

Materials Science

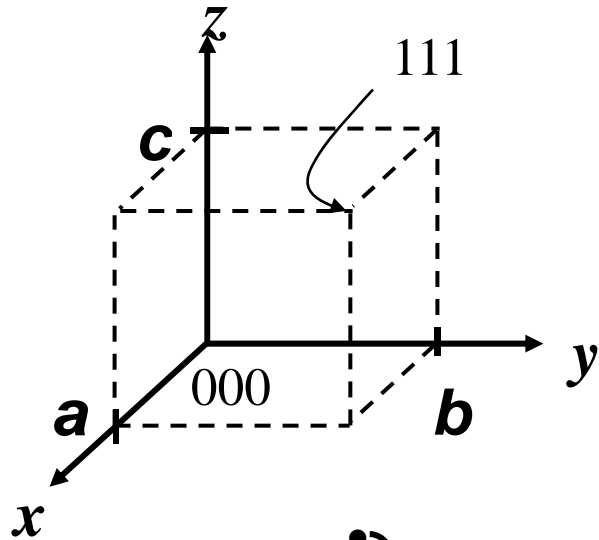
ME 274

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Crystallographic Points, Directions & Planes

- When dealing with crystalline materials, it is often necessary to specify a particular point within the unit cell, a crystallographic direction, or some crystallographic plane of atoms.
- Labeling conventions have been established in which three numbers or indices are used to designate point locations, directions, and planes.
- The basis for determining index values is the unit cell, with a right-handed coordinate system consisting of three (x, y, and z) axes situated at one of the corners and coinciding with the unit cell edges.
- For some crystal systems, the three axes are not mutually perpendicular, e.g. hexagonal, rhombohedral, monoclinic and triclinic.

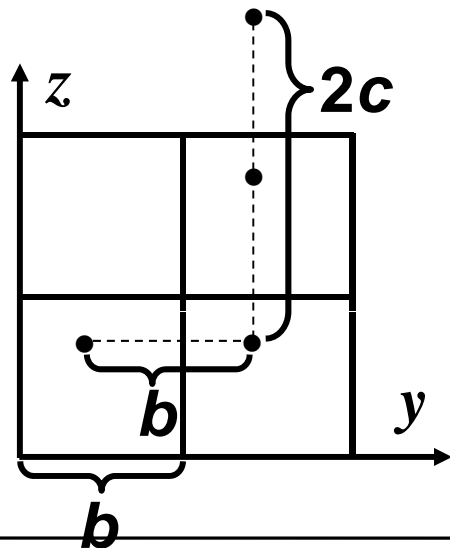
Crystallographic Points, Directions & Planes



Point coordinates for unit cell center are

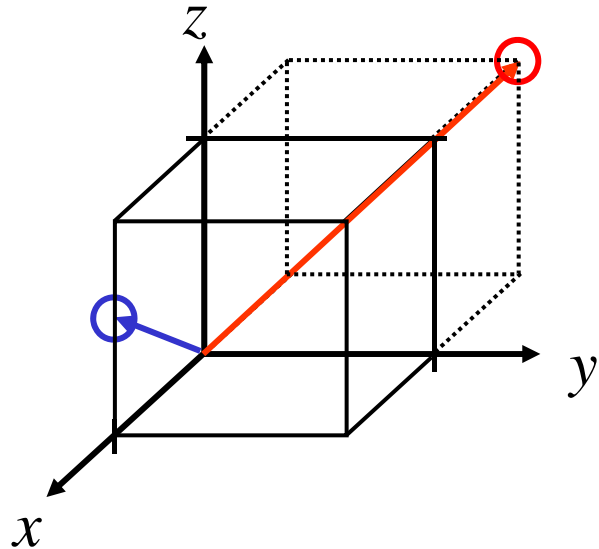
$$a/2, b/2, c/2 \quad \frac{1}{2} \frac{1}{2} \frac{1}{2}$$

