Materials Science (C)

By

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Safety

- Students must wear:
  - Closed shoes
  - All skin from neck to toes covered
  - Lab coat or lab apron
  - Indirect vent or unvented chemical splash proof goggles.
  - All skin from neck to wrists covered
  - Long hair (shoulder length or longer) must be tied back
  - N95 or KN95 Mask while puck testing going on

What Students May Bring

- One non-image capable calculator per student.
- One unique 8.5 X 11” sheet of paper, two sided containing information in any form from any source per team member
- A writing instrument
- Chemistry “C” lab kit
- Concrete puck for testing
- Design Log

Students can bring Chemistry C kit consisting of:

- Spot plate or something to do reactions in
- Microspatula or something to get powders out
- Forceps/ Metal Tongs
- Hydron paper
- Hand lens

Chemistry C kit

- Test Tubes
- Test Tube rack
- Test Tube holder
- Eye droppers
- Funnel
- Filter Paper
- Battery Conductivity meter
- Flame loop/cobalt blue glass
- Ruler
- Nail, Zn, & Cu metals

Chemistry C kit

- Stirring rods or something to stir with
- Slide & cover slip
- Pencil
- Paper towels
- A test tube brush
- Thermometer
- Petri Dish

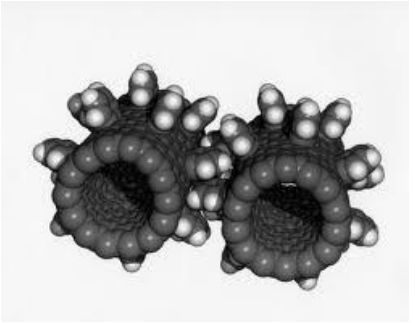
Chemistry C kit

- Graduated Cylinders
- Erlenmeyer Flasks
- Battery multimeter
- Alligator clip wires
- Calipers
- Will all of this be any good to Materials Scientist?
- No, but we are going for one kit
- Nothing else is allowed!!!!!!

What Supervisors Will Supply

- Everything the student will need
  - This may include:
    - Glassware
    - Reagents
    - Balances
    - Hot plates
    - Probes
    - Stirrers
    - Model materials
    - Concrete testing area with meter stick & concrete or metal base

Materials Science



- Materials Science - a relatively new interdisciplinary field
- It merges Metallurgy, Ceramics, Polymers, & Composites
- It merges Chemistry, Physics, Biology and Geology
- Materials Science takes advantage of the fact that we can not make pure crystals of anything & the interesting effects of the impurities.
- It also focuses on how to make purer crystals
- Materials Science is a field where many of our students will find lucrative employment in the future.
- Materials Science also incorporates the fascinating area of nano-technology

Main Focus

- The competition will focus on the chemical structure, synthesis, characterization, performance, processing and applications of ceramic and composite materials
- How to prepare Students
- Experiment ideas
- Resources

Ceramics

- This year the focus of Materials Science will be Ceramics
- Ceramic materials are nonmetallic inorganic materials that have typically gone through a heating and cooling cycle
- They can be crystalline or glassy or both crystalline and glassy
- They are relatively chemically inert
- They are often grouped into 5 types:
  - Structural
  - Refractory
  - Electrical
  - Magnetic
  - Abrasive

Event Parameters

- Pre-build Puck Testing 10%
- A log of student experimentation 8%
- Laboratory Activities 32%
- Written Test 50%

Pre-build Puck

- Students will determine the best composition of Portland type cement, sand, gravel, and water to use to make an ~4 cm ± 0.2 cm in diameter concrete puck 1.5 cm thick for Invitationals & Regionals, 1.0 cm thick for State, & 0.5 cm thick for Nationals. These are maximum thicknesses.
- Toilet tissue rolls can be used for forms

Puck Testing

- The pucks will be dropped from heights from 20 cm to 100 cm at 20 cm intervals onto a cement or steel area/pad.
- Tournaments will announce ahead of time what the pucks will be dropped on to.
- Any sign of cracking, chipping, or breaking will be declared a failure & prevent higher drops.
  - In other words if there is any alteration to the surface, after the drop, it is not allowed to be dropped again

Puck Testing Continued

- If pucks show any sign of wetness when they fail, they will be disqualified
- Everyone present in testing area must wear an N95 or KN95 mask as well as safety goggles
- If pucks are tested in the same room as the rest of the activities, everyone in the room must wear both masks & goggles
- If the testing is done in a separate room, only those present must mask & goggle
- Goggles will be worn during any laboratory activities

More Puck Testing

- If concrete floors are not available, non-porcelain ring stand basses can be used
- Pieces of steel or cement slabs can also be purchased inexpensively and used.

Design Log Continued

- The design log will have a cover that lists
  - The school name
  - The students names
  - The team code for the tournament
- A page with the composition of the puck being tested at that tournament

Design Log

- Students will make tests on at least 10 different combinations of
  - Portland type cement
  - Sand
  - Gravel
  - Water
- The failure heights will be recorded & graphed
- So the 4 pages (max 2 pts each) are:
  - 1) Title page
  - 2) Particular concrete composition being tested that day
  - 3) Chart with at least 10 concrete compositions and their fail height
  - 4) Graph of the above chart

Lab Activities

- In addition to the puck testing, the event must contain at least one lab activity dealing with ceramics, crystal structure, characterization of ceramic or composite materials, etc.
- Lab activity ideas might include, but are not limited to:
  - Asking the students to make a crystal structure by choosing which metal to use with Borax in a Bunsen burner flame
  - Asking students to make a crystalline structure out of toothpicks & marshmallows
- Determining the elastic modulus of a candy bar
- Students might be asked to make a “glass” rod of a given length from molten Jolly Ranchers
- Students might be asked to light an LED with a piezoelectric device

The Written Test

- The written test will make up 50% of the event points
- This year we are focusing on ceramics and the topics of materials science that are important to ceramics.

