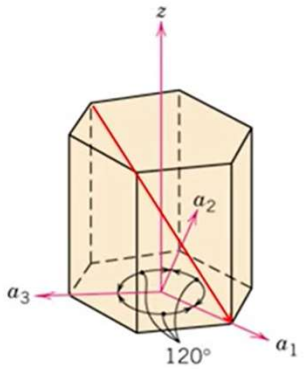


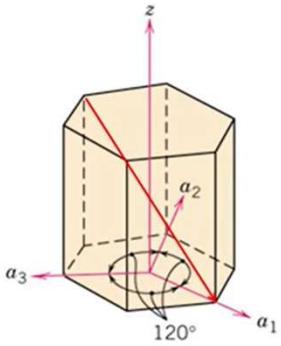
Direction of red arrow in 3 indices

Head point

Tail Point

Head-tail

25



Direction of red arrow in 3 indices

Head point

1 0 0

Tail Point

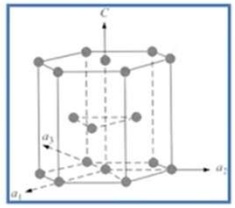
-1 0 1

Head-tail

2 0 -1

26

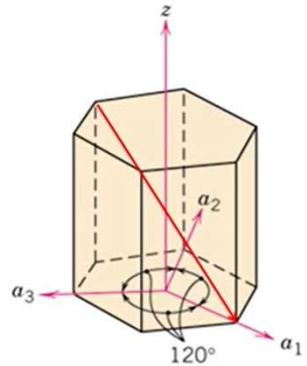
- directional indices denoted by 4 digits:
  [*u v t w*], where $t = -(u + v)$
- Conversion from 3-index system to 4-index system:
  [*u′,v′,w′*] ⇨ [*u v t w*]



$$u = \frac{1}{3}\left(2u' - v'\right) \quad v = \frac{1}{3}\left(2v' - u'\right) \quad t = -\left(u + v\right) \quad w = w'$$

Reduction to the lowest set of integers may be necessary.

27



Head-tail

2 0 -1

U = 1/3 (2x2-0)=4/3

V = 1/3(2x0-2)=-2/3

T = -(4/3+(-2/3))=-2/3

W = -1

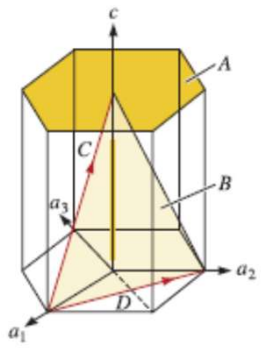
28

Direction C

1. Two points are 0, 0, 1 and 1, 0, 0.
2. 0, 0, 1 – 1, 0, 0 = –1, 0, 1
3. No fractions to clear or integers to reduce.
4. [$\bar{1}01$] or [$\bar{2}113$]

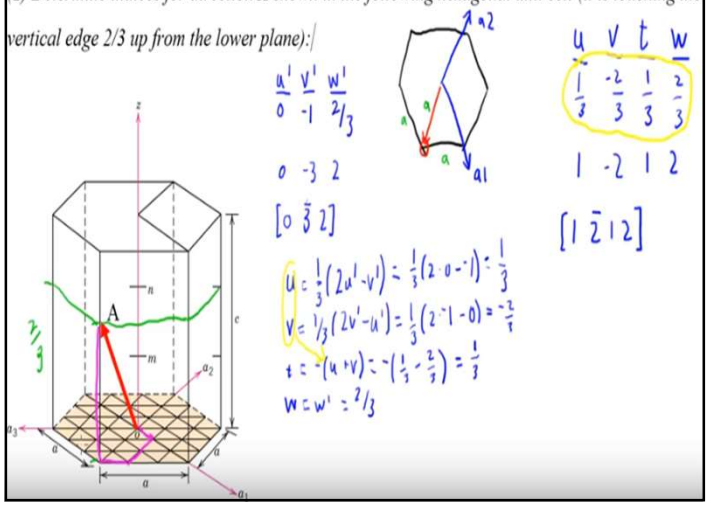
Direction D

1. Two points are 0, 1, 0 and 1, 0, 0.
2. 0, 1, 0 – 1, 0, 0 = –1, 1, 0
3. No fractions to clear or integers to reduce.
4. [$\bar{1}10$] or [$\bar{1}100$]



29

(2) Determine indices for direction A shown in the following hexagonal unit cell (it is touching the vertical edge 2/3 up from the lower plane):



u'	v'	w'
0	-1	2/3

0 -3 2

[0 $\bar{3}$ 2]

u	v	t	w
1/3	-2/3	1/3	2/3

1 -2 1 2

[1 $\bar{2}$ 1 2]

