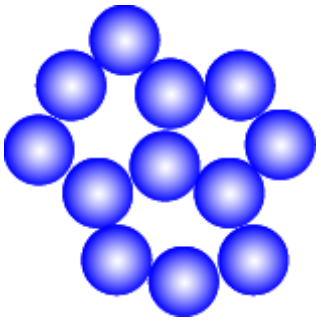
Chapter 3: Fundamentals of Structure of Crystalline Solids

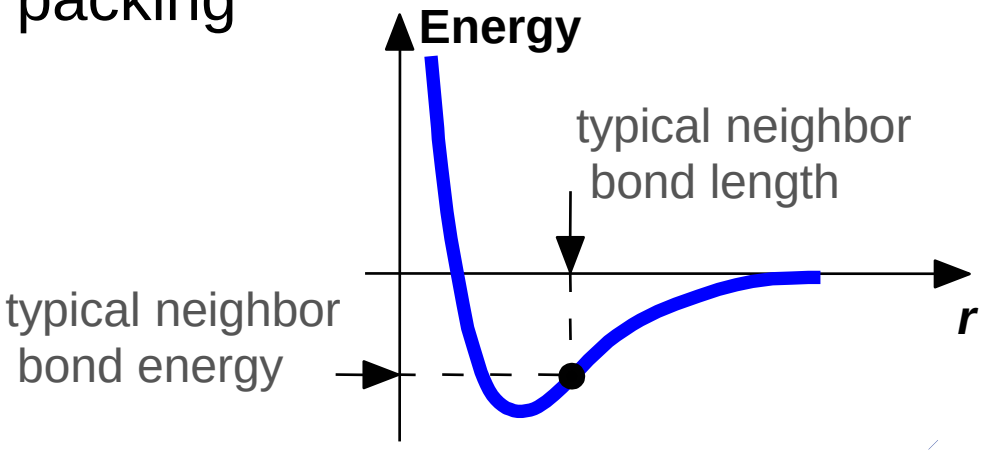
ISSUES TO ADDRESS...

- How do atoms assemble into solid structures in crystalline and non-crystalline materials?
- How do we specify directions and planes in unit cells?
- How do we distinguish between single crystals and polycrystalline materials?
- When do material properties vary with the sample (i.e., part) orientation?

