Chemical Engineering 378

Science of Materials Engineering

Lecture 4

Crystal Directions and Planes

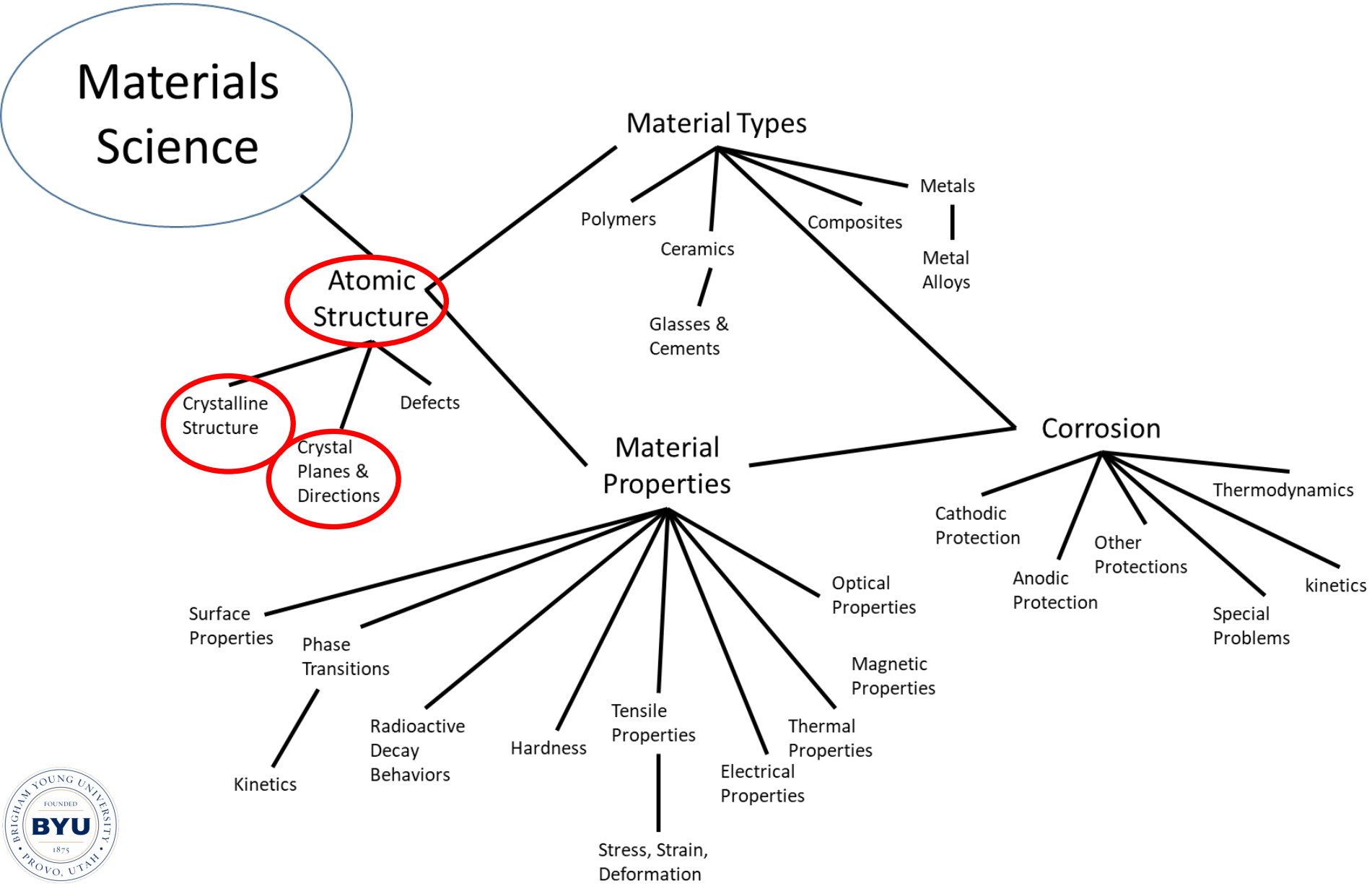
Spiritual Thought

Sooner or later, I believe that all of us experience times when the very fabric of our world tears at the seams, leaving us feeling alone, frustrated, and adrift. It can happen to anyone. No one is immune. Everyone's situation is different, and the details of each life are unique. Nevertheless, I have learned that there is something that would take away the bitterness that may come into our lives. There is one thing we can do to make life sweeter, more joyful, even glorious.

We can be grateful!

Dieter F. Uchtdorf

Materials Roadmap



OEP #2

https://www.youtube.com/watch?v=b_HhiU1mOwU

OEP#2 Problem Statement

Open Ended Problem #2 The Core
Individual work only, Due 9/20/23 at beginning of class

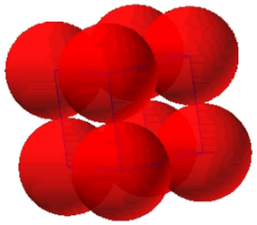
(Don't be afraid to "Google" for reasonable assumptions; just provide references!)