$u = \frac{1}{3}(2u' - v') = \frac{1}{3}(2 \cdot 0 - -1) = \frac{1}{3}$

$v = \frac{1}{3}(2v' - u') = \frac{1}{3}(2 \cdot -1 - 0) = -\frac{2}{3}$

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

$w = w' = 2/3$

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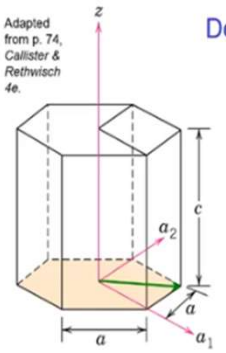
Determination of HCP Crystallographic Directions (ii)

Adapted from p. 74, *Callister & Rethwisch 4e.*



Determine indices for green vector

Example		a_1	a_2	z
1.	Reposition	not needed		
2.	Projections	a	a	0c
		1	1	0
3.	Reduction	1	1	0
4.	Brackets	[110]		

5. Convert to 4-axis parameters

$u = \frac{1}{3}[(2)(1) - (1)] = \frac{1}{3}$ $\quad v = \frac{1}{3}[(2)(1) - (1)] = \frac{1}{3}$

$t = -(\frac{1}{3} + \frac{1}{3}) = -\frac{2}{3}$ $\quad w = 0$

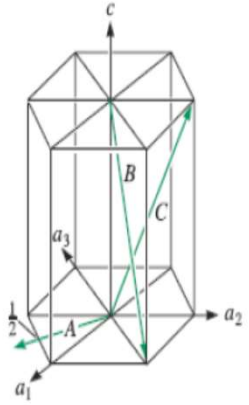
6. Reduction & Brackets

1/3, 1/3, -2/3, 0 => 1, 1, -2, 0 => [11$\bar{2}$0]

31

31

Determine the indices for the directions in the hexagonal lattice shown in Figure using both the three-digit and four-digit systems.



A:

(1, -1, 0) – (0, 0, 0) = (1, -1, 0) = [1$\bar{1}$0]

$h = \frac{1}{3}(2 + 1) = 1$

$k = \frac{1}{3}(-2 - 1) = -1$

$i = -\frac{1}{3}(1 - 1) = 0$

$l = 0$

Therefore, [1$\bar{1}$00]

B:

(1, 1, 0) – (0, 0, 1) = (1, 1, -1) = [11$\bar{1}$]

$h = \frac{1}{3}(2 - 1) = \frac{1}{3}$

$k = \frac{1}{3}(2 - 1) = \frac{1}{3}$

$i = -\frac{1}{3}(1 + 1) = -\frac{2}{3}$

$l = -1$

Therefore, [11$\bar{2}\bar{3}$]

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C:

(0, 1, 1) – (0, 0, 0) = (0, 1, 1) = [011]

h = ⅓(0 - 1) = -⅓

k = ⅓(2 - 0) = ⅔

i = -⅓(0 + 1) = -⅓

l = 1

Therefore, $[\bar{1}2\bar{1}3]$

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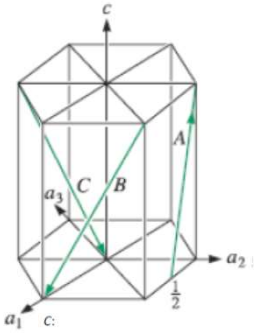

A:

(0, 1, 1) – (½, 1, 0) = (-½, 0, 1) = $[\bar{1}02]$

h = ½(-2 - 0) = -⅔

k = ½(0 + 1) = ⅔

i = -⅔(-1 + 0) = ⅔

l = 2

Therefore, $[\bar{2}116]$

B:

(1, 0, 0) – (1, 1, 1) = (0,-1, -1) = $[0\bar{1}\bar{1}]$

h = ⅔(0 + 1) = ⅔

k = ⅔(-2 + 0) = -⅔

i = -⅔(0 - 1) = ⅔

l = -1

$[1\bar{2}\bar{1}3]$

C:

(0, 0, 0) – (1, 0, 1) = (-1, 0, -1) = $[\bar{1}0\bar{1}]$

h = ½(-2 + 0) = -⅔

k = ½(0 + 1) = ⅔

i = -⅔(-1 + 0) = ⅔

l = -1

$[\bar{2}11\bar{3}]$

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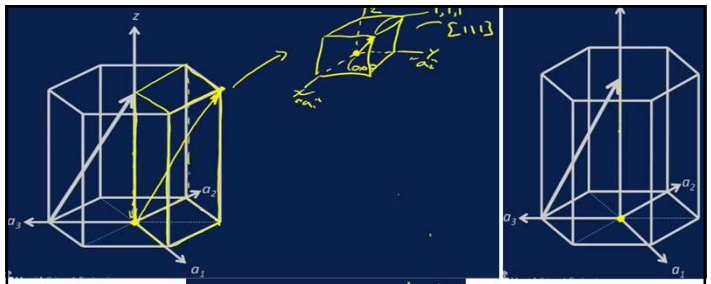
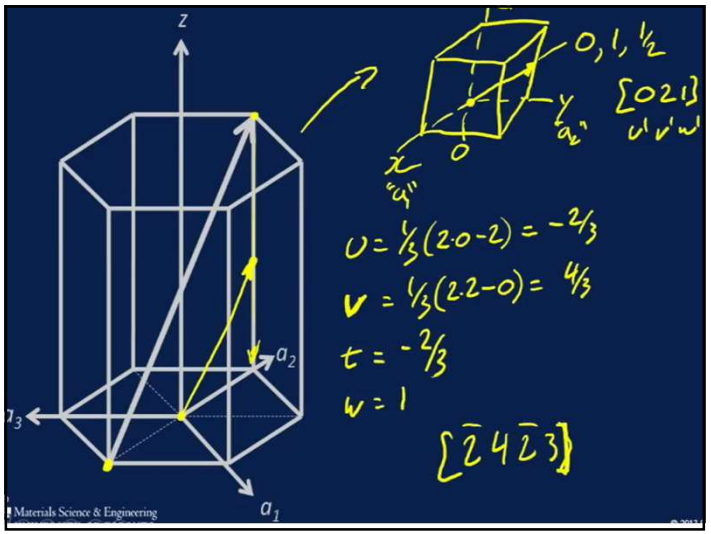
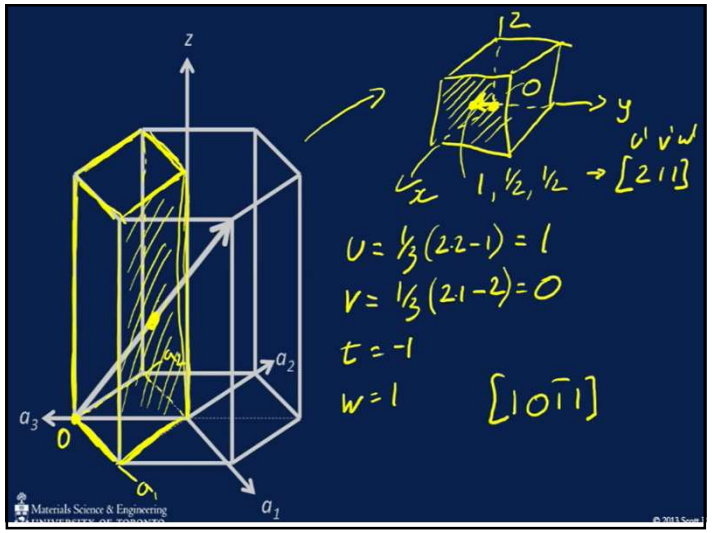


35



36



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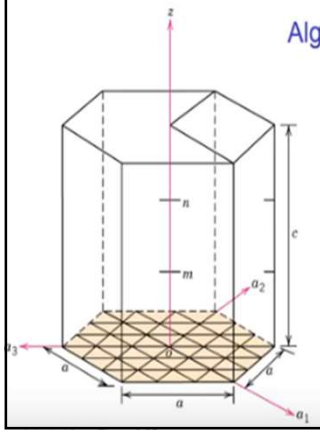
Drawing HCP Crystallographic Directions (i)



Algorithm (Miller-Bravais coordinates)

1. Remove brackets
2. Divide by largest integer so all values are ≤ 1
3. Multiply terms by appropriate unit cell dimension a (for a_1, a_2, and a_3 axes) or c (for z-axis) to produce projections

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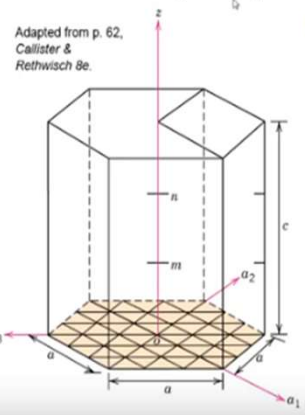
Drawing HCP Crystallographic Directions (ii)

- Draw the $[\bar{1}\,\bar{2}13]$ direction in a hexagonal unit cell.



Algorithm	a_1	a_2	a_3	z

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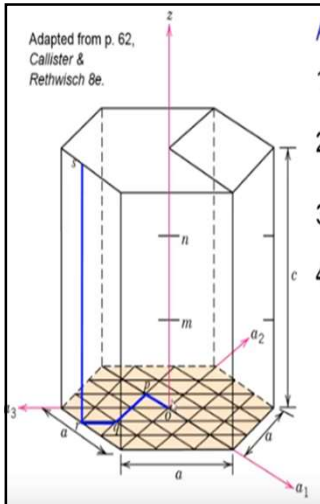