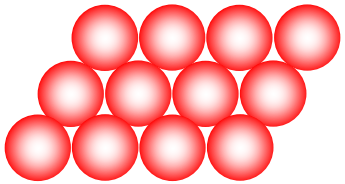
Energy and Packing

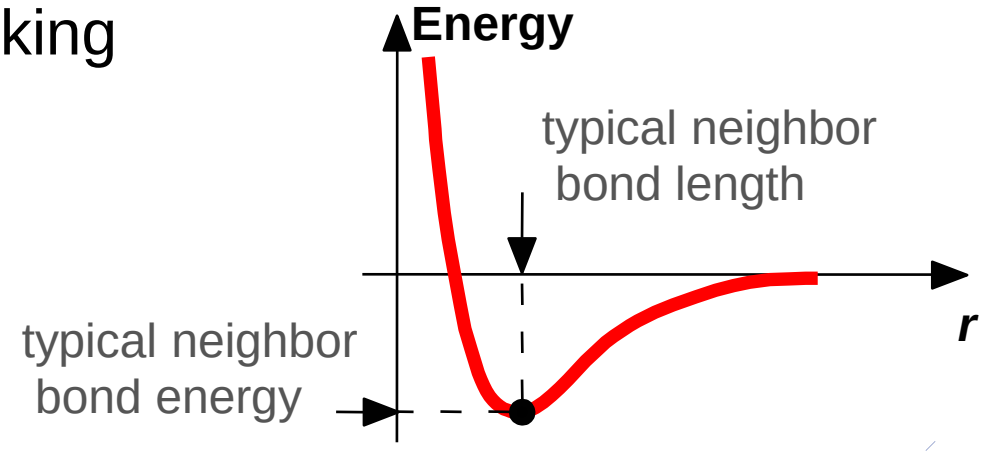
- Non dense, random packing





- Dense, ordered packing



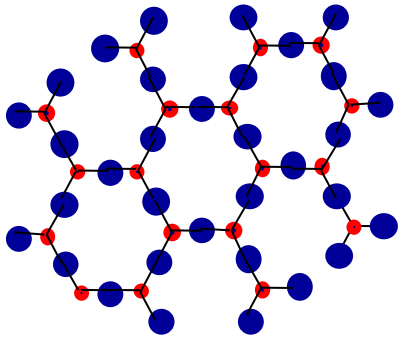


Dense, ordered packed structures tend to have lower energies.

Materials and Packing

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers



crystalline SiO_2

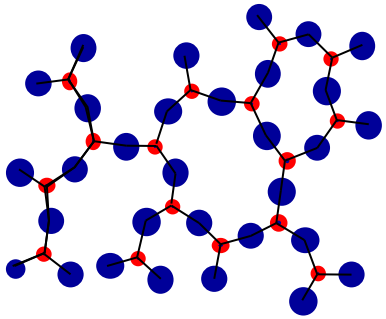
From Fig. 3.10(a)
Callister's Materials Science and Engineering, Adapted Version.

• Si ● Oxygen

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
  -rapid cooling

"Amorphous" = Noncrystalline



noncrystalline SiO_2

From Fig. 3.10(b)
Callister's Materials Science and Engineering, Adapted Version.

Section 3.3 – Crystal Systems

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.

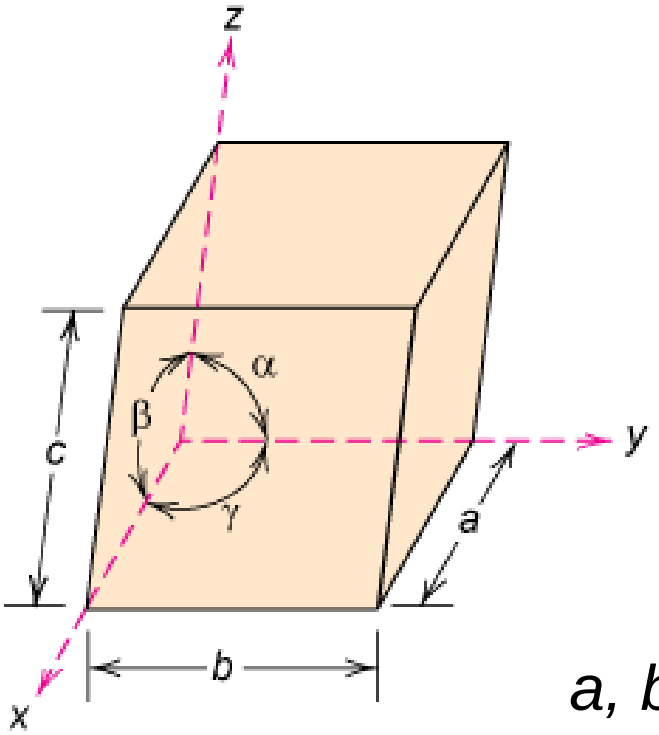


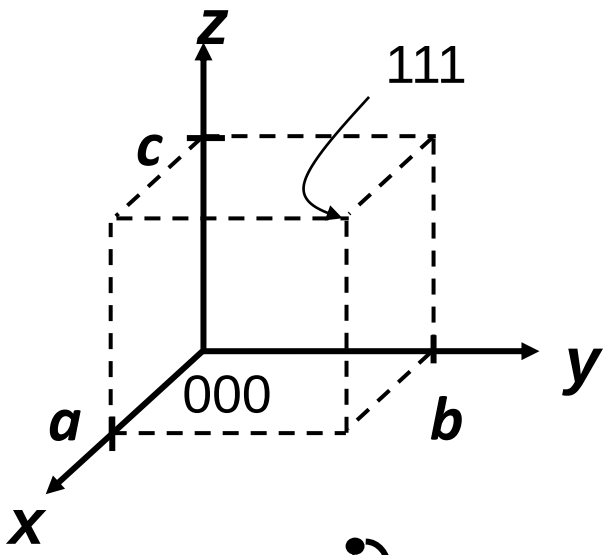
Fig. 3.2
Callister's Materials Science and Engineering, Adapted Version.