Structure, Performance, Processing, & Application Topics

- Characterization
- Performance
- Processing
  - Stress-Strain behavior
  - Materials Selection
  - Elastic Modulus (Young's Modulus)
  - Flexural strength
  - Sheer Modulus
- Phase diagrams
  - TTT Diagrams
- Fracture toughness
- Brittle fracture
- Breaking Strength (Yield strength)
- Transverse Strain (Poisson's ratio)

Structure, Performance, Processing, & Application Topics

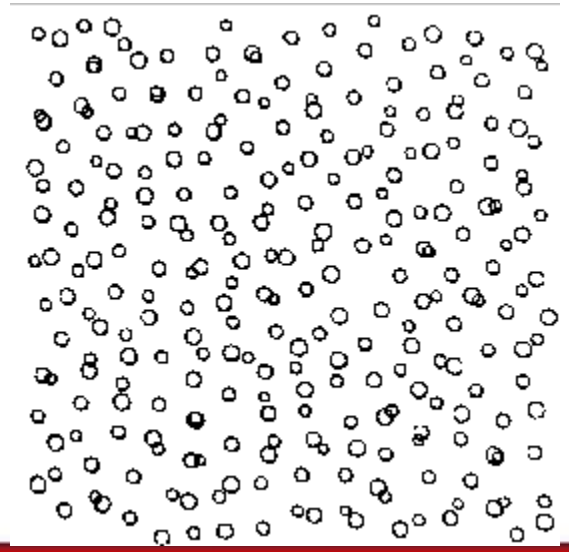
- Chemical Structure
- Crystal Structures
- Interatomic bonding
- Ion Size Ratios
- Grain Boundaries
- Microscopy
- State & Nationals
- Imperfections
- Atomic point defects
- Vacancy
- Interstitial cations
- Impurities
- Frenkel Defects
- Schottky defects

Applications

Types of ceramics/glasses and their uses

Materials Selection

- Properties
  - Stiffness
  - Heat Resistance
  - Cost



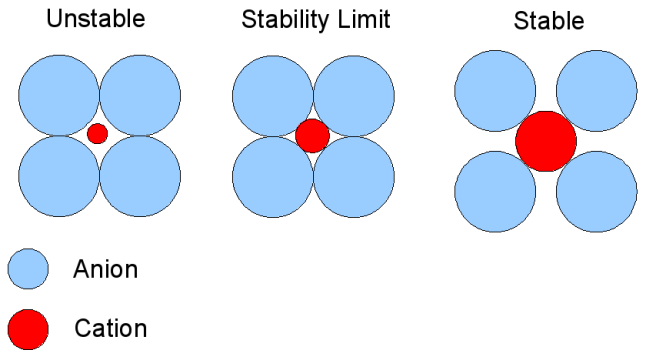
Composition	*Property*	*Use*
	Glasses	
Al_2O_3, MgO, CaO, SiO_2	Translucent, chemically resistant	Window glass, bottles
PbO, SiO_2	High refractive index	Lead crystal
B_2O_3, SiO_2, Na_2O	Acid resistant, low expansion on heating	Pyrex
	Glass Ceramics	
MgO, Al_2O_3, SiO_2	Insulator with high mechanical strength at high temperatures	Spark plug insulators
$CaSiO_3$, $CaMgSi_2O_6$, $CaAl_2Si_2O_8$	Wear resistant	Building materials
$Li_2Si_2O_5$	Resistant to thermal shock	Nose cones on rockets, cookware

Ceramics

- Any inorganic, non-metal solid
- Classified as:
- Structural – generally clay based – strong chemical bonding that can endure stress heat and corrosion - bricks, statues, plates – pressed or extruded
- Refractory – heat resistant can withstand temperatures in excess of 1,00 °F (538°C) – more heat resistant than metals – typically xoides, carbides, or nitrides of Si, Al, Mg, Ca, B, Cr, & Zr
- Electrical – great insulators – vitrification-process of transforming clay into glass, an amorphous, non-crystalline solid
- Magnetic
- Abrasive – Brakes, clutches, bullet proof vests – Diamond, sand, WC

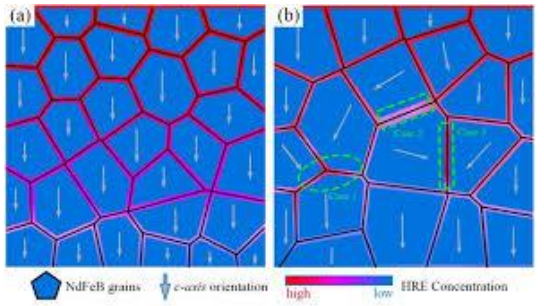
Chrystal Structures

- Crystal structures are predicted by the ratio of the cation radius to the anion radius
- Only works about 2/3^{rds} of the time
- Ratio calculated by equation $\frac{Radius_{cation}}{Radius_{anion}}$
- The type of crystal structure can be predicted from the Ratio by the equation R = $\sqrt{\frac{12}{12-CN}} - 1$
- Where CN is the coordination number



Critical Radius Ratio	Coordination Number	Structure
0.1547	3	Trigonal planar
0.2247	4	Tetrahedral
0.4142	6	Octahedral
0.7320	8	Cubic