Algorithm	a_1	a_2	a_3	z
1. Remove brackets	-1	-2	1	3
2. Divide by 3	$-\frac{1}{3}$	$-\frac{2}{3}$	$\frac{1}{3}$	1
3. Projections	$-\frac{a}{3}$	$-\frac{2a}{3}$	$\frac{a}{3}$	c

4. Construct Vector
   - start at point o
   - proceed $-a/3$ units along a_1 axis to point p
   - $-2a/3$ units parallel to a_2 axis to point q
   - $a/3$ units parallel to a_3 axis to point r
   - c units parallel to z axis to point s

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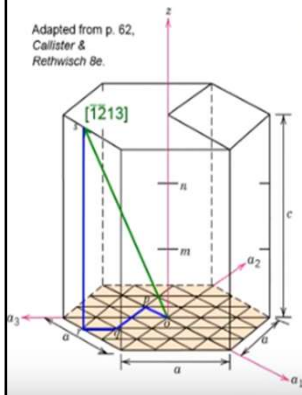
Drawing HCP Crystallographic Directions (ii)

- Draw the $[\bar{1}\,\bar{2}13]$ direction in a hexagonal unit cell.

Adapted from p. 62, *Callister & Rethwisch 8e.*



Algorithm	a_1	a_2	a_3	z
1. Remove brackets	-1	-2	1	3
2. Divide by 3	$-\frac{1}{3}$	$-\frac{2}{3}$	$\frac{1}{3}$	1
3. Projections	$-\frac{a}{3}$	$-\frac{2a}{3}$	$\frac{a}{3}$	c

4. Construct Vector
   - start at point o
   - proceed $-a/3$ units along a_1 axis to point p
   - $-2a/3$ units parallel to a_2 axis to point q
   - $a/3$ units parallel to a_3 axis to point r
   - c units parallel to z axis to point s

$[\bar{1}\bar{2}13]$ direction represented by vector from point o to point s

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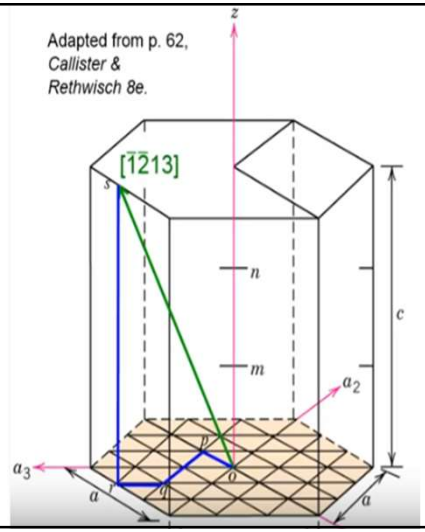
Adapted from p. 62, *Callister & Rethwisch 8e.*



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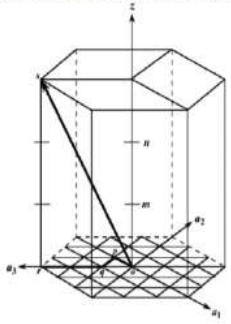
3.36 *Sketch the* $[\bar{1}\,\bar{1}\,23]$ *and* $[10\bar{1}\,0]$ *directions in a hexagonal unit cell.*

Solution

The first portion of this problem asks that we plot the $[\bar{1}\,\bar{1}\,23]$ within a hexagonal unit cell. Below is shown this direction plotted within a hexagonal unit cell having a reduced-scale coordinate scheme.



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For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, -1, -1, 2, and 3, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the $-a_1$ axis (to point p), from here 1 unit distance parallel to $-a_2$ axis (to point q), then 2 unit distances parallel (or along) the a_3 axis (to point r), and finally, 3 unit distances parallel to the z axis (to point s). Thus, the $[\bar{1}\,\bar{1}\,23]$ direction is that vector that extends from point o to point s as shown.

Now we are asked to plot the $[10\bar{1}\,0]$ within a hexagonal unit cell. In the figure below is plotted this direction within a hexagonal unit cell having a reduced-scale coordinate scheme.

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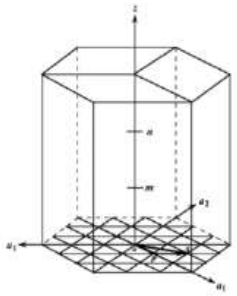

For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, 1, 0, −1, and 0, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the a_1 axis (to point p). Since there is no projection on the a_2 axis it is not necessary to move parallel to this axis. Therefore, from point p we proceed 1 unit distance parallel to $-a_3$ axis (to point q). And, finally, inasmuch as there is no projection along the z axis, it is not necessary to move parallel to this axis. Thus, the $[10\bar{1}0]$ direction is that vector that extends from point o to point q as shown.