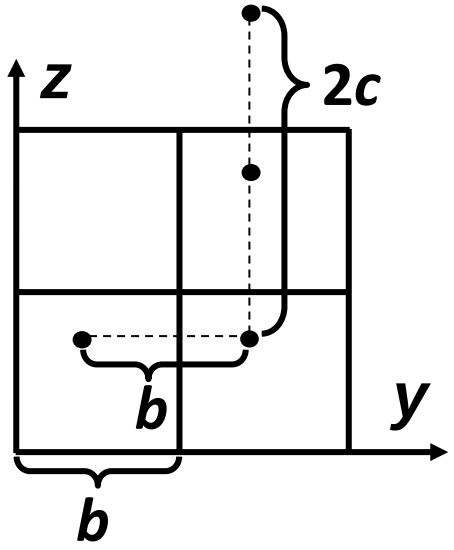
7 crystal systems

14 crystal lattices

a, b, and *c* are the lattice constants

Section 3.5 Point Coordinates





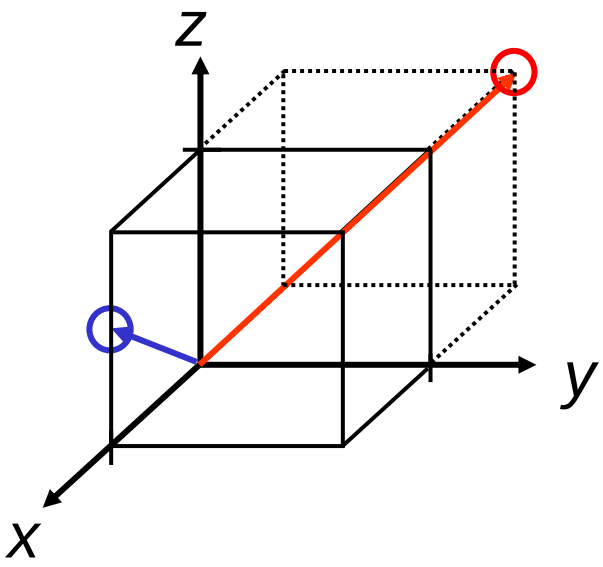
Point coordinates for unit cell center are

a/2, *b*/2, *c*/2 ½ ½ ½

Point coordinates for unit cell corner are 111

Translation: integer multiple of lattice constants → 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

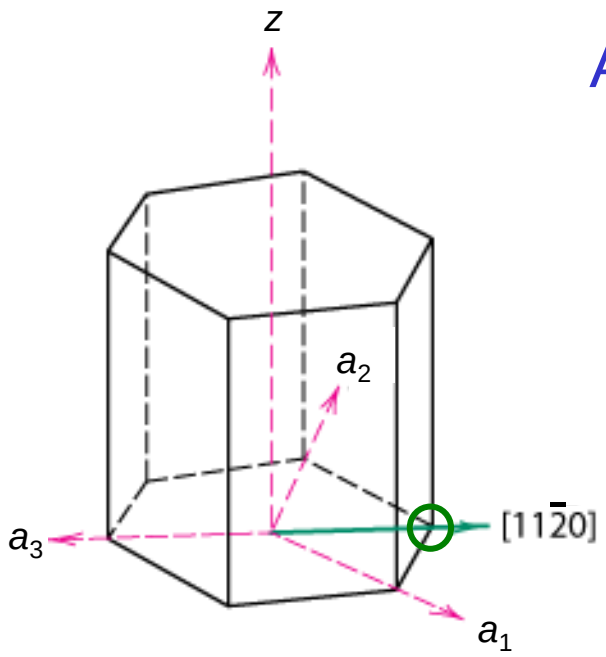
[*uvw*]

ex: 1, 0, ½ => 2, 0, 1 => [201]