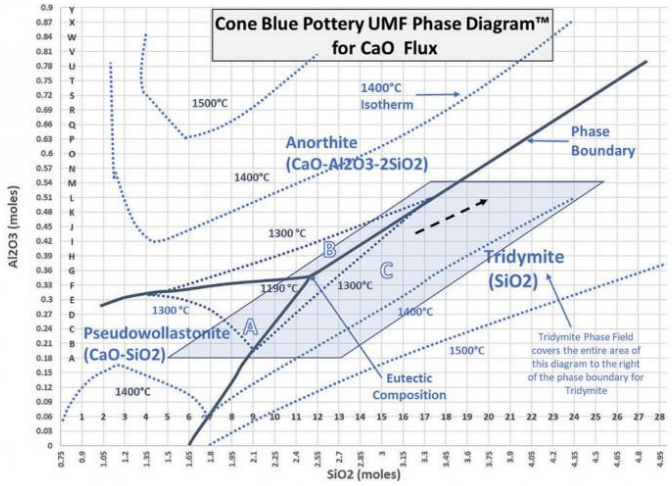
Chemical Structure-Bonding

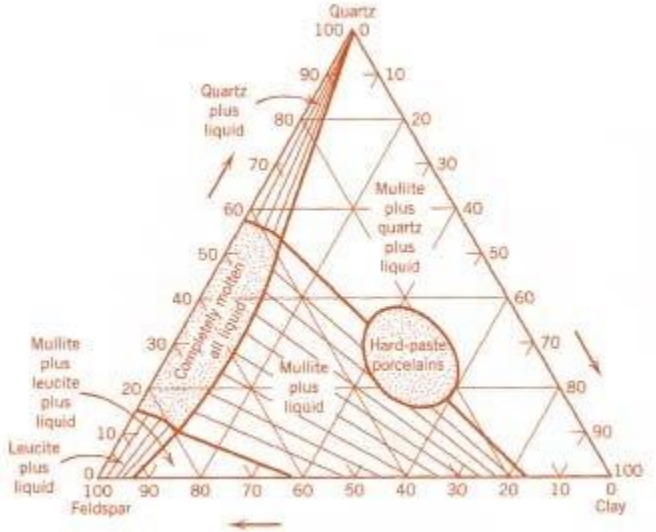


- Bonding in ceramics is more complex
- Both ionic and covalent bonding exist in the same piece
- Ionic bonding is usually the most prevalent
- Some metallic bonding may also be present
- When ceramics start to solidify, many different crystals will form
- When the crystals form so far, they will meet another crystal forming
- The space between the crystals is the grain boundary.

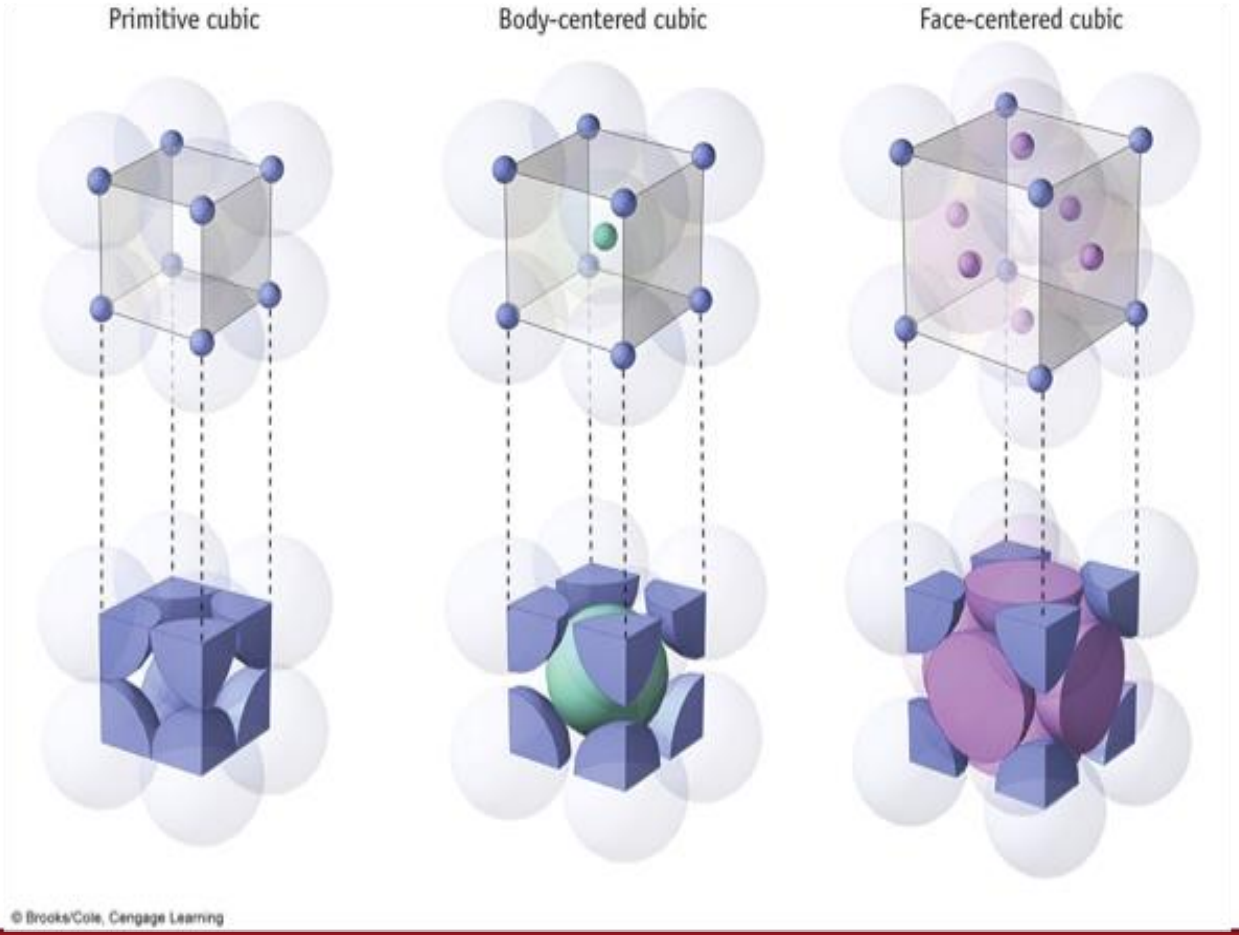
Phase Diagrams

- A phase diagram plots the temperature vs. time for a ceramic material and lays out where the ceramic will be solid, liquid, or gas.
- TTT diagrams stand for time, temperature, and transformation.
  - Also known as isothermal plots



