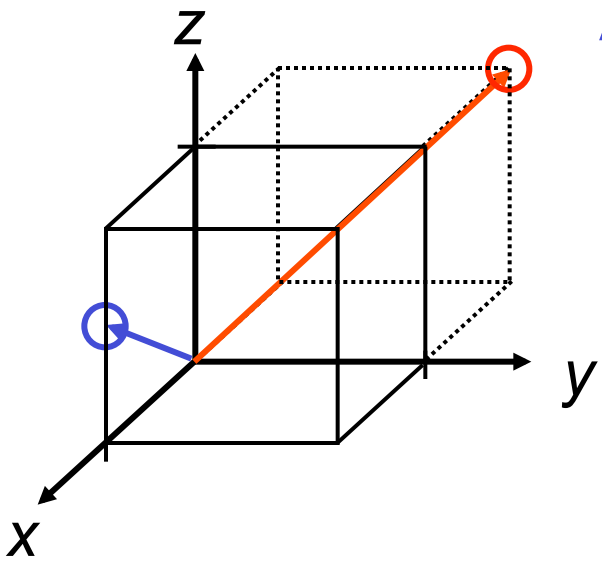
Point coordinates for unit cell center are

a/2, *b*/2, *c*/2 ½ ½ ½

Point coordinates for unit cell corner are 111

Translation: integer multiple of lattice constants → 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, ½ => 2, 0, 1 => [201]

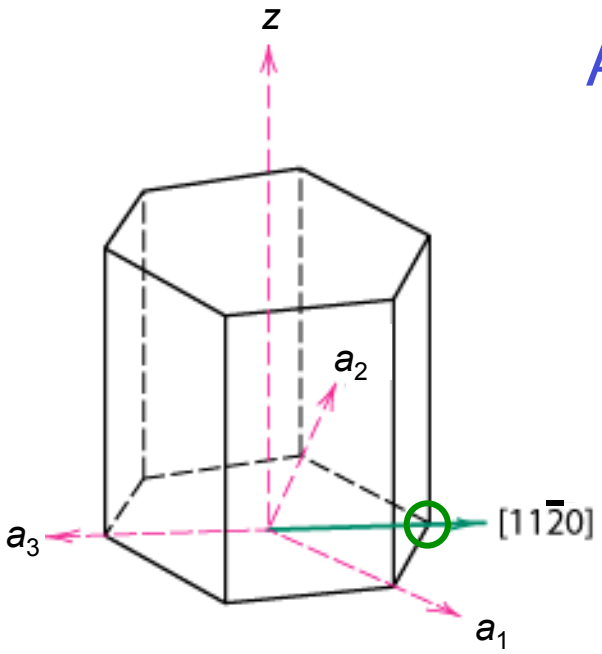
-1, 1, 1 => $[\bar{1}11]$ where overbar represents a negative index

families of directions <*uvw*>

Examples

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

HCP Crystallographic Directions



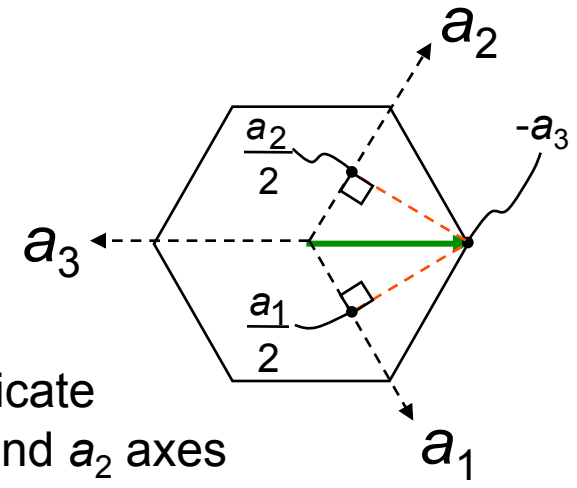
Adapted from Fig. 3.8(a), *Callister 7e.*

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1, a_2, a_3, or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

[*uvtw*]

ex: ½, ½, -1, 0 => [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.

