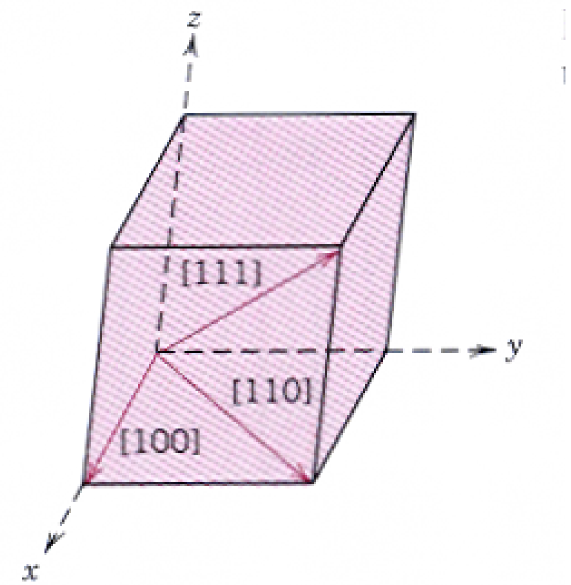
Chapter 3: Crystallographic directions and planes

Outline

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

Crystallographic directions

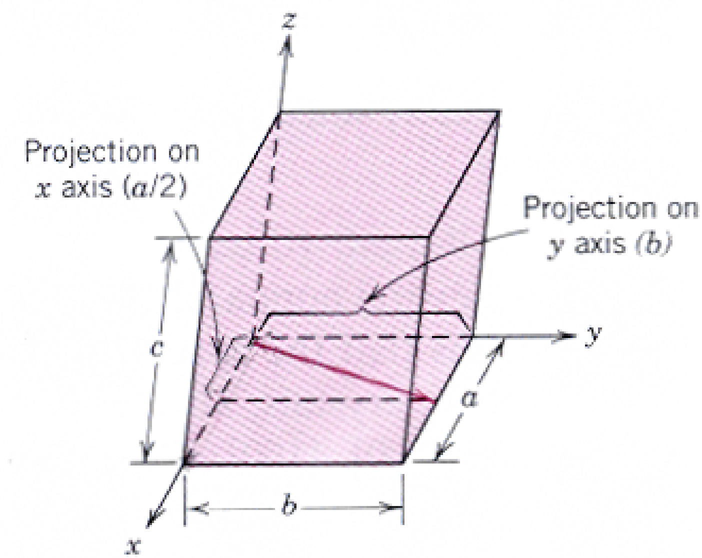
- Direction: a line between two points and a vector
- General rules for defining a crystallographic direction
  - pass through the origin of a coordinate system
  - determine length of the vector projection in the unit cell dimensions a, b, and c
  - remove the units $[u_a\ v_b\ w_c]$---[uvw] e.g [2a 3b 5c]--[2 3 5]
  - uvw are multiplied and divided by a common factor to reduce them to smallest integer values



Crystallographic directions (continue)

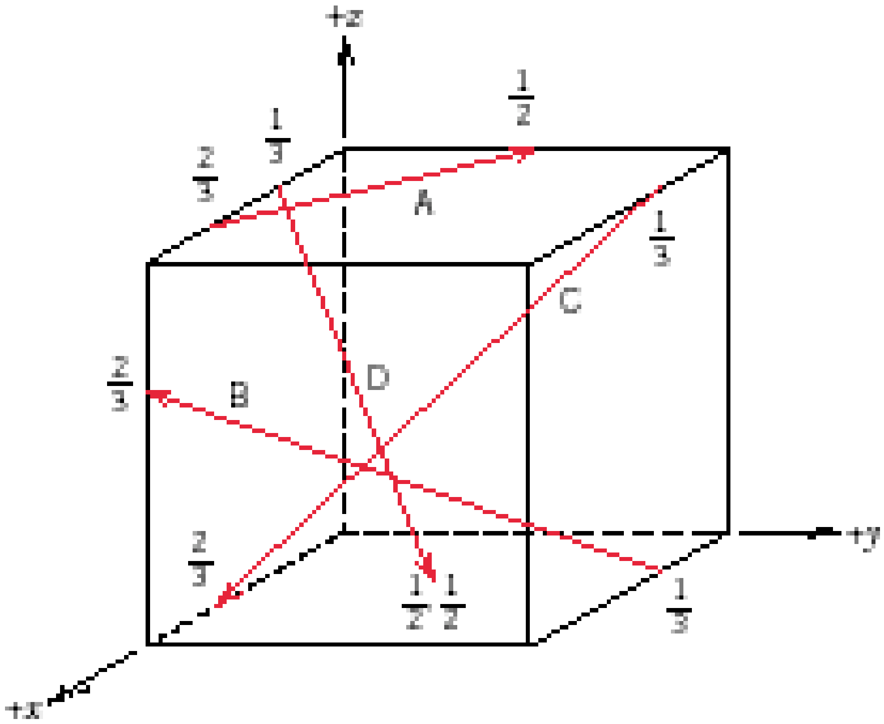
- denote the direction by [uvw]
- family direction <u v w>, defined by transformation
- material properties along any direction in a family are the same, e.g. [100] [100] [010] in simple cubic are same.
- for uniform crystal materials, all parallel directions have the same properties
- negative index: a bar over the index