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

$[uvw]$

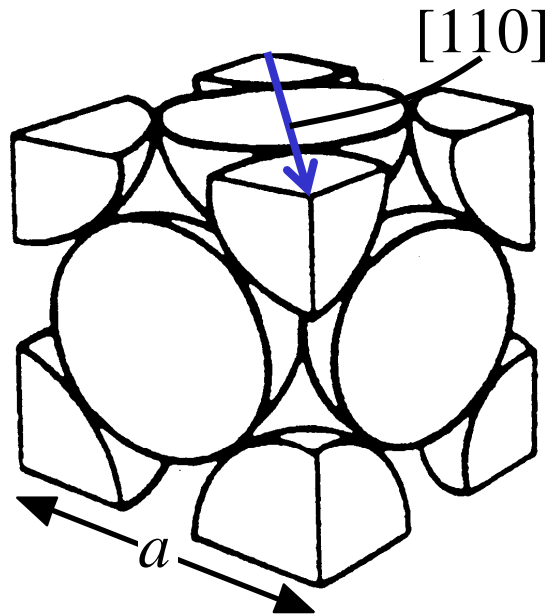
ex: $1, 0, \frac{1}{2} \Rightarrow 2, 0, 1 \Rightarrow [201]$

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

families of directions $\langle uvw \rangle$

Linear Density

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

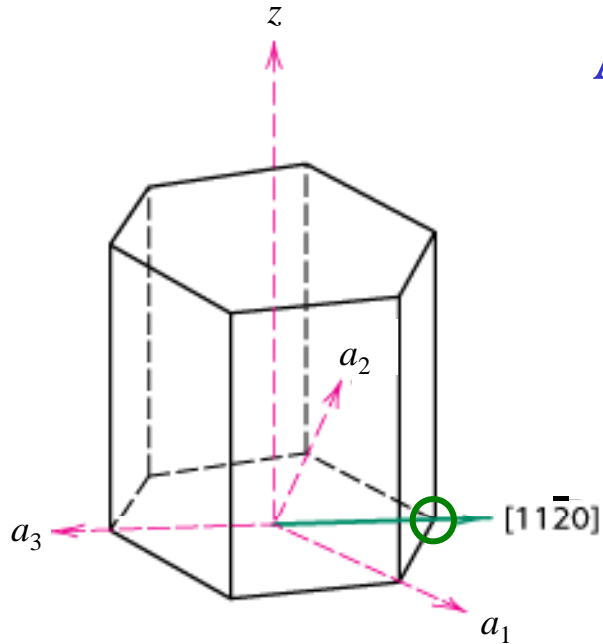


ex: linear density of Al in [110] direction

$$a = 0.405 \text{ nm}$$

$$LD = \frac{\text{\# atoms}}{\text{length}} = \frac{2}{\sqrt{2}a} = 3.5 \text{ nm}^{-1}$$