Unobtanium

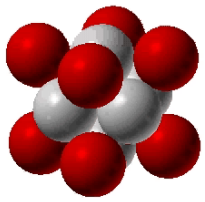
I'm fairly certain that this movie won awards for the worst science ever, at least in my mind. The plot and characters didn't help it much. Either way, this movie involves people traveling to the core of the earth to avert an environmental disaster, and they do so by using "unobtainium" to build a heat-impervious vehicle. This material is supposedly a tungsten/titanium (WTi) matrix that includes crystals inserted throughout. Assuming the scientist's claims are real regarding the heat absorbing properties, this would be amazing (read that as unrealistic) stuff! Let's evaluate some properties, shall we? We won't worry about the crystals, but I want you to evaluate the matrix. What is the likely unit cell type for this matrix? (keep in mind similar unit cells form matrixes much more easily than different unit cells) What would be the APF for the Ti and W crystals? What would you predict the density of the matrix to be?

Crystal System Review

Property	SC	FCC	BCC	HCP
# atoms/cell	1	4	2	6
Lattice Parameter				
Coordination #	6	12	8	12
APF	0.52	0.74	0.68	0.74

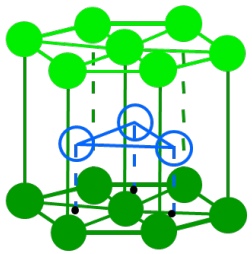


Polonium



Gold

Tungsten



Zinc

Densities of Material Classes

In general

$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$

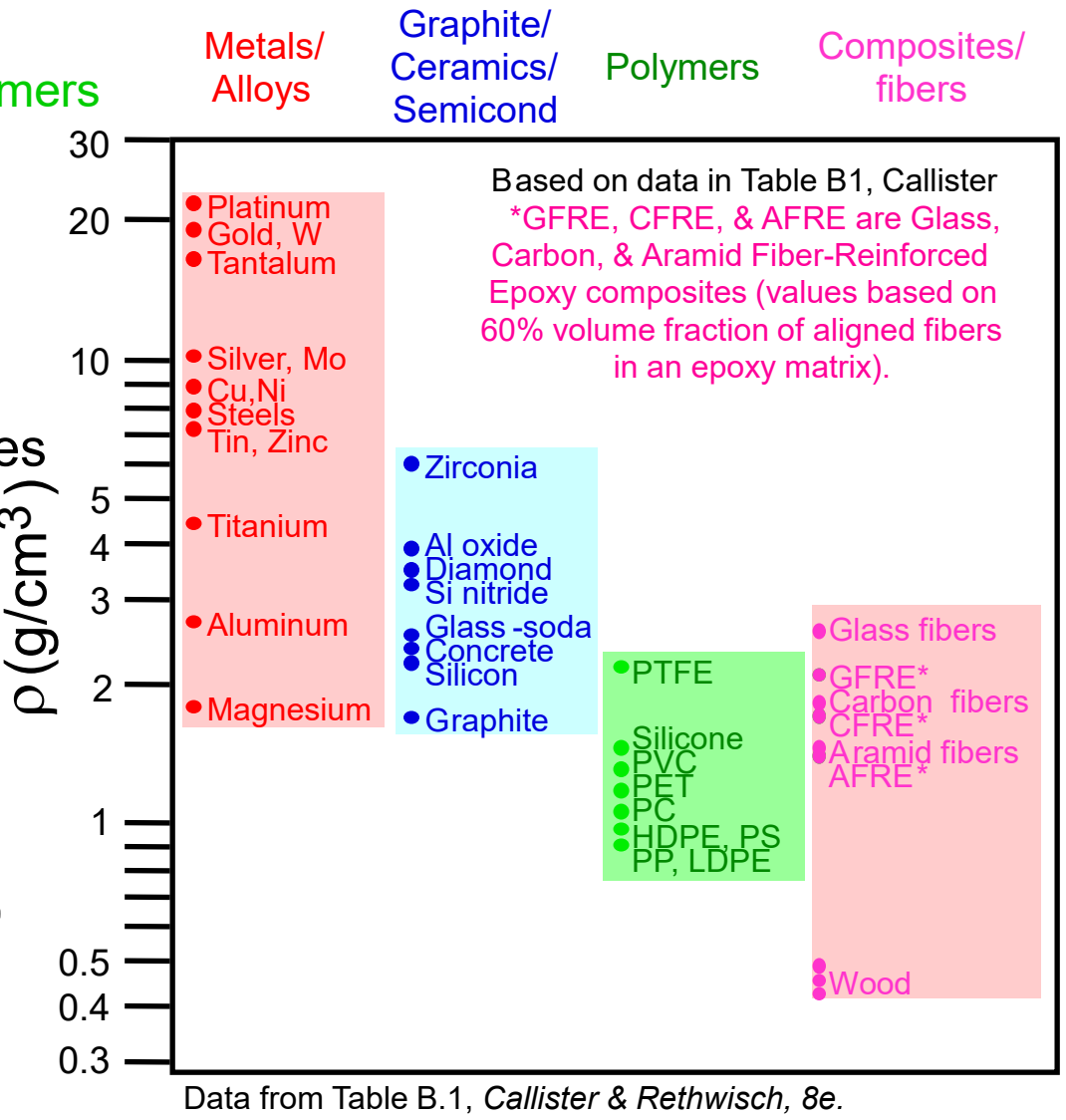
Why?