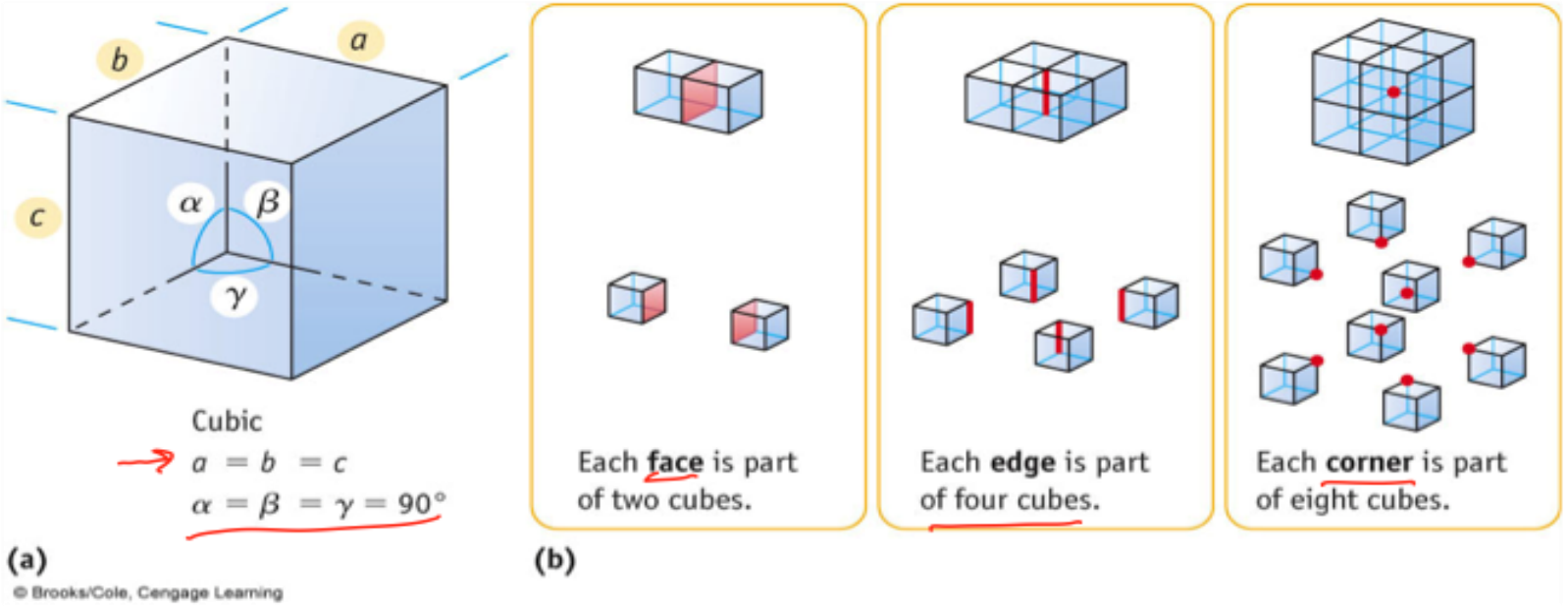


Crystal Structure



Cubic Crystal Lattices

$\gamma = 90^{o}$

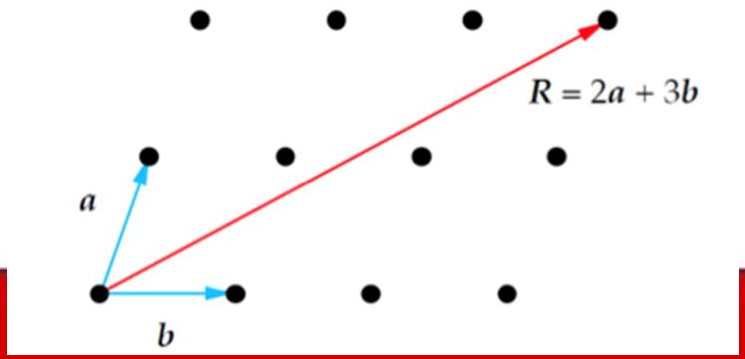


The size and shape of a unit cell is described, in three dimensions, by the lengths of the three edges (a, b, and c) and the angles between the edges (α, β, and γ).

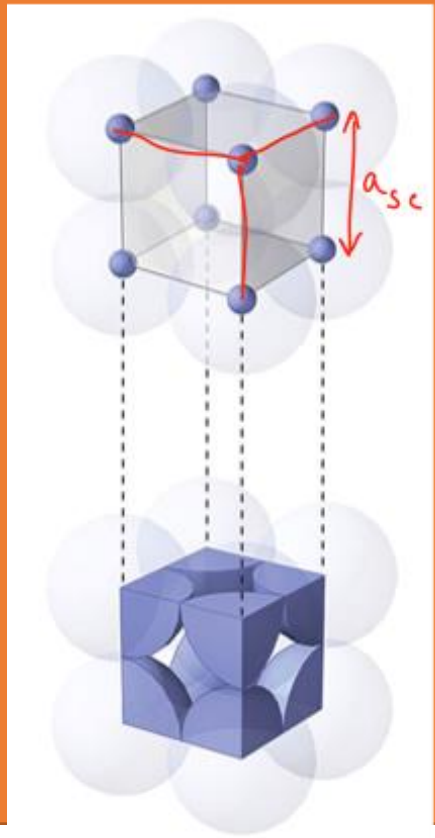
These quantities are referred to as the lattice parameters of the unit cell.