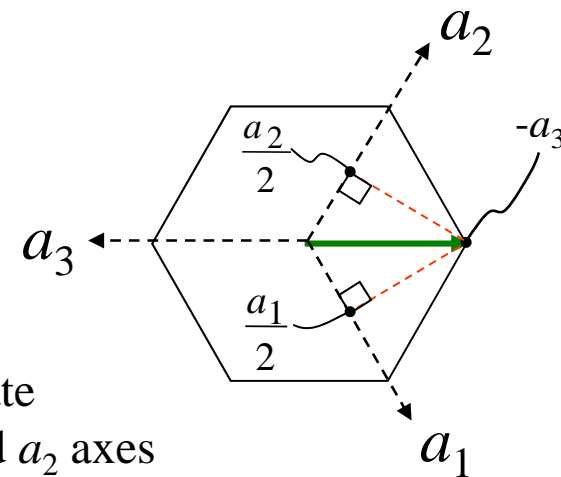
HCP Crystallographic Directions



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



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

$$[uvw]$$

HCP Crystallographic Directions

- Hexagonal Crystals

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

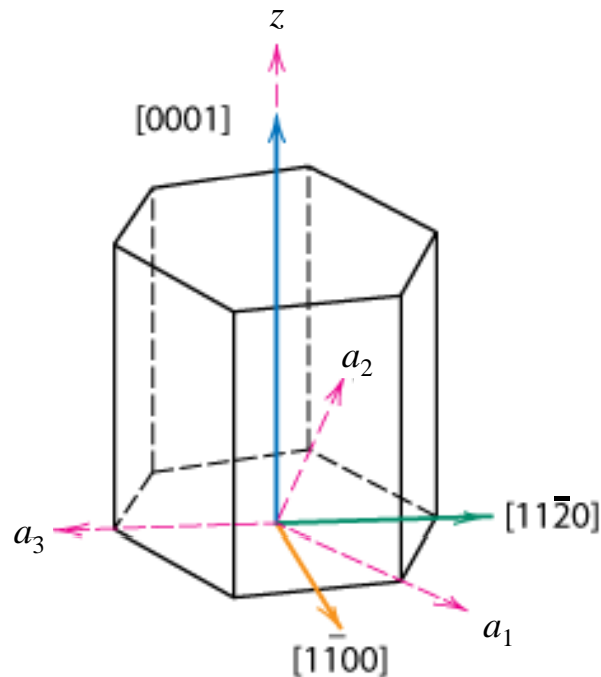


Fig. 3.8(a), Callister 7e.