Metals have...
- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...
- less dense packing
- often lighter elements

Polymers have...
- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...
- intermediate values

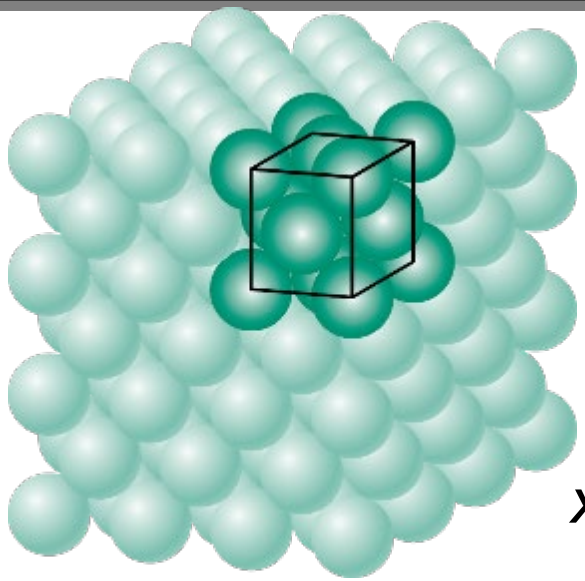


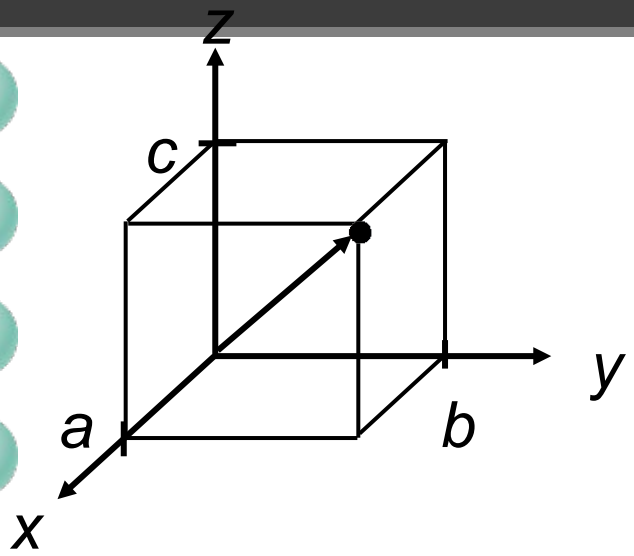
Data from Table B.1, *Callister & Rethwisch, 8e.*

Crystal Coordinates, Directions, Planes

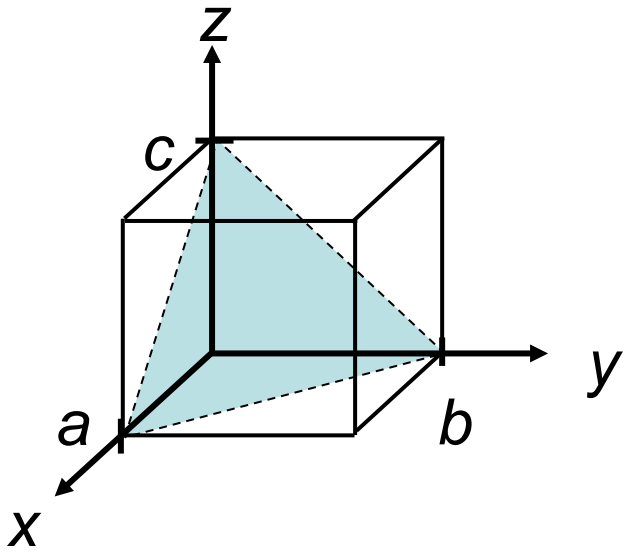
- How can we identify crystal coordinates, directions, and planes?
  - Or how we talk a common language about crystals

How We Do It





- Points
  - 111
- Directions
  - [111]
  - Families <111>
    - Will be used in Ch 7
- Planes
  - (111)
  - Families {111}
    - Will be used in Ch 7



The direction of the red arrow is:

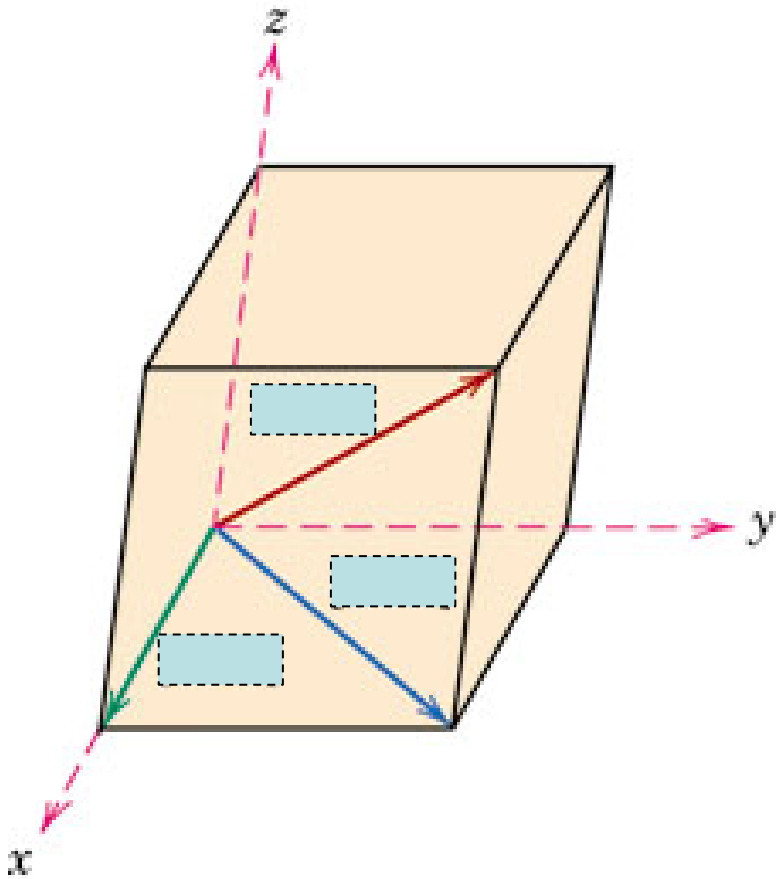
A. [1 0 0]

B. <1 0 1>

C. <1 1 1>

D. [1 1 0]

E. [1 1 1]



Which of the following has the highest atomic packing factor (APF)?

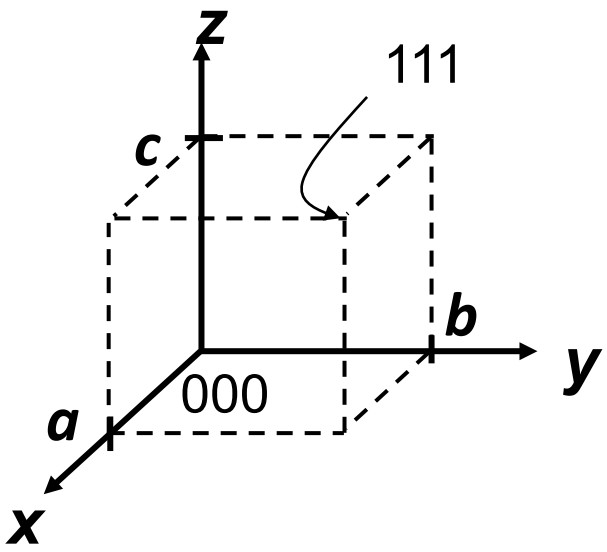
A. Simple Cubic

B. FCC

C. BCC

D. HCP

Point Coordinates

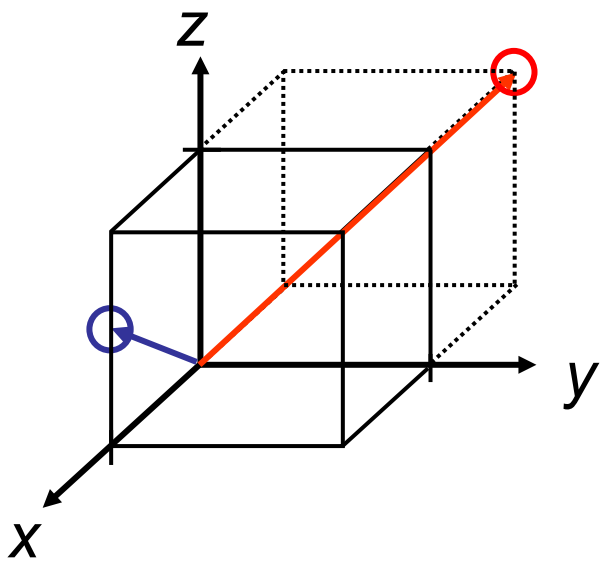


Point coordinates for unit cell center are

a/2, *b*/2, *c*/2 ½ ½ ½

Point coordinates for unit cell corner are 111

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*]

families of directions <uvw>

ex: 1, 0, ½ → × 2 → 2, 0, 1 → [201]