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(a) $[01\bar{1}0]$ (b) $[11\bar{2}0]$ (c) $[\bar{1}011]$

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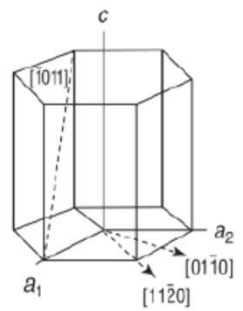
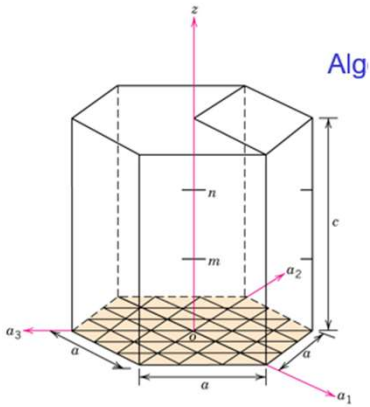
- Sketch the following and directions within a hexagonal unit cell

(a) $[01\bar{1}0]$ (b) $[11\bar{2}0]$ (c) $[\bar{1}011]$

(a) $[\bar{2}110]$ (b) $[11\bar{2}1]$ (c) $[10\bar{1}0]$





Alg

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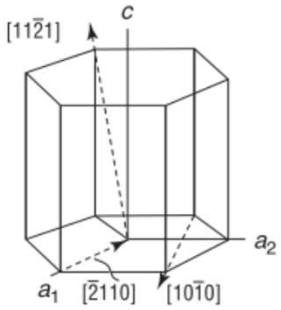

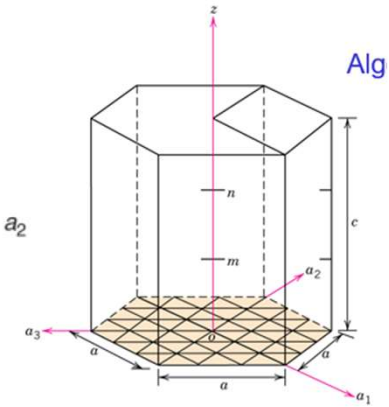

Alg

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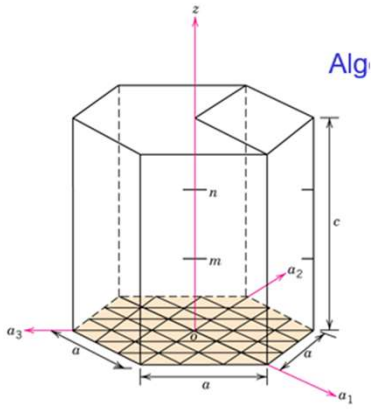
Sketch the [0110] and [2 2 4 3] directions in a hexagonal unit cell.



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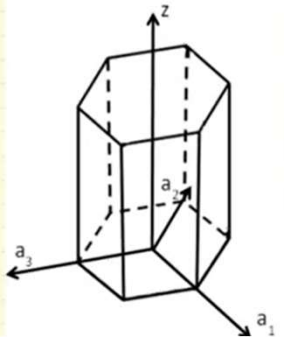
Sketch on the unit cell the [1 $\bar{1}$ 0 1] direction for a hexagonal close-packed crystal.



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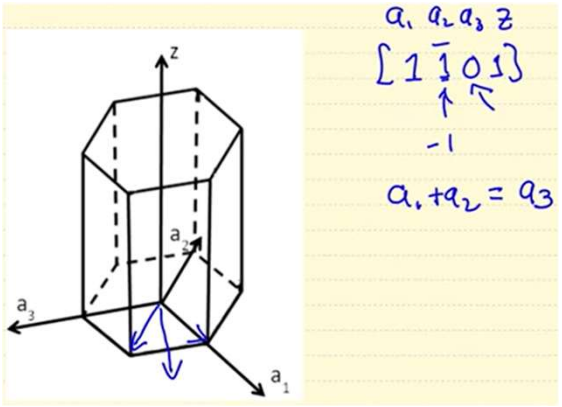

$a_1\ a_2\ a_3\ z$

$[1\ \bar{1}\ 0\ 1]$

-1

$a_1 + a_2 = a_3$

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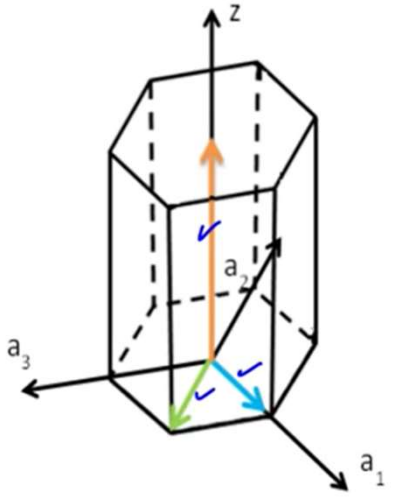