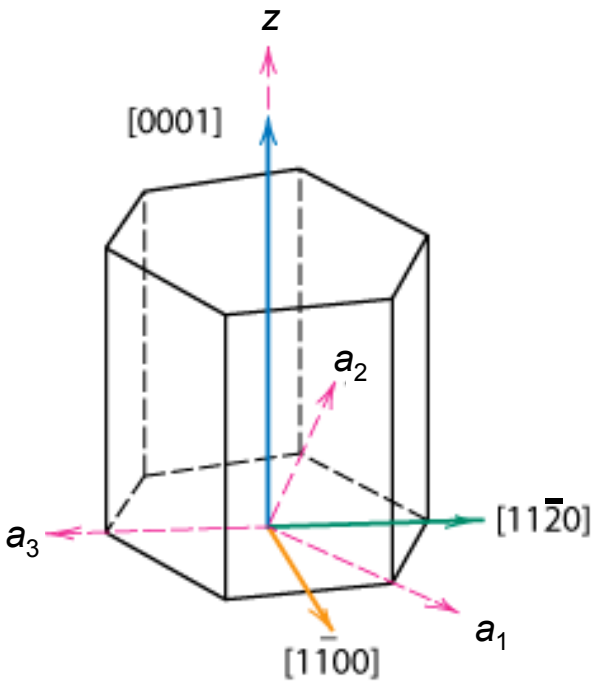


Fig. 3.8(a), *Callister 7e.*

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

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

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

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

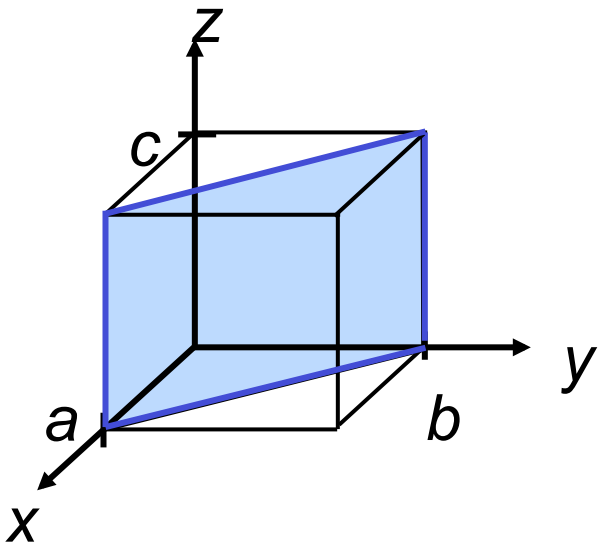
$$w = w'$$

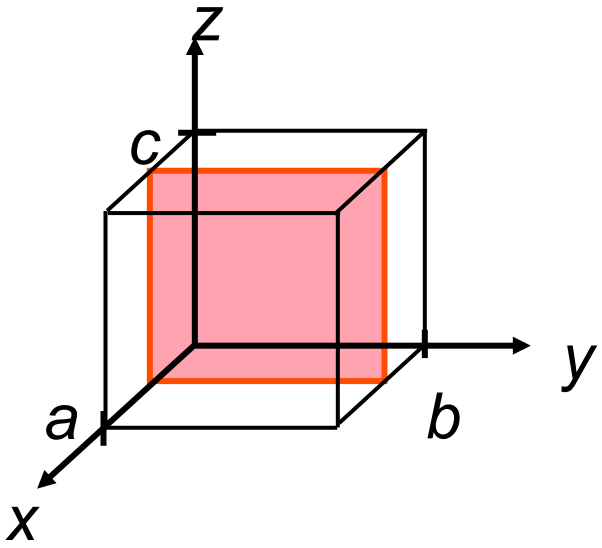
Crystallographic Planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

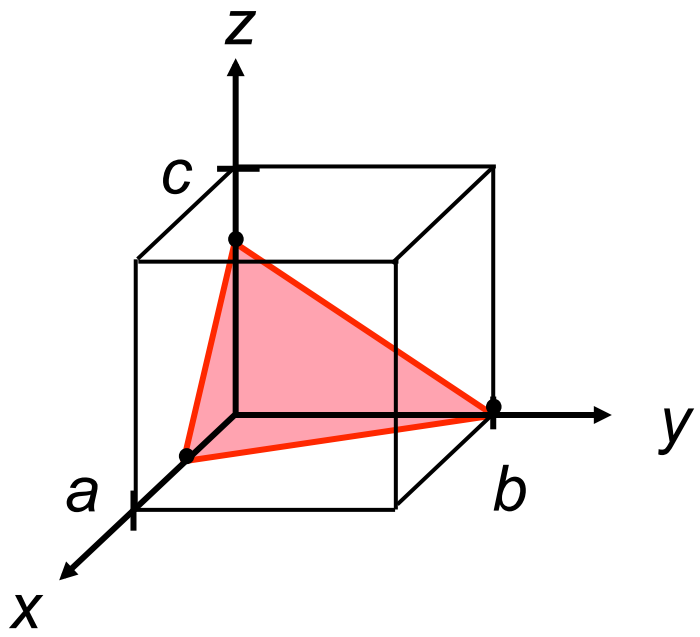
- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