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

Crystallographic planes are typically identified with which of the following:

A. Direction indices

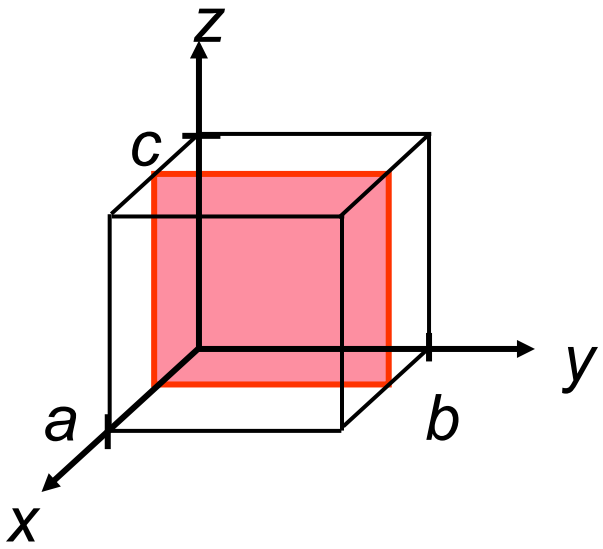
B. Planar Directions

C. Miller Indices

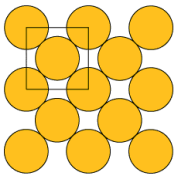
Crystallographic Planes

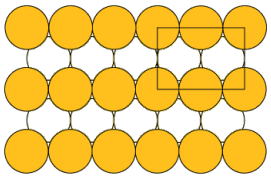
- Miller Indices: **Reciprocals** of the (three) axial intercepts for a plane, cleared of fractions & common multiples.
  All parallel planes have same Miller indices.

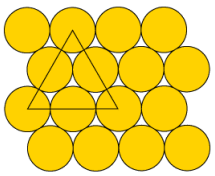
- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)



Why? (FCC)

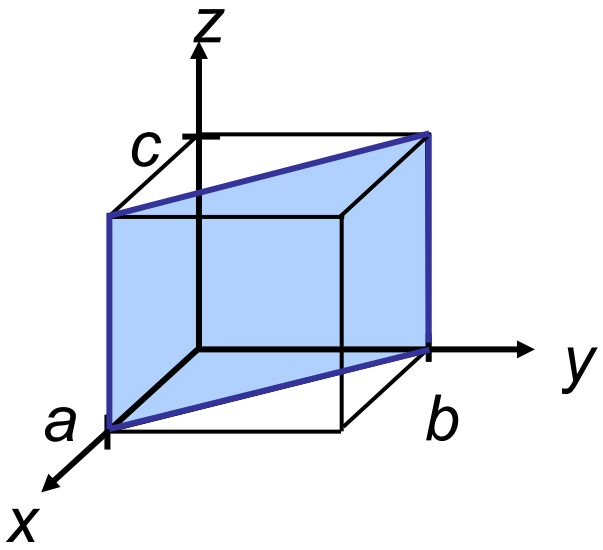

(100)


(110)

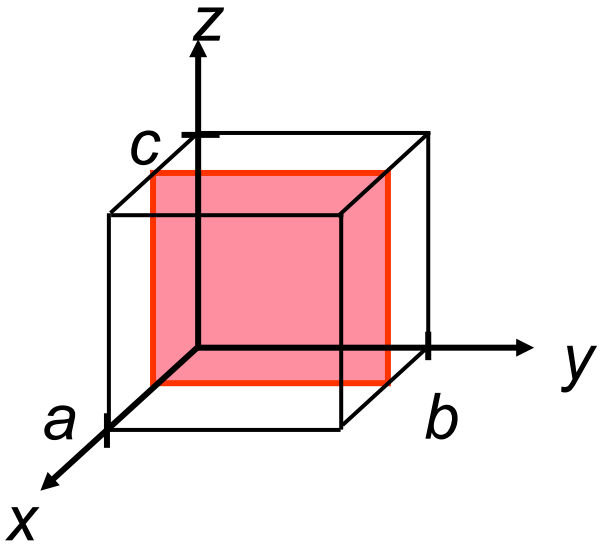

(111)

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)**	

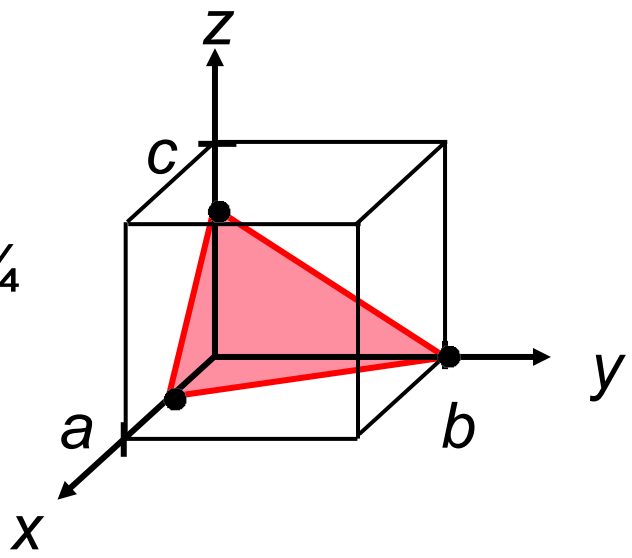


example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	1	0	0
4.	Miller Indices		**(100)**	