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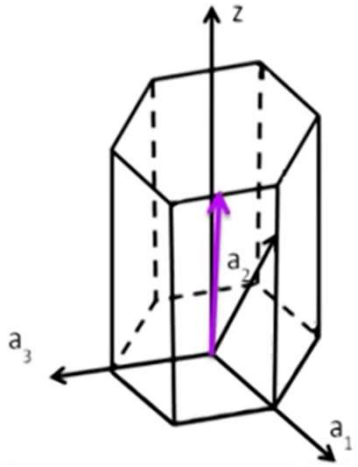

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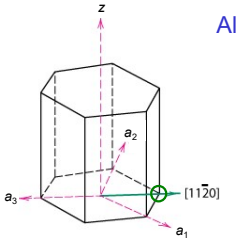
HCP Crystallographic Directions



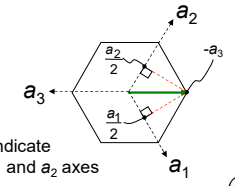
Adapted from Fig. 3.8(a), *Callister 7e.*

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

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HCP Crystallographic Directions

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

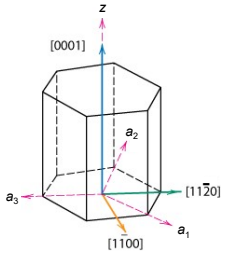

Fig. 3.8(a), *Callister 7e.*

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

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

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

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

$$w = w'$$

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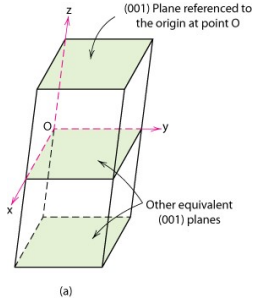
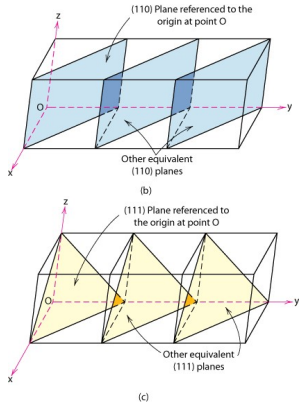
Crystallographic Planes





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

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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*)

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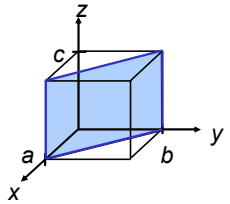
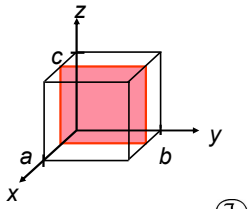
Crystallographic Planes

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)		



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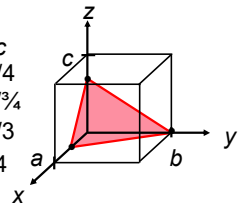
Crystallographic Planes

example	*a*	*b*	*c*
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



Family of Planes {*hkl*}

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

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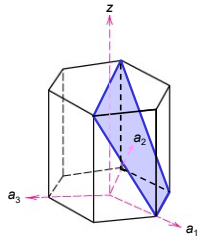
Crystallographic Planes (HCP)

- 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.*

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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.

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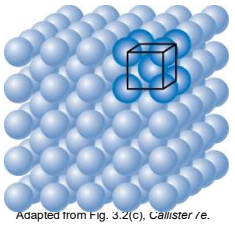
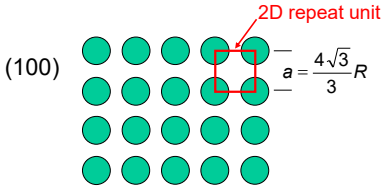
Planar Density of (100) Iron

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



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



Radius of iron R = 0.1241 nm

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

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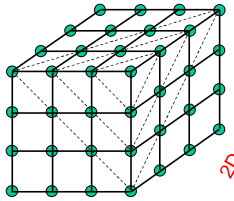
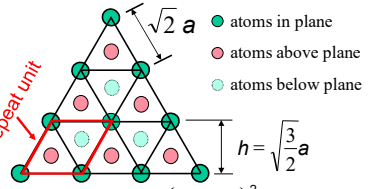
Planar Density of (111) Iron

Solution (cont): (111) plane

1 atom in plane/ unit surface cell





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

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

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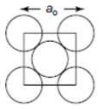
- Determine the planar density and packing fraction for FCC nickel in the (100),
- (110), and (111) planes. Which, if any, of these planes is close-packed?
- Solution: *ao* = 3.5167 Å

For (100):



$$\text{planar density} = \frac{2}{(3.5167 \times 10^{-8}\ \text{cm})^2} = 0.1617 \times 10^{16}\ \text{points/cm}^2$$

$$\text{packing fraction} = \frac{2\pi r^2}{\left(4r/\sqrt{2}\right)^2} = 0.7854$$