Space Lattice

- A lattice is an array of points repeated through space
- A translation from any point through a vector R_{lmn}+la+mb+nc, where l, m, & n are integers, locates an exactly equivalent point. a, b, & c are known as lattice vectors.

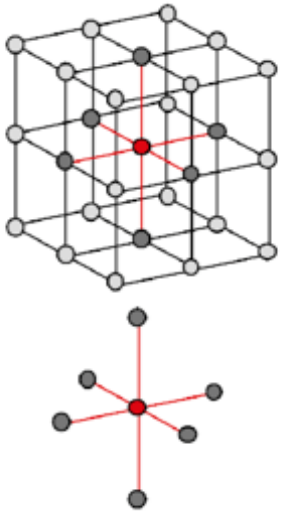


Simple Cubic



- Atoms per unit cell
  $(\frac{1}{8}) \cdot 8 = 1$
- Cell Edge Distance, $a_{SC} = 2 \cdot r$
- Cell Volume, $V_{SC} = a_{SC}^{\ 3} = 8 \cdot r^3$
- Each atom has 6 nearest neighbors

Coordination # = 6
(# nearest neighbors)

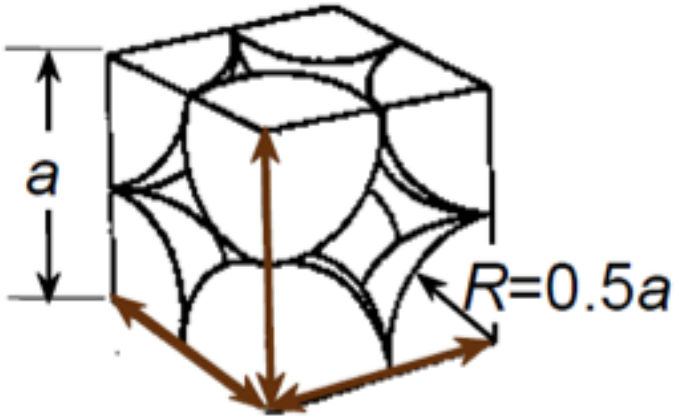


Simple Cubic Atomic Packing Factor

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



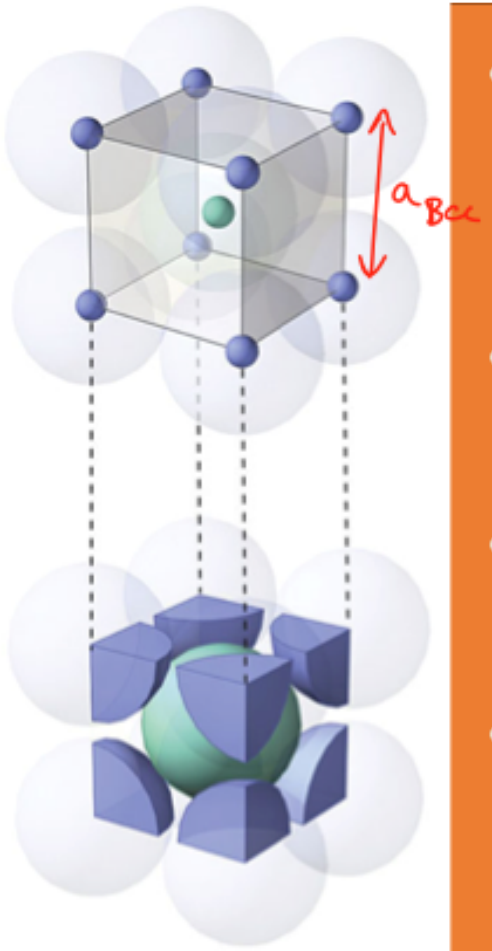
close-packed directions

contains 8 x 1/8 =

1 atom/unit cell

$$APF = \frac{\dfrac{\text{atoms}}{\text{unit cell}} \cdot \dfrac{\text{volume}}{\text{atom}}}{\dfrac{\text{volume}}{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

Body-Centered Cubic (BCC)



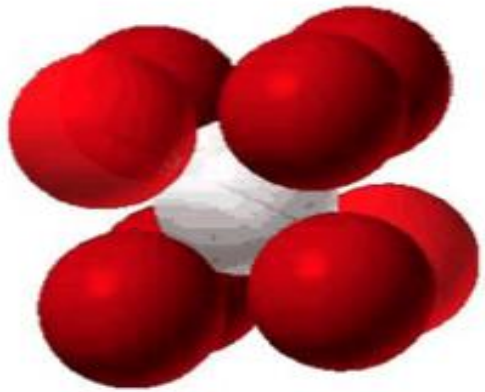
- Atoms per unit cell
  $(\frac{1}{8}) \cdot 8 + 1 = 2$
- Cell Edge Distance, $a_{BCC} = \frac{4 \cdot r}{\sqrt{3}}$
- Cell Volume, $V_{BCC} = a_{BCC}^{\ 3} = 64 \cdot \left(\frac{r}{\sqrt{3}}\right)^3$
- Each atom has 8 nearest neighbors

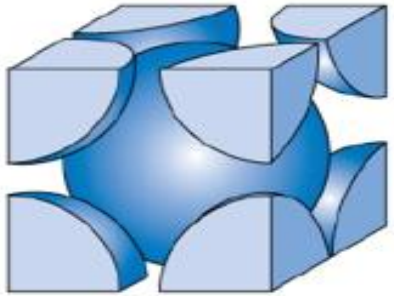
Body Centered Cubic

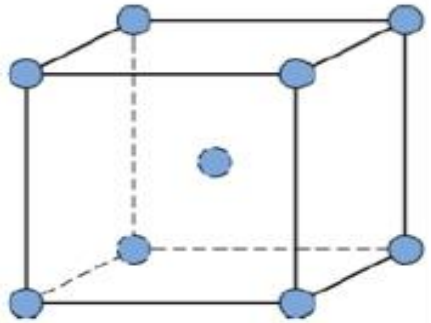
- Atoms touch each other along cube diagonals.
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8