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), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$

Select the correct set of indices for this plane

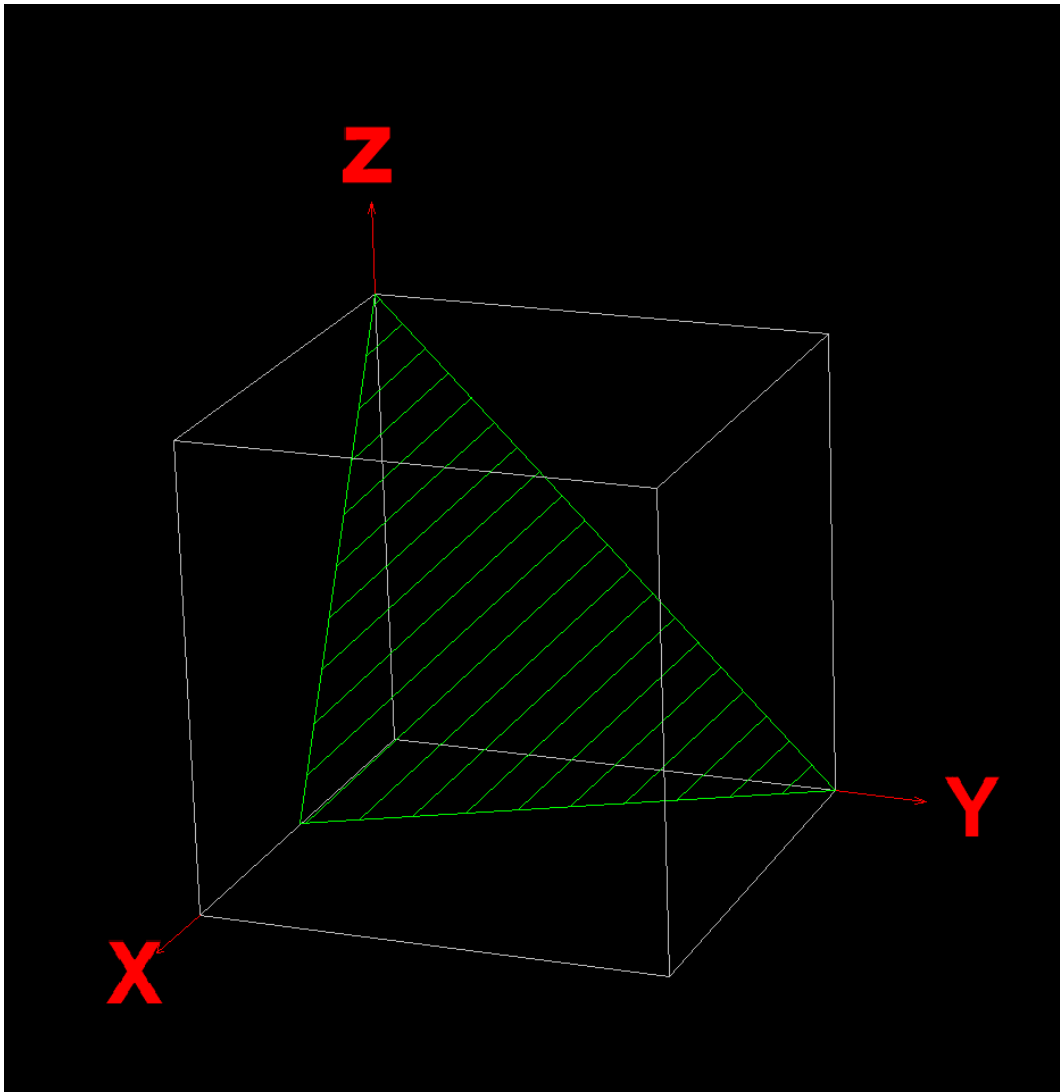
A. (211)