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

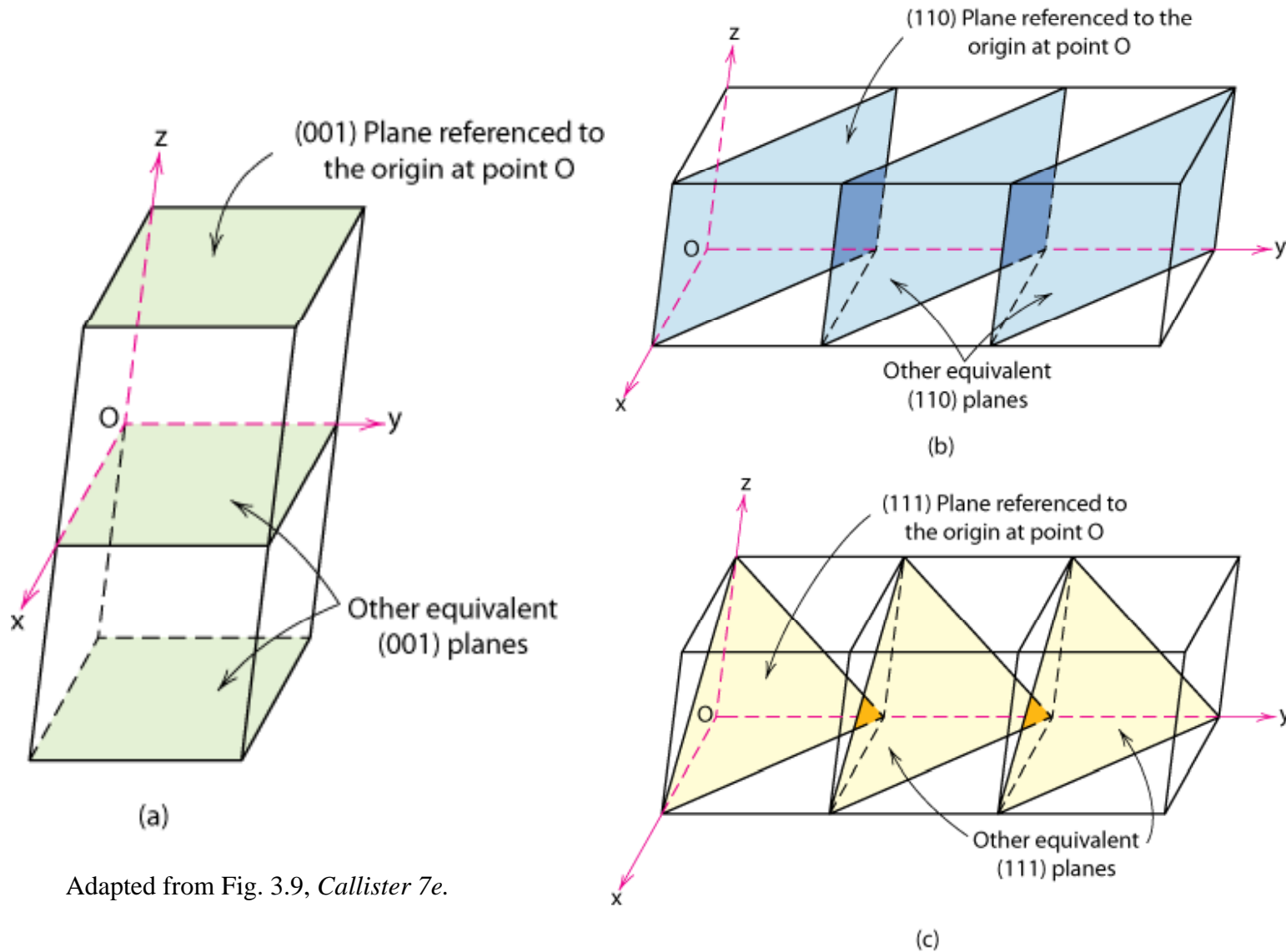
$$u = \frac{1}{3}(2u' - v')$$

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

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

$$w = w'$$

Crystallographic Planes



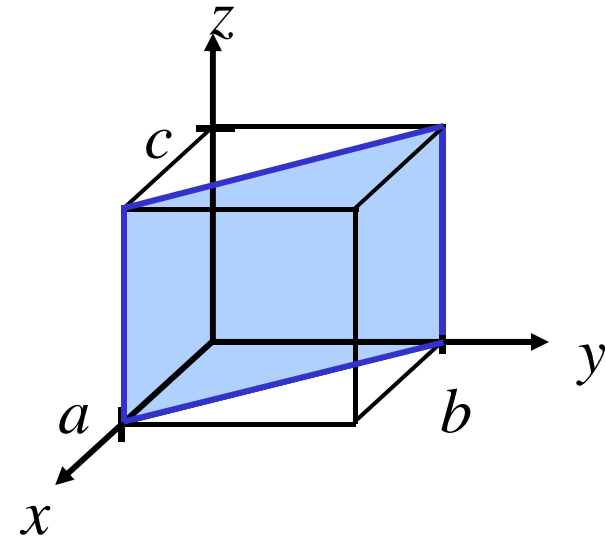
Adapted from Fig. 3.9, *Callister 7e*.

Crystallographic Planes

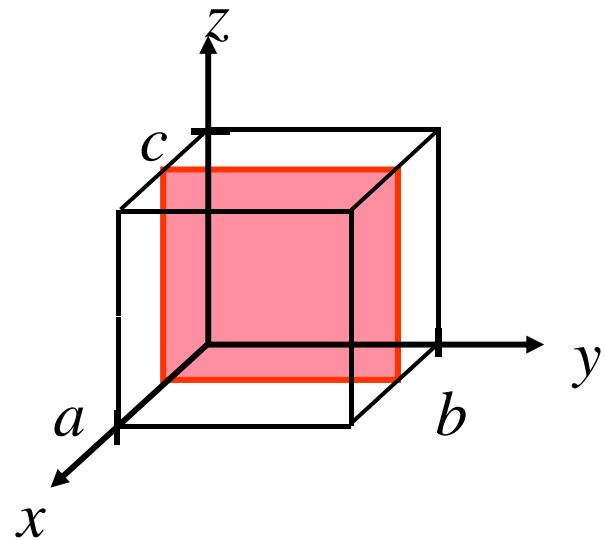
- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.
- Algorithm
 1. Read off intercepts of plane with axes in terms of a , b , c
 2. Take reciprocals of intercepts
 3. Reduce to smallest integer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

Crystallographic Planes

<u>Example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1	1	∞
2. Reciprocals	1/1	1/1	1/ ∞
	1	1	0
3. Reduction	1	1	0
4. Miller Indices	(110)		

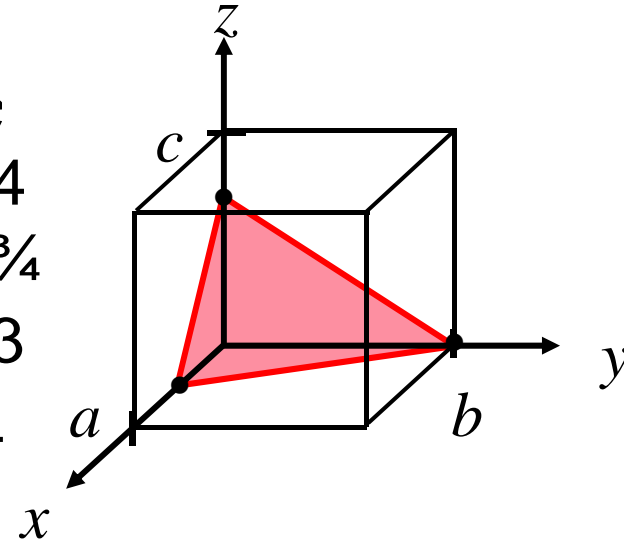


<u>Example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/1/2	1/ ∞	1/ ∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(100)		