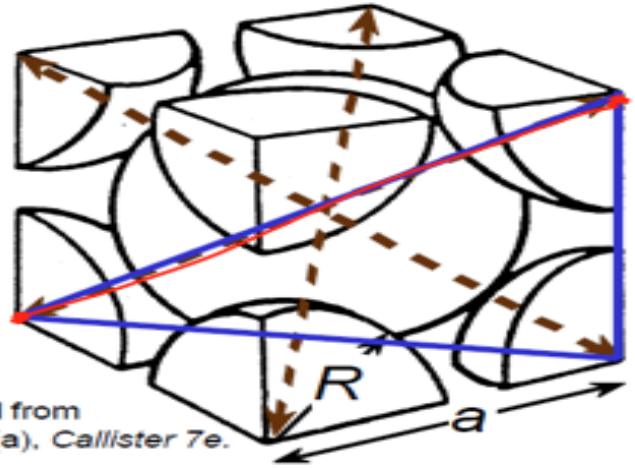


Adapted from Fig. 3.2, *Callister 7e.*

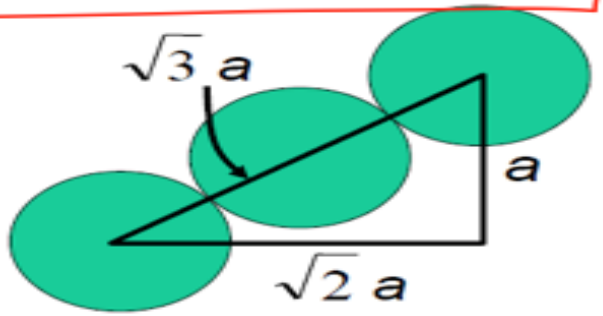
2 atoms/unit cell: 1 center + 8 corners x 1/8

Body Centered Cubic

- APF for a body-centered cubic structure = 0.68



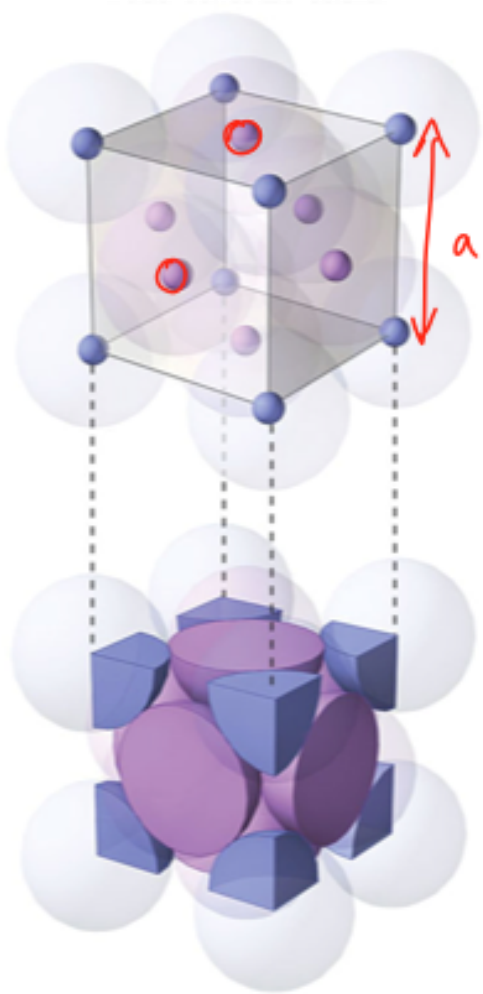
Adapted from Fig. 3.2(a), *Callister 7e.*



Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3\right)}{a^3}$$

Face-Centered Cubic (Cubic Close-Packed)



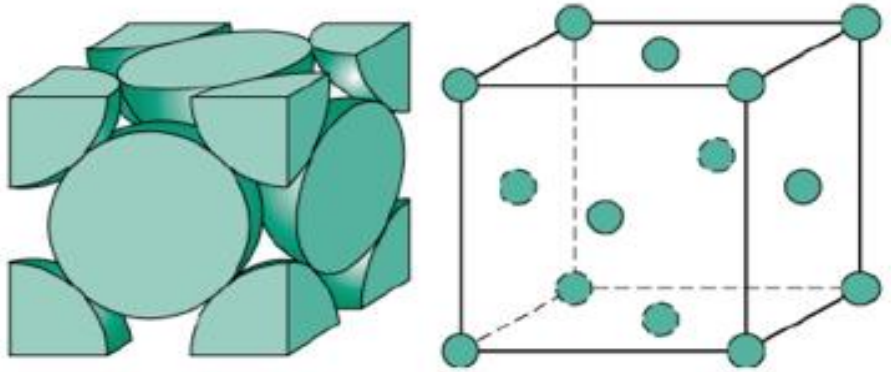
- Atoms per unit cell
  $(\frac{1}{8}) \cdot 8 + (\frac{1}{2}) \cdot 6 = 4$
- Cell Edge Distance, $a_{FCC} = 2\sqrt{2} \cdot r$
- Cell Volume, $V_{FCC} = a_{FCC}^{\ 3} = 8 \cdot (\sqrt{2} \cdot r)^3$
- Each atom has 12 nearest neighbors

Face Centered Cubic

- Atoms touch each other along face diagonals.
  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12