B. $(21\bar{3})$

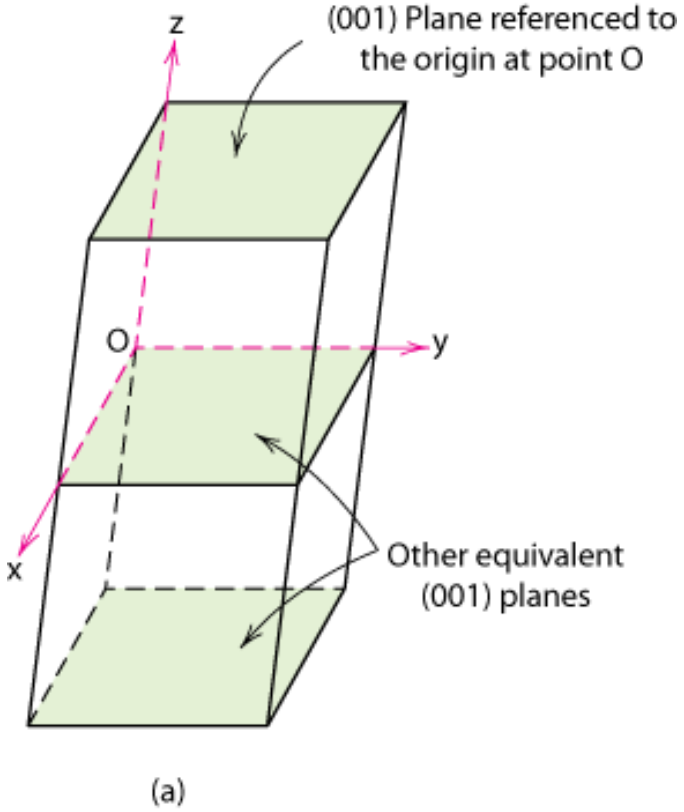
C. $(\bar{3}32)$

D. $(\bar{2}0\bar{1})$

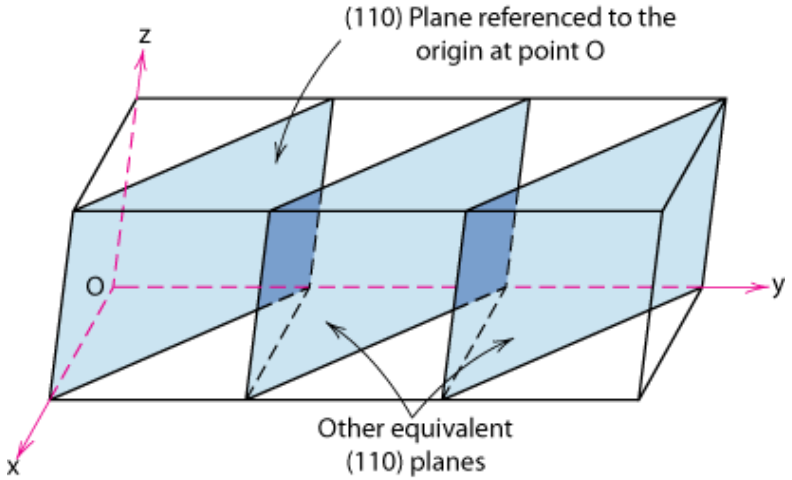
E. $(1\bar{1}0)$



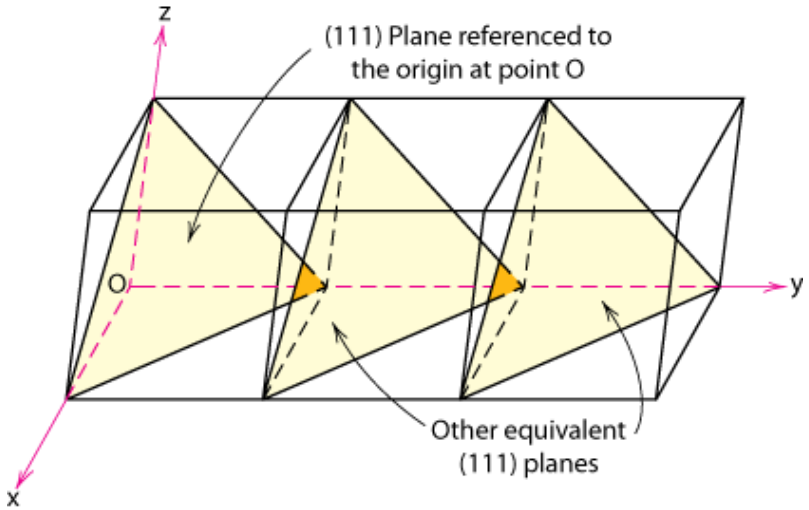
Crystallographic Planes



(a)



(b)



(c)

Adapted from Fig. 3.10,
Callister & Rethwisch 8e.