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

families of directions <*uvw*>

HCP Crystallographic Directions



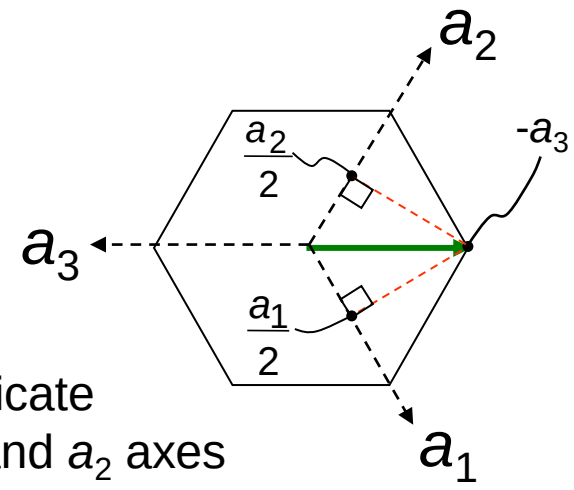
From Fig. 3.6(a)
Callister's Materials Science and Engineering, Adapted Version.

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

HCP Crystallographic Directions

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

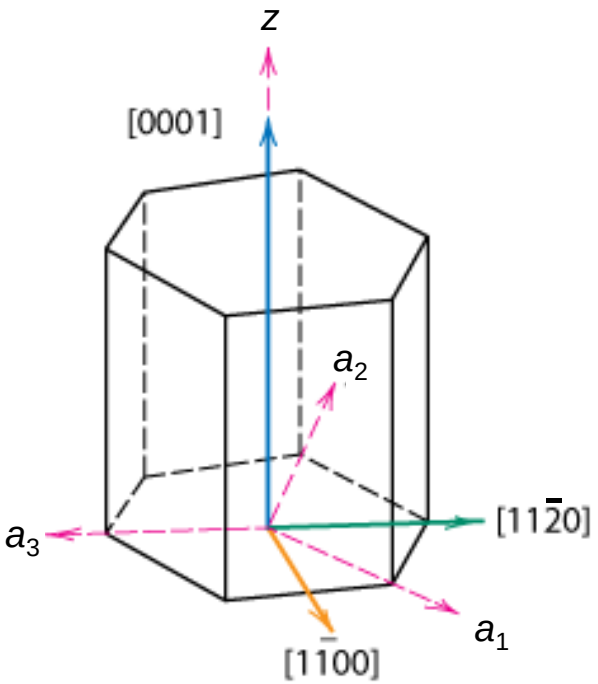


Fig. 3.6(a)
Callister's Materials Science and Engineering, Adapted Version.