Crystallographic Planes

<u>Example</u>	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/1/2	1/1	1/3/4
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



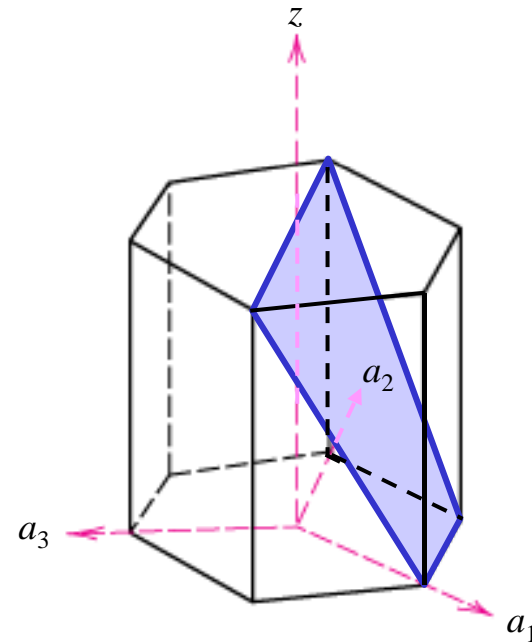
Family of Planes $\{hkl\}$

Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

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



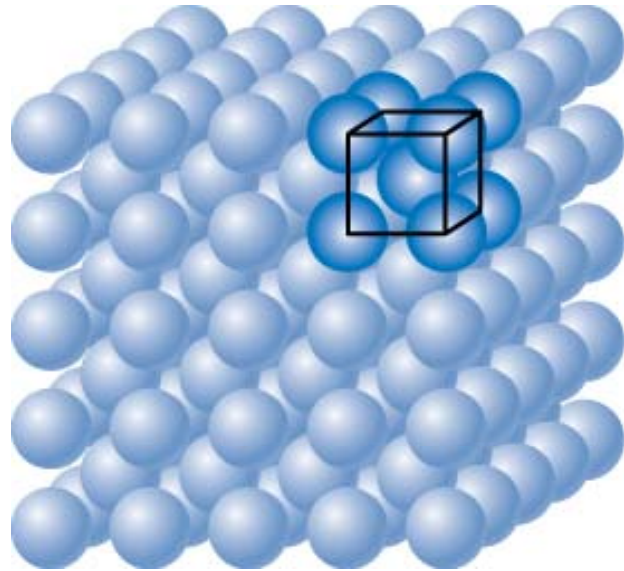
Adapted from Fig. 3.8(a), Callister 7e.

Crystallographic Planes

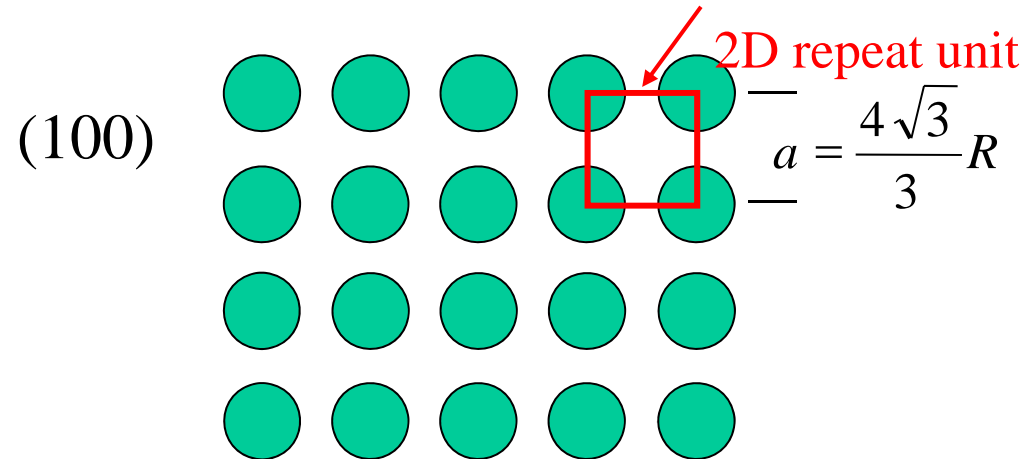
- We want to examine the atomic packing of crystallographic planes
- Iron foil can be used as a catalyst. The atomic packing of the exposed planes is important.
 - a) Draw (100) and (111) crystallographic planes for Fe.
 - b) Calculate the planar density for each of these planes.