Review Summary

- Points
  - 111
- Directions
  - [111]
  - Families <111>
    - Will be used in Ch 7
- Planes
  - (111)
  - Families {111}
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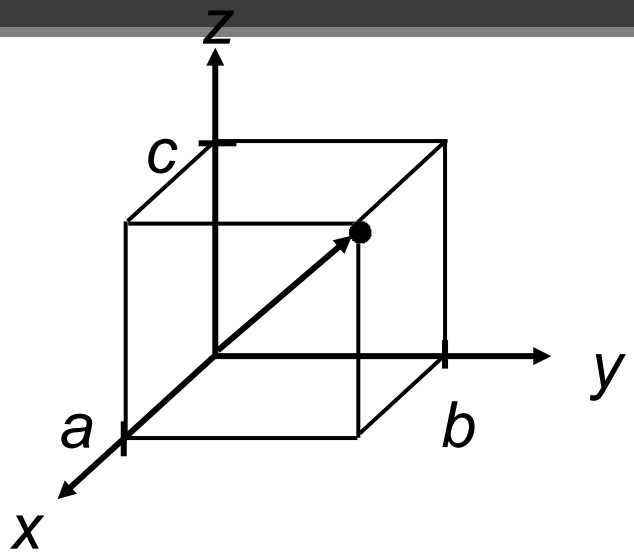
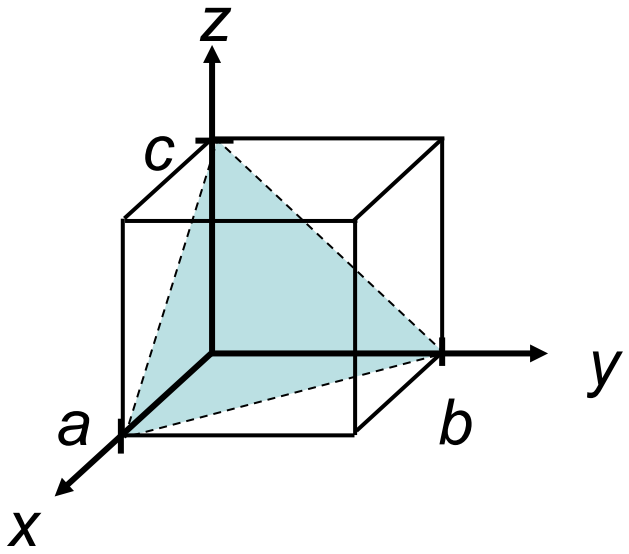


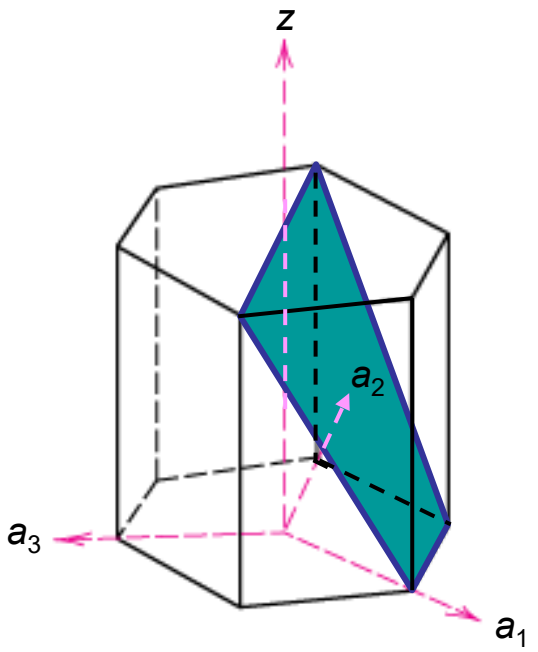


Crystallographic Planes (HCP)

- 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	$1/\infty$	-1	1
	1	0	-1	1
3. Reduction	1	0	-1	1

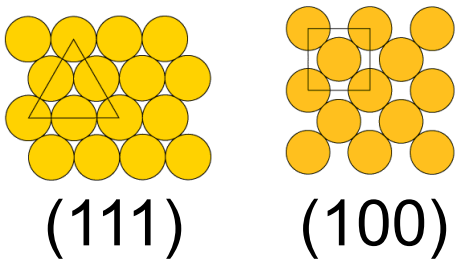
4. Miller-Bravais Indices $(10\bar{1}1)$



Adapted from Fig. 3.8(b), *Callister & Rethwisch 8e.*

Bigger Picture

- Classifying crystals
  - Metrics ✔
  - Planes/directions ✔
  - Densities
- Real Materials
  - Single/Polycrystal
  - Anisotropy
  - Characterization



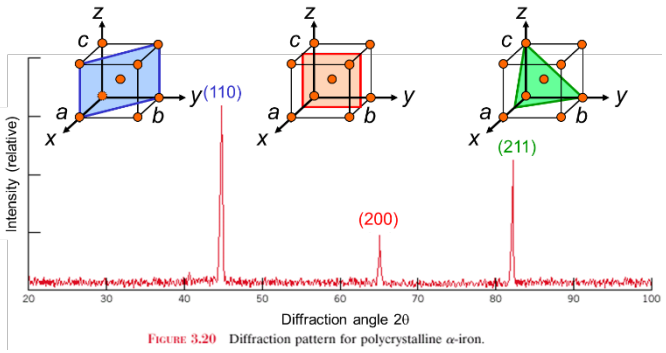


FIGURE 3.20 Diffraction pattern for polycrystalline α-iron.