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

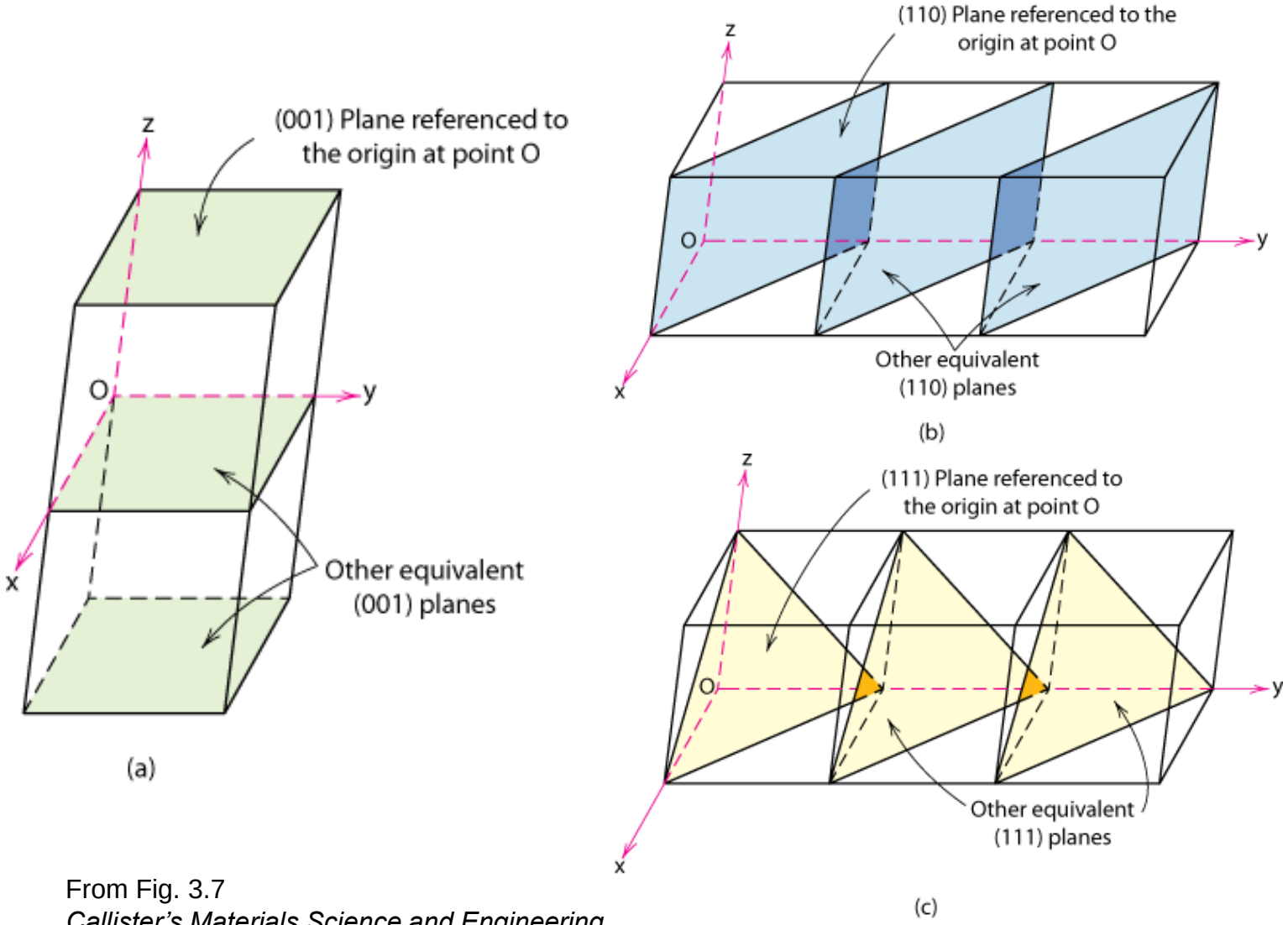
$$u = \frac{1}{3}(2u' - v')$$

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

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

$$w = w'$$

Crystallographic Planes



From Fig. 3.7
Callister's Materials Science and Engineering, Adapted Version.