Crystallographic Planes





Crystallographic Planes



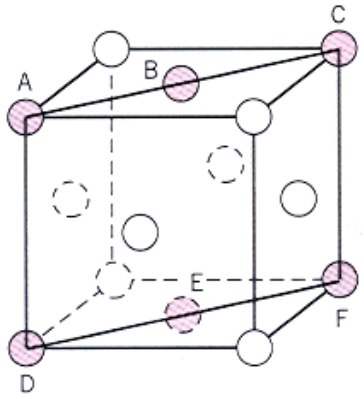
Crystallographic planes (*continued*)

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

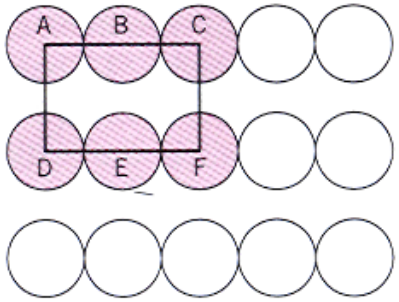
Atomic arrangements

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

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

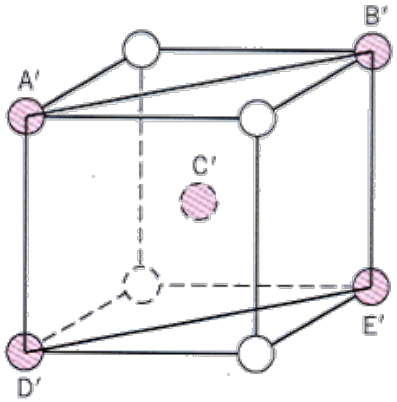


(a)

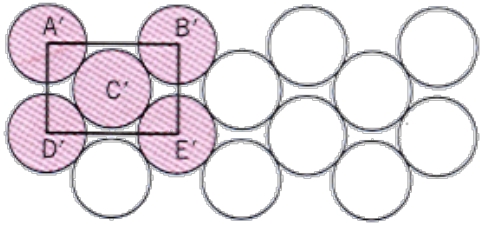


(b)

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



(a)



(b)

Atomic arrangements

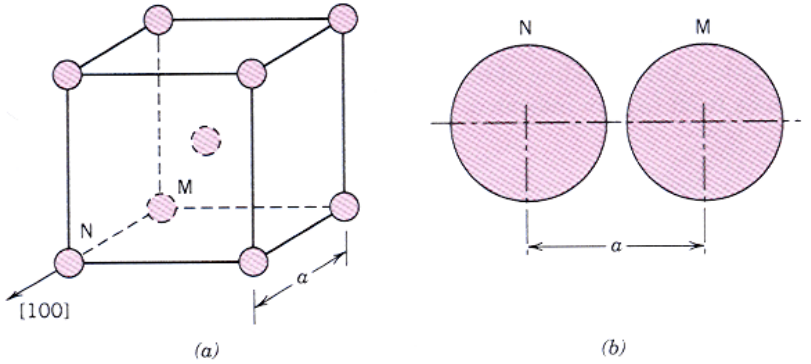
- **A family of planes contains all the planes that are crystallographically equivalent.**

- **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), $(1\bar{2}3)$, $(312\bar{)}$ 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 ≡ LD = $\frac{\text{Number of atoms}}{\text{Unit length of direction vector}}$