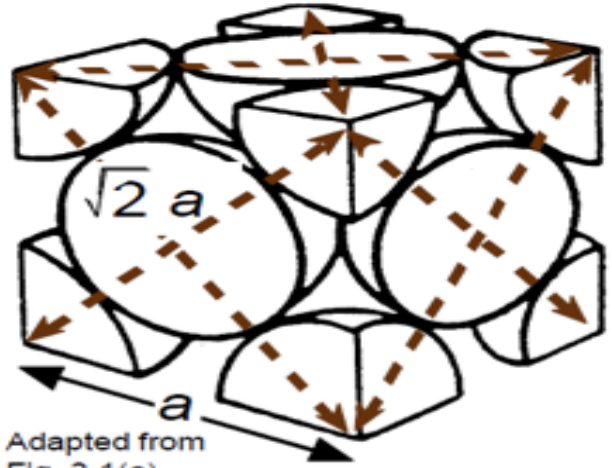


Adapted from Fig. 3.1, *Callister 7e.*

4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

Face Centered Cubic

- APF for a face-centered cubic structure = 0.74
  maximum achievable APF



Adapted from Fig. 3.1(a), *Callister 7e.*

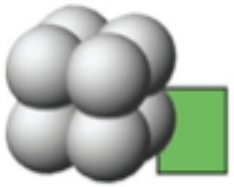
Close-packed directions:
length = $4R = \sqrt{2}\,a$

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \rightarrow \frac{4 \left(\frac{4}{3}\pi (\sqrt{2}a/4)^3\right)}{a^3} \leftarrow \frac{\text{volume}}{\text{atom}}$$

$$a^3 \leftarrow \frac{\text{volume}}{\text{unit cell}}$$

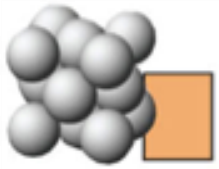
Crystal Structure Summary



Primitive

$$a_{SC} = 2 \cdot r$$

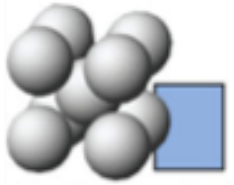
$$V_{SC} = a_{SC}^{\ 3} = 8 \cdot r^3$$



Cubic close packing
(Face-centered cubic)

$$a_{FCC} = 2\sqrt{2} \cdot r$$

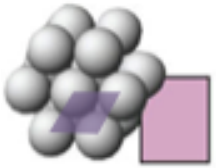
$$V_{FCC} = a_{FCC}^{\ 3} = 8 \cdot (\sqrt{2} \cdot r)^3$$



Body-centered cubic

$$a_{BCC} = \frac{4 \cdot r}{\sqrt{3}}$$

$$V_{BCC} = a_{BCC}^{\ 3} = 64 \cdot \left(\frac{r}{\sqrt{3}}\right)^3$$



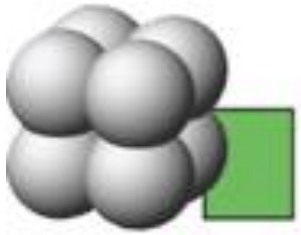
Hexagonal close packing

$$a_{HCP} = 2 \cdot r$$

$$c_{HCP} = \frac{4\sqrt{2} \cdot r}{\sqrt{3}}$$

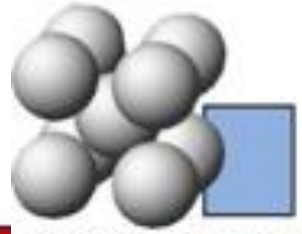
$$V_{HCP} = \sqrt{2} \cdot a_{HCP}^{\ 3} = 8\sqrt{2} \cdot r^3$$

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															

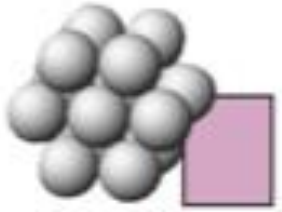


Primitive

Cubic close packing
(Face-centered cubic)



Body-centered cubic



Hexagonal close packing

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Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n\,A}{V_C N_A}$$

where n = number of atoms/unit cell

A = atomic weight

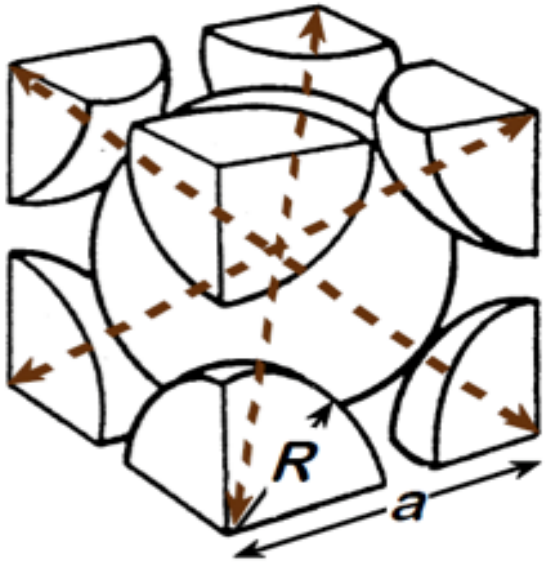
V_C = Volume of unit cell = a^3 for cubic

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

Theoretical Density, ρ

$$\rho = \frac{(\#\ of\ Atoms)\cdot(Atomic\ Mass)}{N_A\cdot(Cell\ Volume)}$$



- Ex: Cr (BCC)