Determine a direction



Examples

Determining the indices of line directions

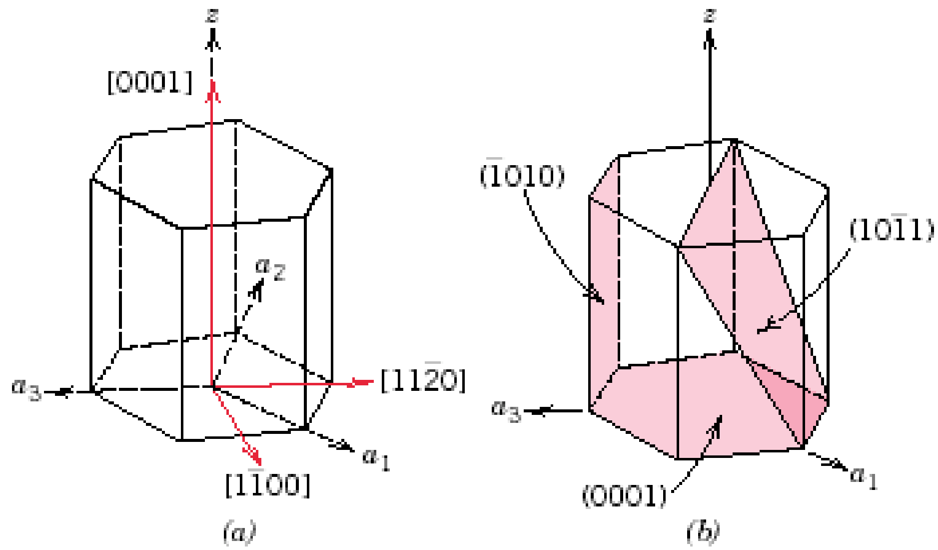


Examples

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

Hexagonal crystal

- 4-index, or Miller-Bravais coordinate system



- Conversion from 3-index index system

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

is accomplished by the following formulas:

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

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

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

$$w = nw'$$

Hexagonal crystal (continue)

- **Convert [100] direction into the four- index Miller-Bravais scheme for hexagonal unit cells.**