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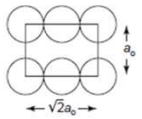
For (110):



$$\text{planar density} = \frac{2 \text{ points}}{(3.5167 \times 10^{-8} \text{ cm})\left(\sqrt{2}\right)(3.5167 \times 10^{-8} \text{ cm})}$$
$$= 0.1144 \times 10^{-16} \text{ points/cm}^2$$

$$\text{packing fraction} = \frac{2\pi r^2}{\sqrt{2}\left(4r/\sqrt{2}\right)^2} = 0.555$$

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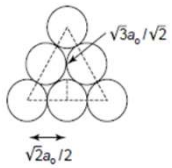
For (111):



From the sketch, we can determine that the area of the (111) plane is $\left(\sqrt{2}a_o/2\right)\left(\sqrt{3}a_o/\sqrt{2}\right) = 0.866a_o^2$. There are $(3)(\frac{1}{2}) + (3)(\frac{1}{6}) = 2$ atoms in this area.

$$\text{planar density} = \frac{2 \text{ points}}{0.866(3.5167 \times 10^{-8} \text{ cm})^2}$$
$$= 0.1867 \times 10^{16} \text{ points/cm}^2$$

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Section 3.6
Interstitial Sites

- Interstitial sites - Locations between the "normal" atoms or ions in a crystal into which another - usually different - atom or ion is placed. Typically, the size of this interstitial location is smaller than the atom or ion that is to be introduced.
- Cubic site - An interstitial position that has a coordination number of eight. An atom or ion in the cubic site touches eight other atoms or ions.
- Octahedral site - An interstitial position that has a coordination number of six. An atom or ion in the octahedral site touches six other atoms or ions.
- Tetrahedral site - An interstitial position that has a coordination number of four. An atom or ion in the tetrahedral site touches four other atoms or ions.

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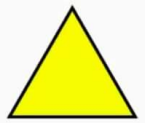
Possible Shapes/Sites

Cubic site

Octahedral site

Tetrahedral site

Triangular site



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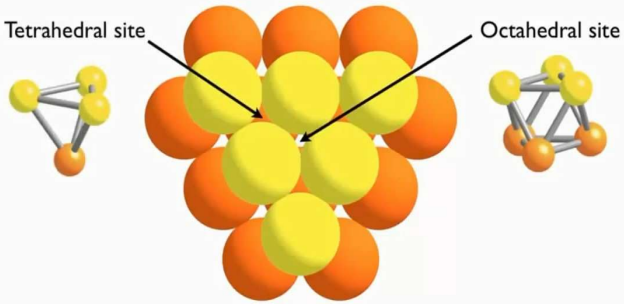
Cubic close-packed structure



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FCC

- Octahedral Void- *4*
- Tetrahedral Void- *8*

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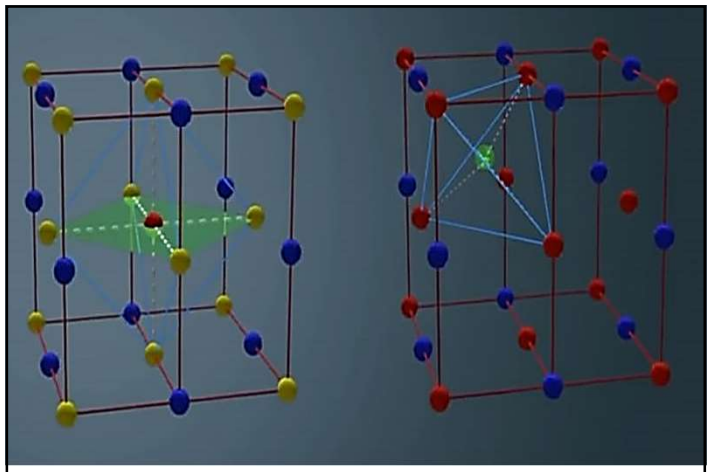

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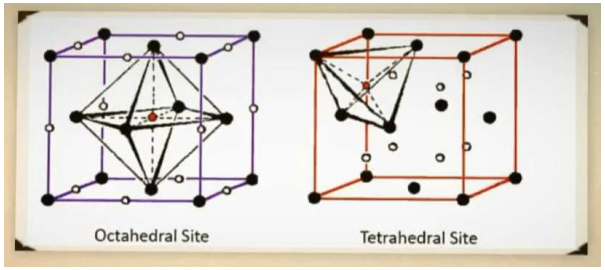

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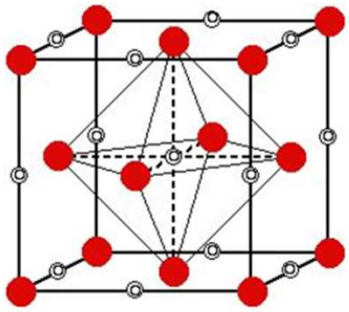
Octahedral sites in FCC

Can you mark all octahedral sites in a FCC unit cell ?