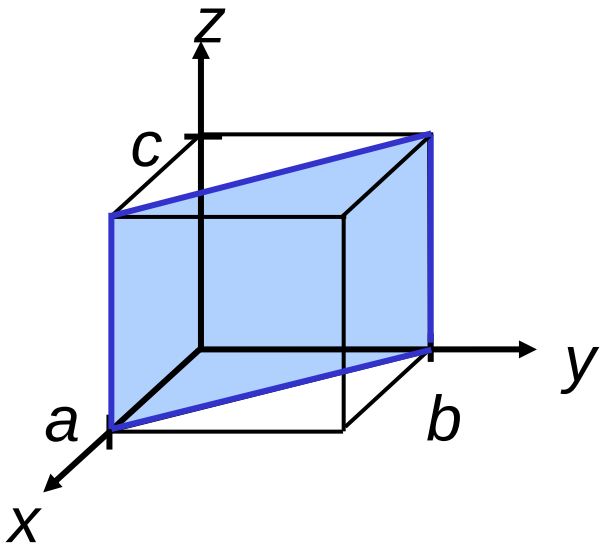
Crystallographic Planes

- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

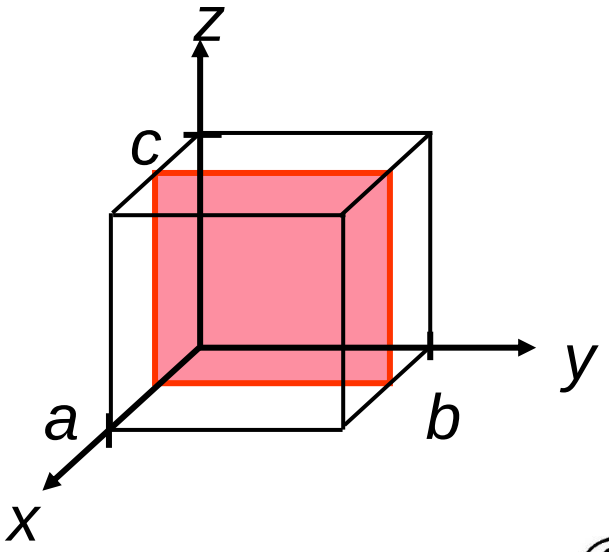
- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

Crystallographic Planes

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)		

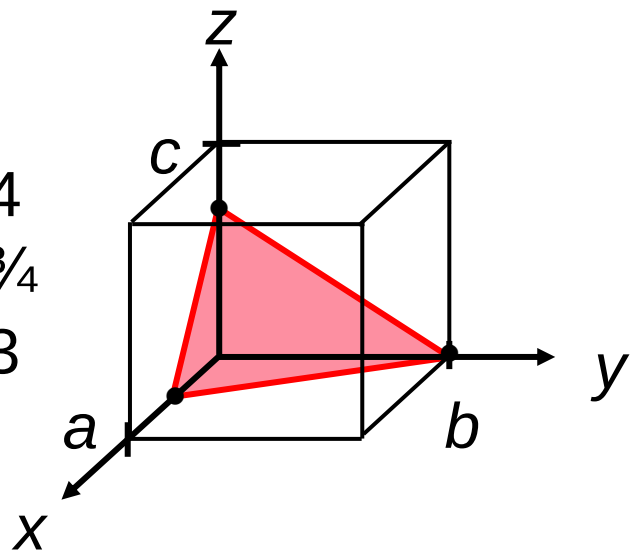


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		



Crystallographic Planes

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)		



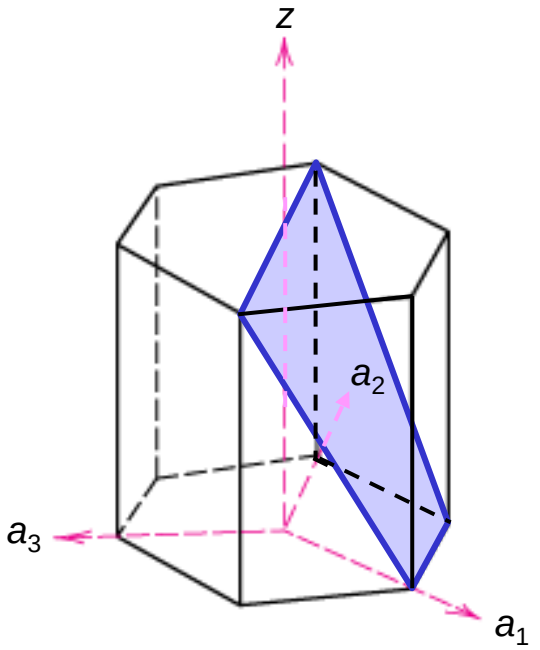
Family of Planes {*hkl*}

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

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	$(10\bar{1}1)$			



From Fig. 3.6(b)
Callister's Materials Science and Engineering, Adapted Version.