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*.

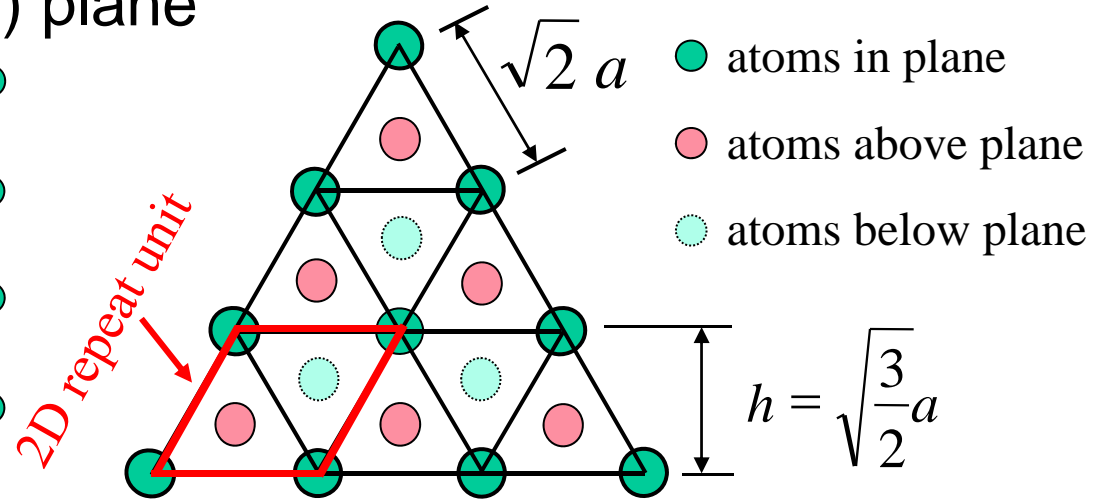
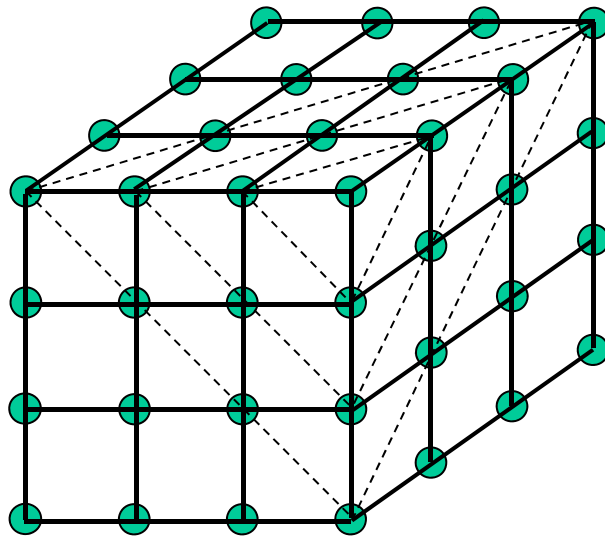


Radius of iron $R = 0.1241 \text{ nm}$

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

Planar Density of (111) Iron

Solution (cont): (111) plane



$$\text{area} = \sqrt{2} ah = \sqrt{3} a^2 = \sqrt{3} \left(\frac{4\sqrt{3}}{3} R \right)^2 = \frac{16\sqrt{3}}{3} R^2$$

atoms
2D repeat unit

area
2D repeat unit

$$\text{Planar Density} = \frac{1}{\frac{16\sqrt{3}}{3} R^2} = 7.0 \frac{\text{atoms}}{\text{nm}^2} = 0.70 \times 10^{19} \frac{\text{atoms}}{\text{m}^2}$$