How many (whole) sites are there?

$$1\times 1+12\times\frac{1}{4}=4$$

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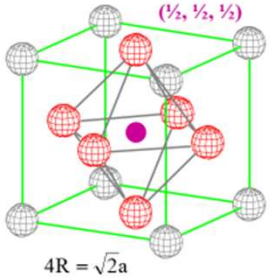
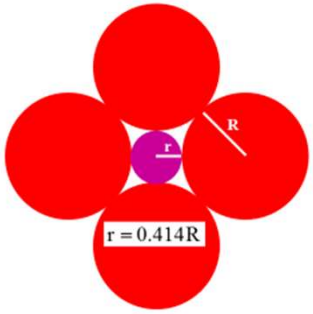
Octahedral sites in FCC



$4R=\sqrt{2}a$



$2(r+R)=a=2\sqrt{2}R$

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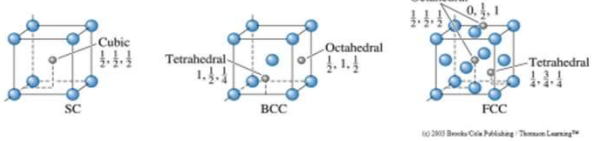

Figure 3.29 The location of the interstitial sites in cubic unit cells. Only representative sites are shown.

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Calculate the number of octahedral sites that *uniquely* belong to one FCC unit cell.

Example 3.12 SOLUTION

The octahedral sites include the 12 edges of the unit cell, with the coordinates

$$\frac{1}{2},0,0 \quad \frac{1}{2},1,0 \quad \frac{1}{2},0,1 \quad \frac{1}{2},1,1$$

$$0,\frac{1}{2},0 \quad 1,\frac{1}{2},0 \quad 1,\frac{1}{2},1 \quad 0,\frac{1}{2},1$$

$$0,0,\frac{1}{2} \quad 1,0,\frac{1}{2} \quad 1,1,\frac{1}{2} \quad 0,1,\frac{1}{2}$$

plus the center position, 1/2, 1/2, 1/2.

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Example 3.12 SOLUTION (Continued)

Each of the sites on the edge of the unit cell is shared between four unit cells, so only 1/4 of each site belongs uniquely to each unit cell.

Therefore, the number of sites belonging uniquely to each cell is:

(12 edges) (1/4 per cell) + 1 center location
= 4 octahedral sites

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TABLE 3-6 ■ *The coordination number and the radius ratio*

Coordination Location of Number	Interstitial	Radius Ratio	Representation
2	Linear	0–0.155	
3	Center of triangle	0.155–0.225	
4	Center of tetrahedron	0.225–0.414	
6	Center of octahedron	0.414–0.732	
8	Center of cube	0.732–1.000	

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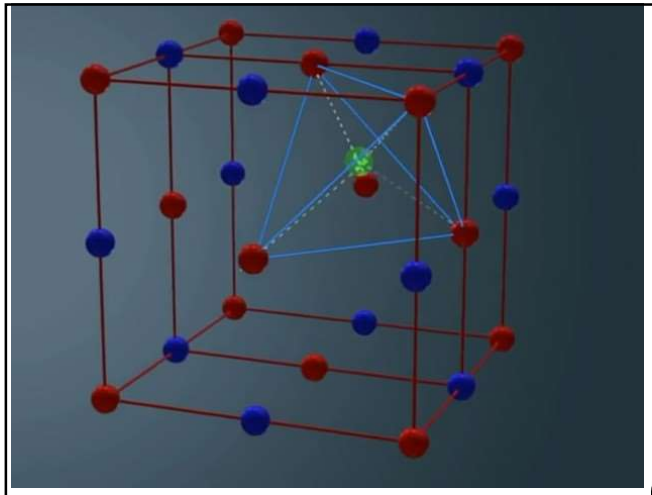

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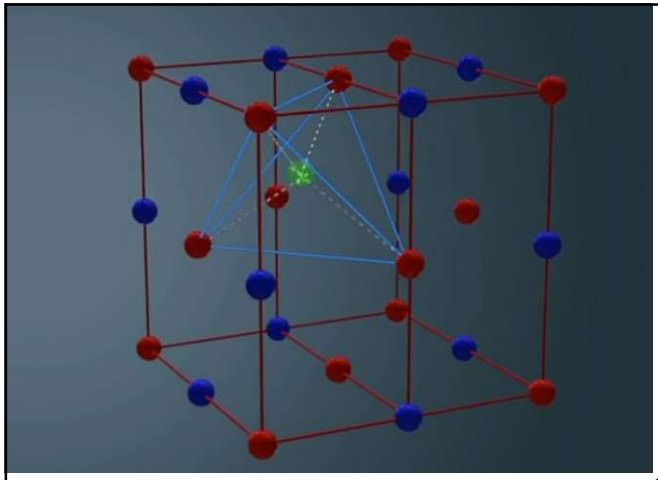

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