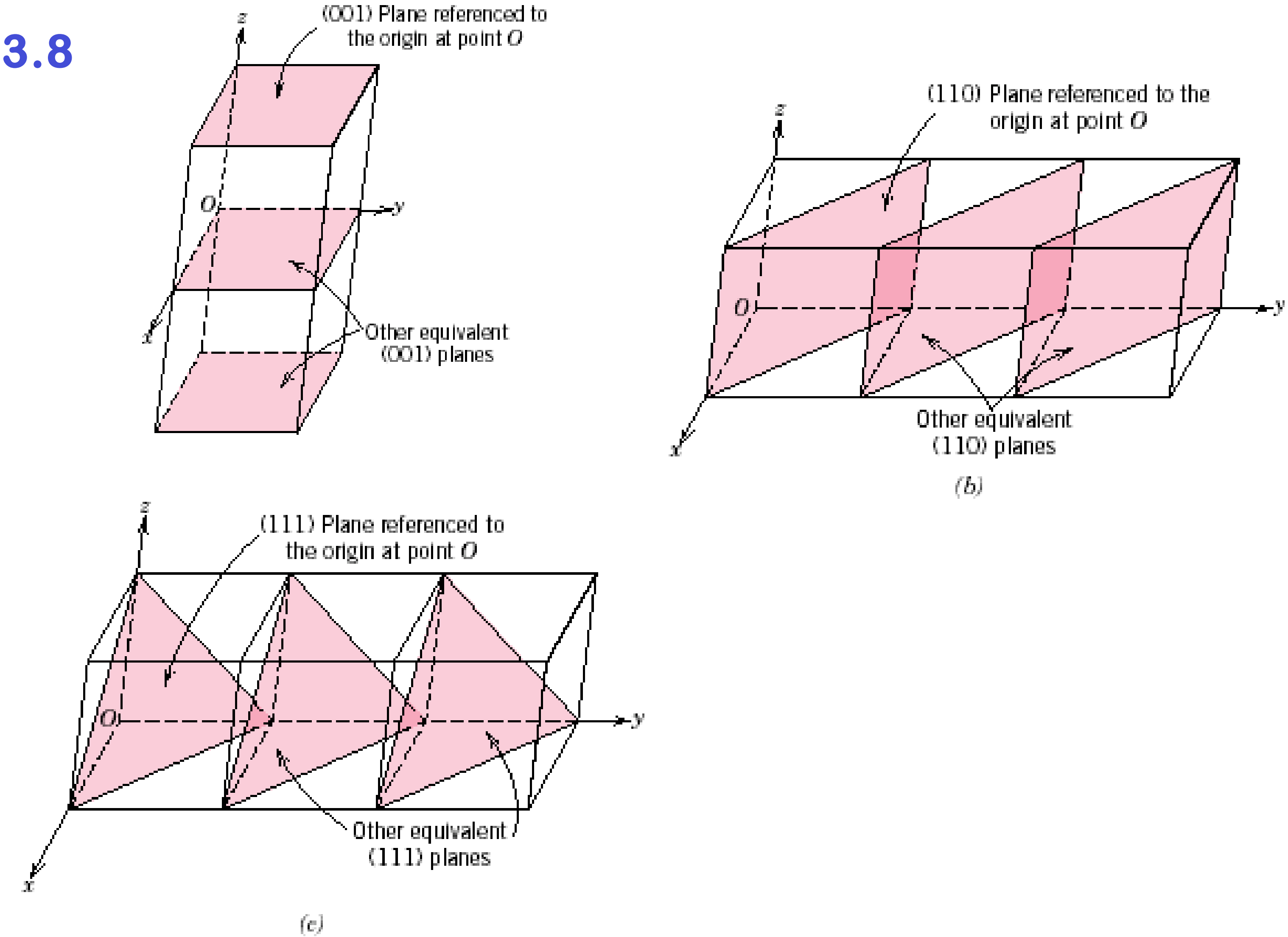
Crystallographic planes

- Orientation representation (hkl)--Miller indices
- Parallel planes have same miller indices
- Determine (hkl)
  - A plane can not pass the chosen origin
  - A plane must intersect or parallel any axis
  - If the above is not met, translation of the plane or origin is needed
  - Get the intercepts a, b, c. (infinite if the plane is parallel to an axis)
  - take the reciprocal
  - smallest integer rule
- (hkl) // $(\bar{h}\bar{k}\bar{l})$ in opposite side of the origin
- For cubic only, plane orientations and directions with same

  indices are perpendicular to one another

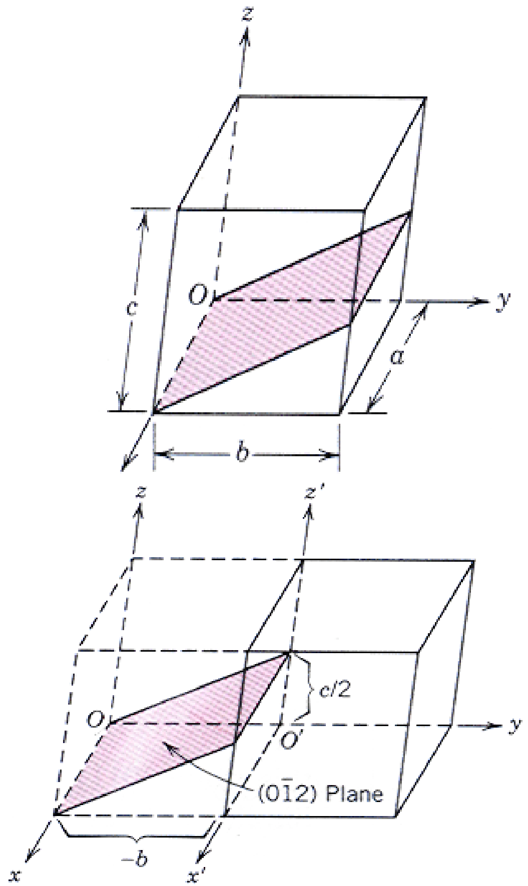
Crystallographic planes (*continue*)

Figure 3.8



Crystallographic planes (*continue*)

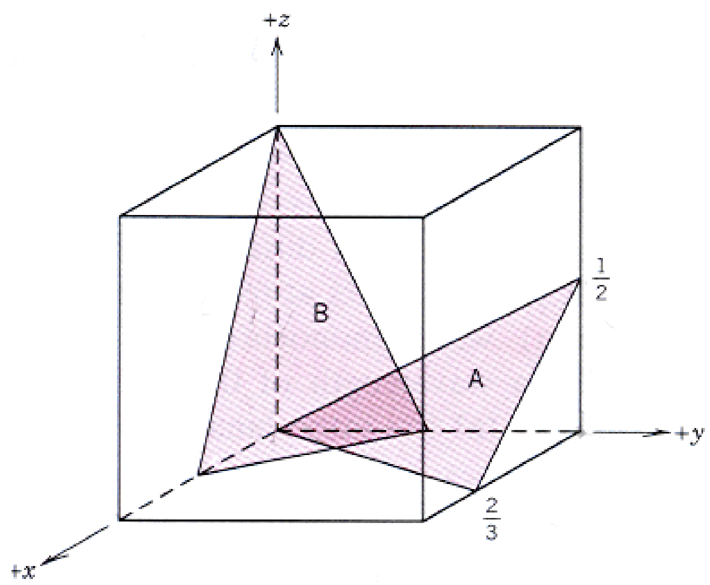
- Determine Miller indices of planes



(b)

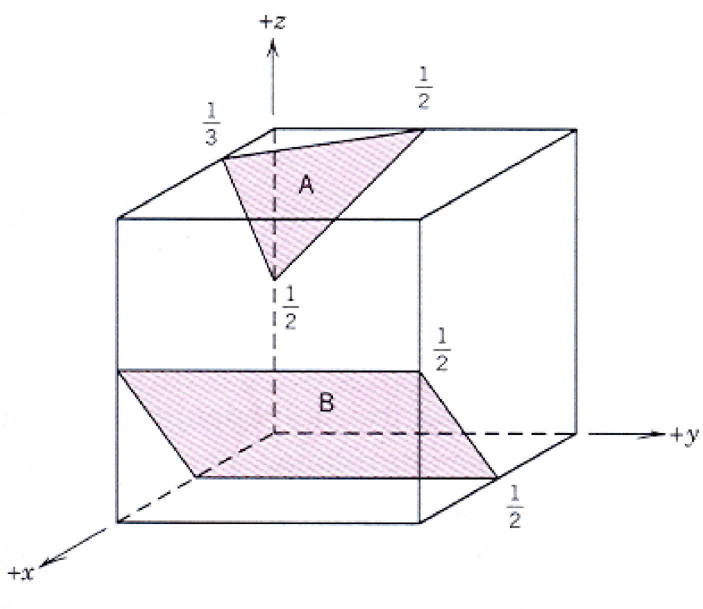
Crystallographic planes (*continue*)

- Determine Miller indices of planes



Crystallographic planes (*continue*)

- **Determine Miller indices of planes**



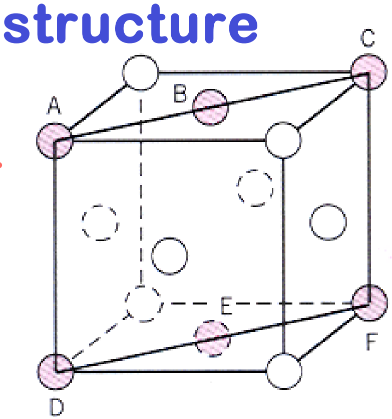
Crystallographic planes (*continue*)

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

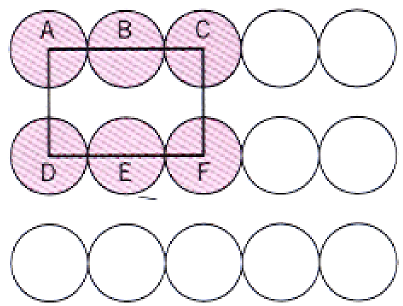
Atomic arrangements

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

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

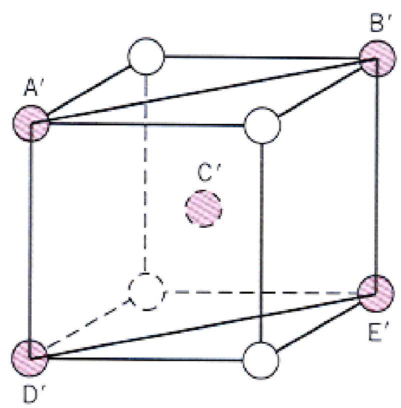


(a)

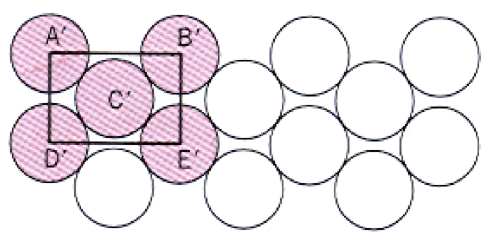


(b)

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), $(\bar{1}\bar{1}1)$, $(\bar{1}11)$ … belong to {111} family**
  - **$(\bar{1}00)$, (100), (010), and (001) belong to {100} family**
  - **(123), $(\bar{1}23)$, $(\bar{3}12)$ in cubic crystals belong to {123} family**

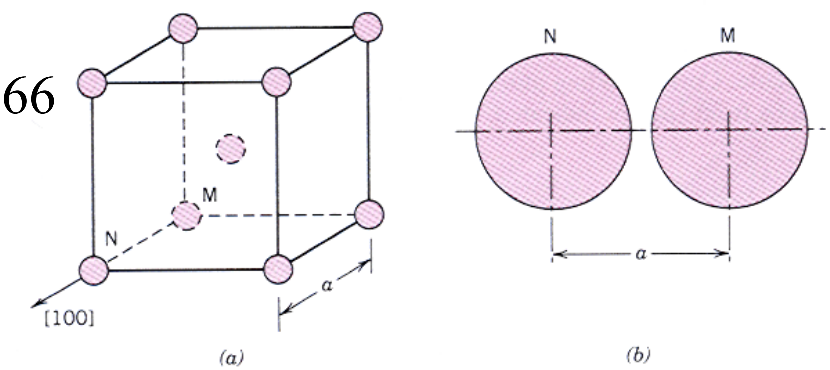
- **In tetragonal, (001) $(00\bar{1})$ are not as same family as (100), $(\bar{1}00)$**

Linear and planar atomic density

- **Linear atomic density: length of intersected atoms/length of edges in a unit cell**

$$LD_{[100]} = \frac{L_{atoms}}{L_{MN}} = \frac{2R}{4R/\sqrt{3}} = 0.866$$

$$LD_{[111]} = 1$$

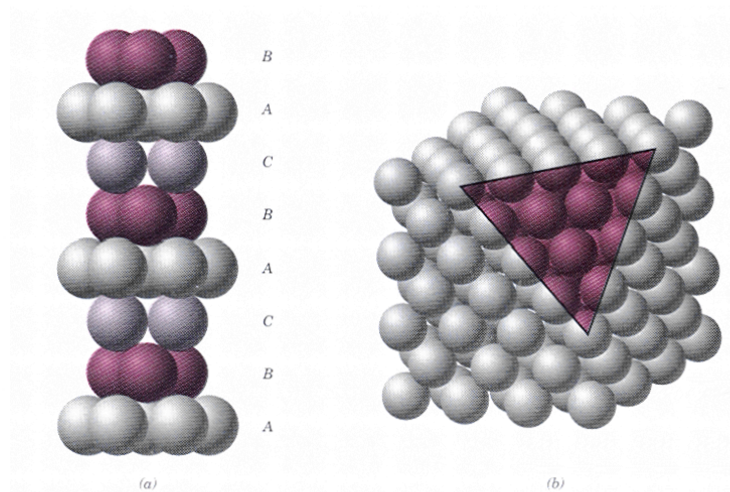


- **Atomic planar density: area occupied by atoms/total area of a crystallographic plane**

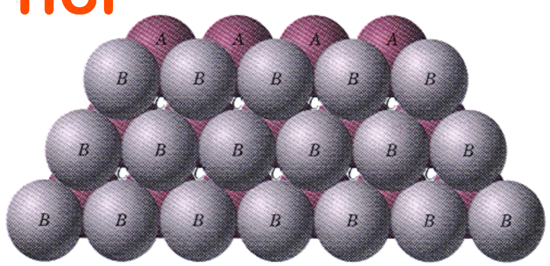
Close-packed crystal structures

Close-packed plane stacking sequence for HCP

(a)



Close-packed plane stacking sequence for HCP



(b)