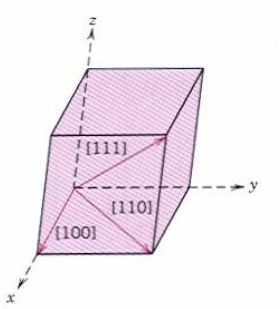
Chapter 3: Crystallographic directions and planes

Outline

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

Crystallographic directions

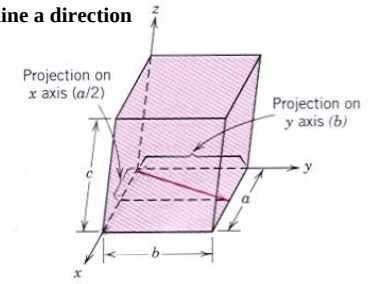
- **Direction: a line between two points and a vector**
- **General rules for defining a crystallographic direction**
  - **pass through the origin of a coordinate system**
  - **determine length of the vector projection in the unit cell dimensions a, b, and c**
  - **remove the units [u_a v_b w_c]---[uvw] 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)

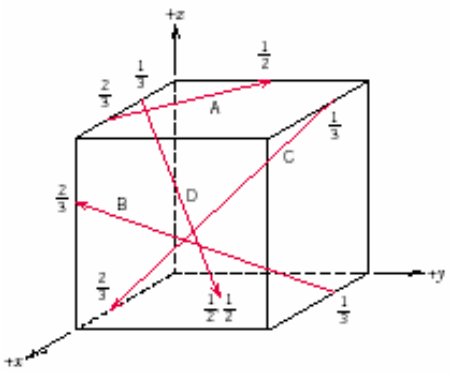
- **denote the direction by [uvw]**
- **family direction <u v w>, defined by transformation**
- **material properties along any direction in a family are the same, e.g. [100] [100] [010] in simple cubic are same.**
- **for uniform crystal materials, all parallel directions have the same properties**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

Determine a direction



Examples

Determining the indices of line directions

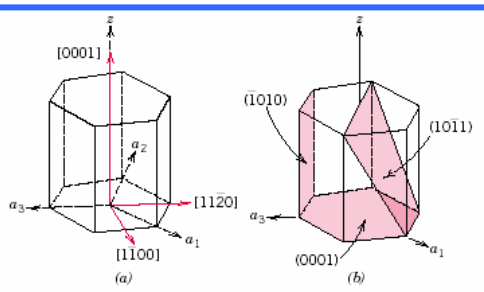


Examples

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

Hexagonal crystal

- **4-index, or Miller-Bravais, coordinate system**



- **Conversion from 3-index to 4-index system**

Hexagonal crystal (continue)

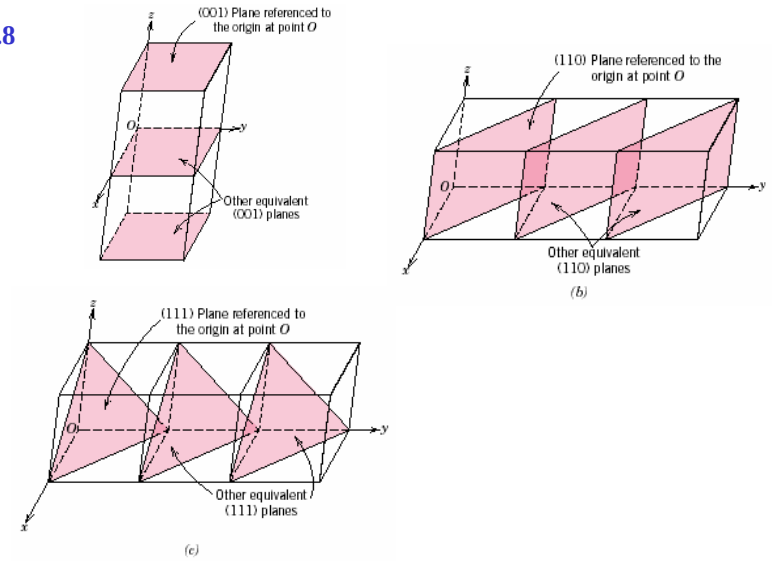
- Convert [100] direction into the four- index Miller-Bravais scheme for hexagonal unit cells.

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

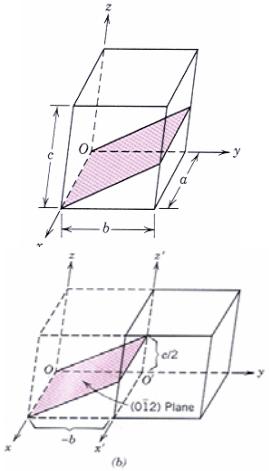
Crystallographic planes (*continue*)

Figure 3.8



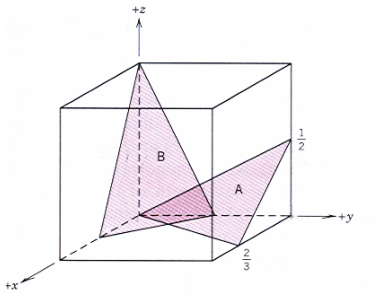
Crystallographic planes (*continue*)

- **Determine Miller indices of planes**



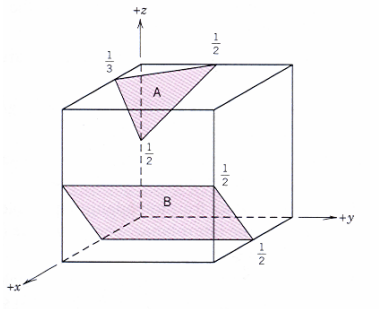
Crystallographic planes (*continue*)

- **Determine Miller indices of planes**



Crystallographic planes (*continue*)

- **Determine Miller indices of planes**



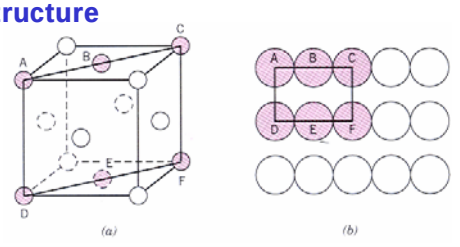
Crystallographic planes (*continue*)

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

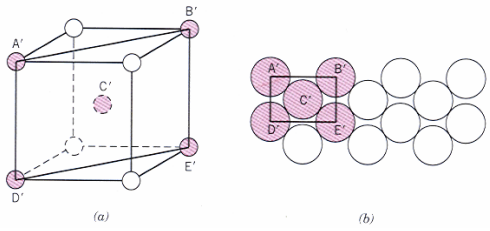
Atomic arrangements

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

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



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

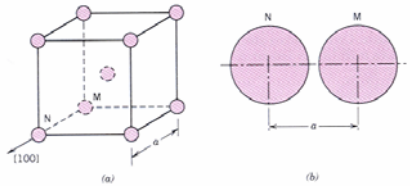


Atomic arrangements

- 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), $(\bar{1}\bar{1}1)$, $(\bar{1}11)$ ... 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

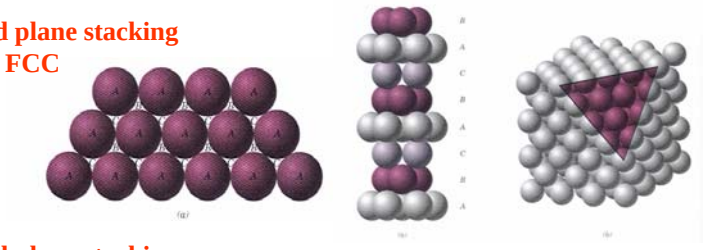
- Linear atomic density: number of atoms centered on a direction vector / length of direction vector



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

Close-packed crystal structures

Close-packed plane stacking sequence for FCC



Close-packed plane stacking sequence for HCP