Crystals as Building Blocks

- *Some* engineering applications require single crystals:
  --diamond single crystals for abrasives

(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

--turbine blades

Fig. 11.33(c) *Callister's Materials Science and Engineering, Adapted Version.* (Fig.11.33(c) courtesy of Pratt and Whitney).

- Properties of crystalline materials often related to crystal structure.

  --Ex: Quartz fractures more easily along some crystal planes than others.

(Courtesy P.M. Anderson)

Polycrystals

- *Most* engineering materials are polycrystals.

From Fig. K, color inset pages of *Callister 5e*. (Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

Anisotropic

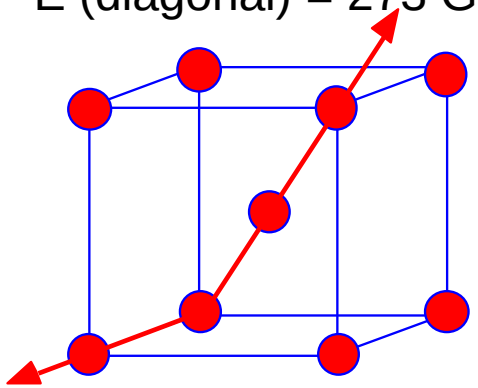
Isotropic

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If grains are randomly oriented,
  overall component properties are not directional.
- Grain sizes typ. range from 1 nm to 2 cm
  (i.e., from a few to millions of atomic layers).

Single vs Polycrystals

- Single Crystals
  - -Properties vary with direction: anisotropic.
  - -Example: the modulus of elasticity (E) in BCC iron:

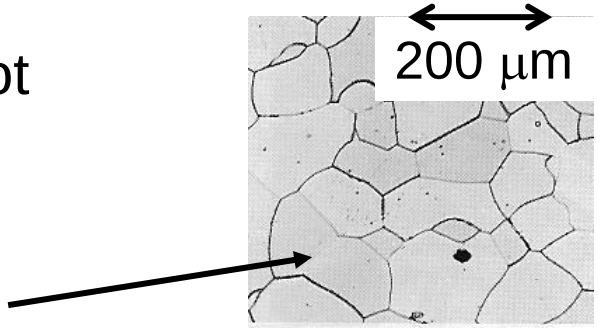
E (diagonal) = 273 GPa

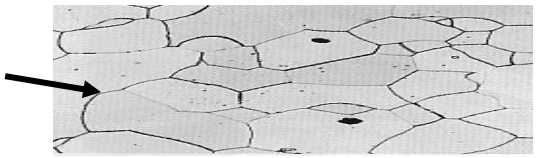


E (edge) = 125 GPa

Data from Table 3.2, *Callister's Materials Science and Engineering, Adapted Version.* (Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals
  - -Properties may/may not vary with direction.
  - -If grains are randomly oriented: isotropic.
    ($E_{poly\ iron}$ = 210 GPa)
  - -If grains are textured, anisotropic.





From Fig. 5.19(b), *Callister's Materials Science and Engineering, Adapted Version.* (Fig. 5.19(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

SUMMARY

- Atoms may assemble into crystalline or amorphous structures.
- Crystallographic points, directions and planes are specified in terms of indexing schemes.
- Materials can be single crystals or polycrystalline. Material properties generally vary with single crystal orientation (i.e., they are anisotropic), but are generally non-directional (i.e., they are isotropic) in polycrystals with randomly oriented grains.

ANNOUNCEMENTS

Reading:

Core Problems:

Self-help Problems: