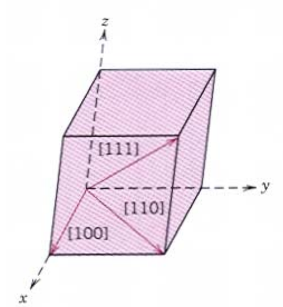
Chapter 3: Crystallographic directions and planes

Outline

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

Crystallographic directions

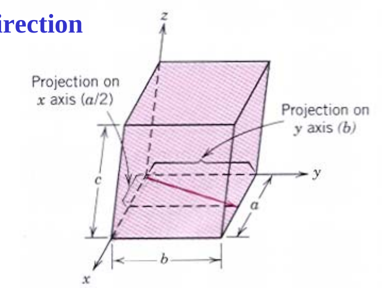
- **Direction: a line between two points and a vector**
- **General rules for defining a crystallographic direction**
  - **pass through the origin of a coordinate system**
  - **determine length of the vector projection in the unit cell dimensions a, b, and c**
  - **remove the units [u_a v_b w_c]---[uvw]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

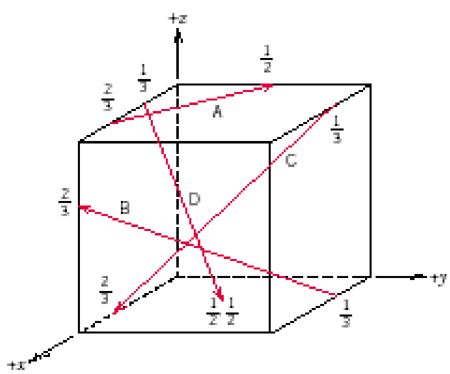
- denote the direction by [uvw]
- family direction <u v w>, defined by transformation
- material properties along any direction in a family are the same, e.g. [100],[010],[001] in simple cubic are same.
- for uniform crystal materials, all parallel directions have the same properties
- negative index: a bar over the index

Determine a direction



Examples

Determine the indices of line directions



Examples

Sketch the following directions : $[110]$, $[\bar{1}\bar{2}1]$, $[\bar{1}02]$

Hexagonal crystal

- **4-index, or Miller-Bravais, coordinate system**
- **Conversion from 3-index to 4-index system**

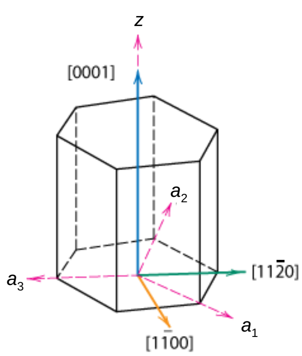


Fig. 3.8(a), *Callister 7e.*

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

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

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

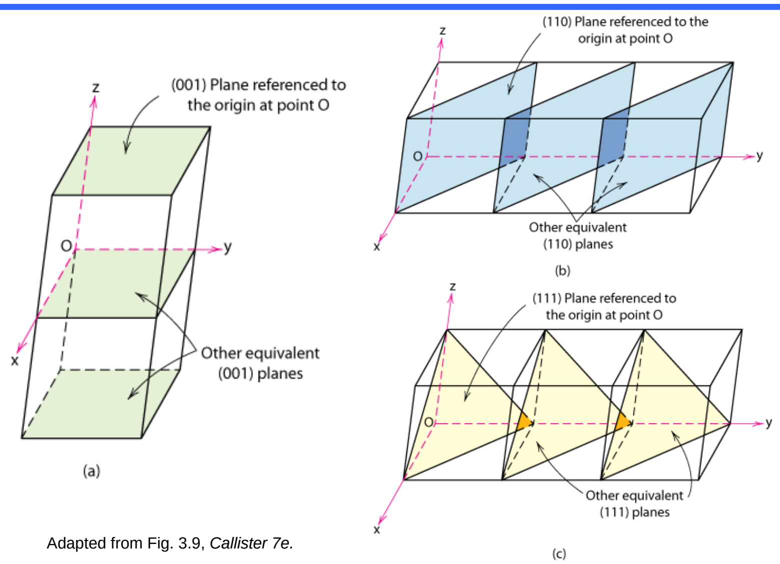
$$t = -(u + v)$$

$$w = w'$$

Crystallographic planes

- 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) // (hk$\bar{l}$) in opposite side of the origin
- For cubic only, plane orientations and directions with same
- indices are perpendicular to one another

Crystallographic planes (*continue*)

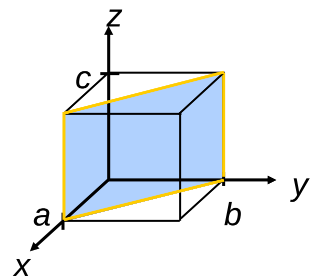


Adapted from Fig. 3.9, *Callister 7e.*

Crystallographic planes (*continue*)

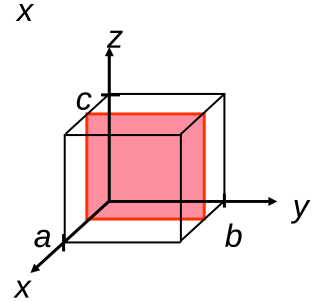
Example

		a	b	c
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		



Example

		a	b	c
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		

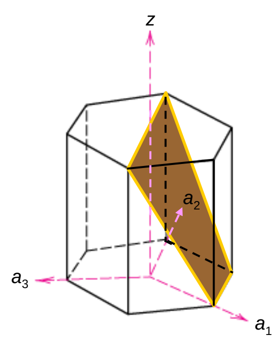


Crystallographic planes (*continue*)

In hexagonal unit cells the same idea is used

Example

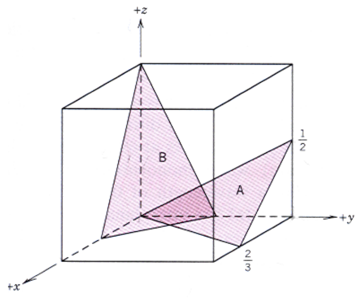
		a_1	a_2	a_3	c
1.	Intercepts	1	∞	-1	1
2.	Reciprocals	1	1/∞	-1	1
		1	0	-1	1
3.	Reduction	1	0	-1	1
4.	Miller-Bravais Indices	$(10\bar{1}1)$			



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

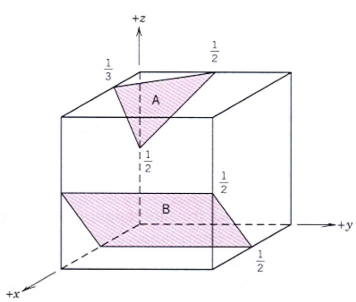
Crystallographic planes (*continue*)

- Determine Miller indices of planes



Crystallographic planes (*continue*)

- Determine Miller indices of planes



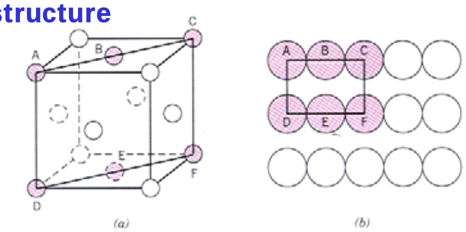
Crystallographic planes (*continue*)

- **Construct planes by Miller indices of planes $(0\ \bar{1}\ \bar{1})$ and $(1\ 1\ \bar{2})$**

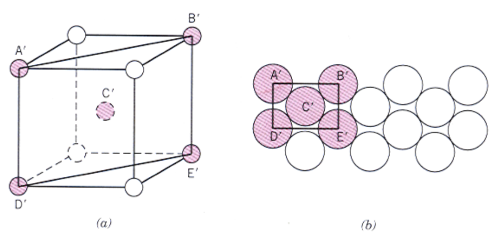
Atomic arrangements

- **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), ($\bar{1}\bar{1}\bar{1}$), ($\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), (100)**

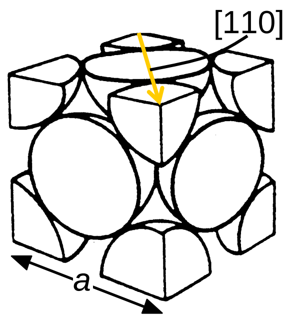
Linear and planar atomic density

- Linear Density of Atoms ≡ LD = $\dfrac{\text{\#atoms}}{\text{Unit length of direction vector}}$

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

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

Linear density (example)



Linear density of Al in [110] direction

a = 0.405 nm

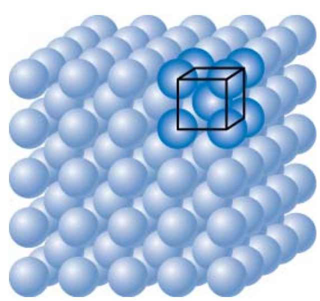
atoms

$$LD = \frac{2}{\sqrt{2}a} = 3.5\ nm^{-1}$$

length

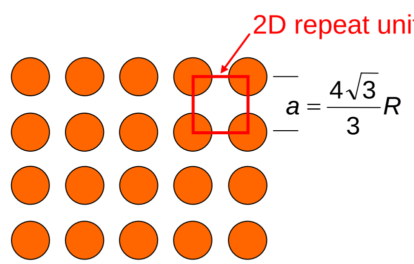
Planar Density of (100) Iron

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



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

(100)



$$a = \frac{4\sqrt{3}}{3}R$$

Radius of iron R = 0.1241 nm

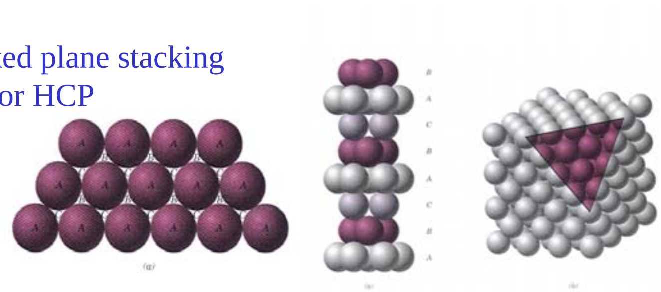
atoms / 2D repeat unit

area / 2D repeat unit

$$\text{Planar Density} = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2} = 12.1\ \frac{\text{atoms}}{\text{nm}^2} = 1.2 \times 10^{19}\ \frac{\text{atoms}}{\text{m}^2}$$

Close-packed crystal structures

- Close-packed plane stacking sequence for HCP



- Close-packed plane stacking sequence for HCP