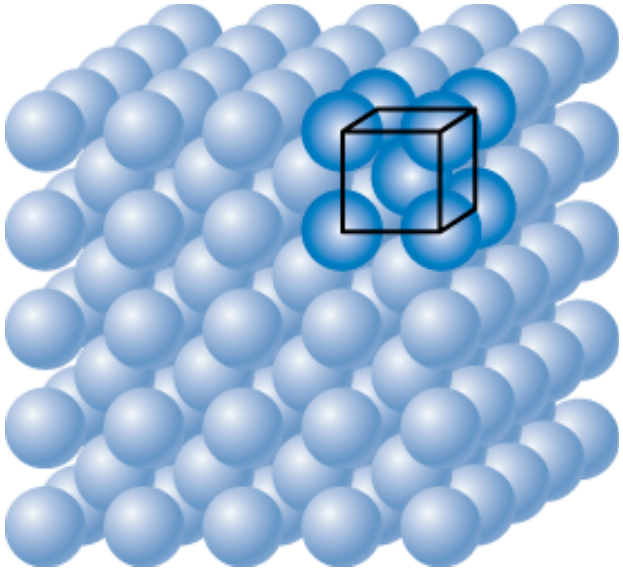


- **Atomic planar density: number of atoms centered on a plane/area of plane**

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

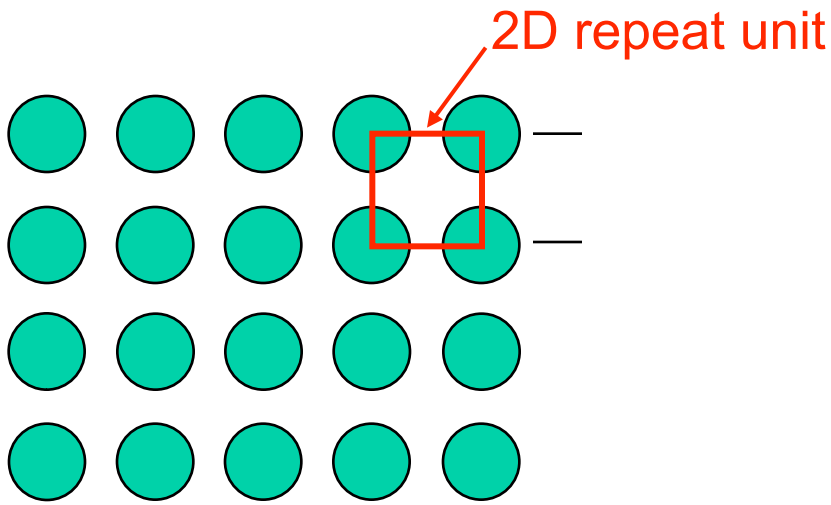
Planar Density of (100) Iron

Solution: At T < 912°C iron has the BCC structure.



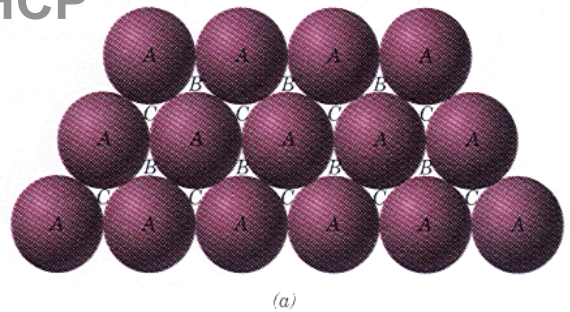
Adapted from Fig. 3.2(c), *Callister 7e.*

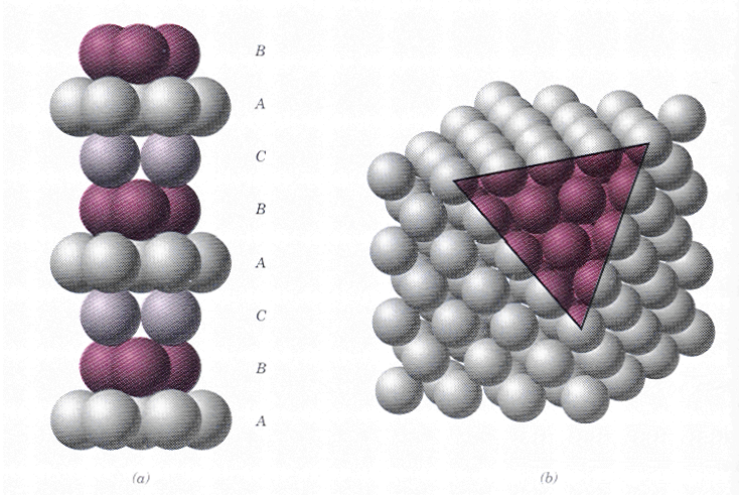
(100)



Close-packed crystal structures

Close-packed plane stacking sequence for HCP





Close-packed plane stacking sequence for HCP