$$\rho = \frac{(\#\ of\ Atoms)\cdot(Atomic\ Mass)}{N_A\cdot(Cell\ Volume)}$$

A = 52.00 g/mol

R = 0.125 nm

n = 2

$a = 4R/\sqrt{3} = 0.2887$ nm

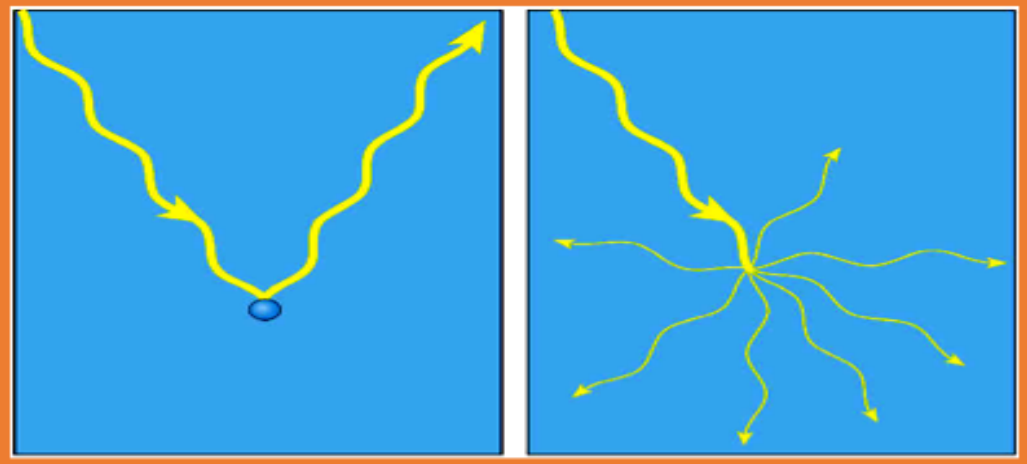
$$\rho = \frac{\frac{atoms}{unit\ cell}\ 2\ \ 52.00\ \frac{g}{mol}}{a^3\ \ 6.023\times10^{23}\ \frac{atoms}{mol}}\ \frac{volume}{unit\ cell}$$

$\rho_{theoretical}$	= 7.18 g/cm^3
ρ_{actual}	= 7.19 g/cm^3

Characterizing a Crystal

Scattering

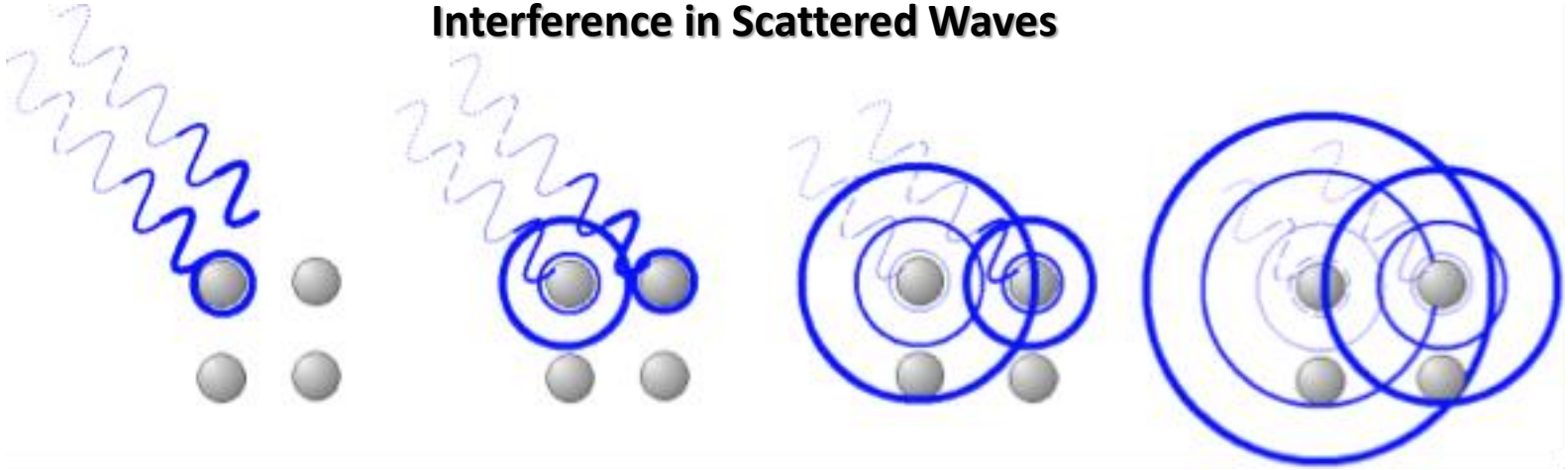
- Scattering occurs when a light wave encounters a particle, droplet, or bubble similar in size to it's own wavelength.



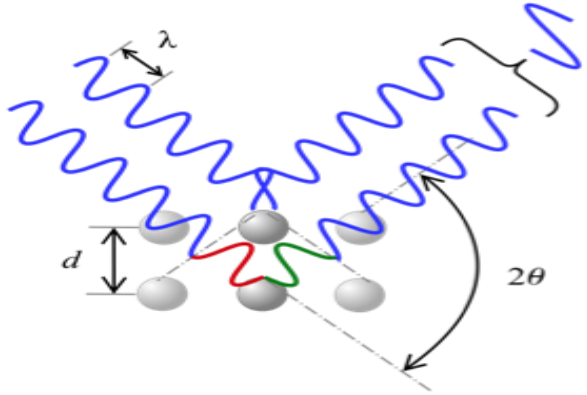
http://www.geography.hunter.cuny.edu/~tbw/wc.notes/2.heating.earth.surface/notes2.htm

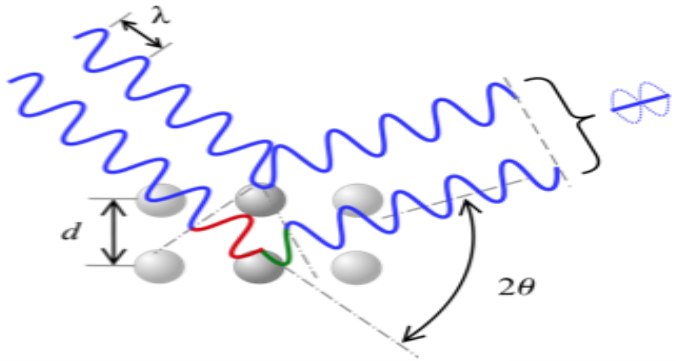
Wave Particle Interaction

Interference in Scattered Waves



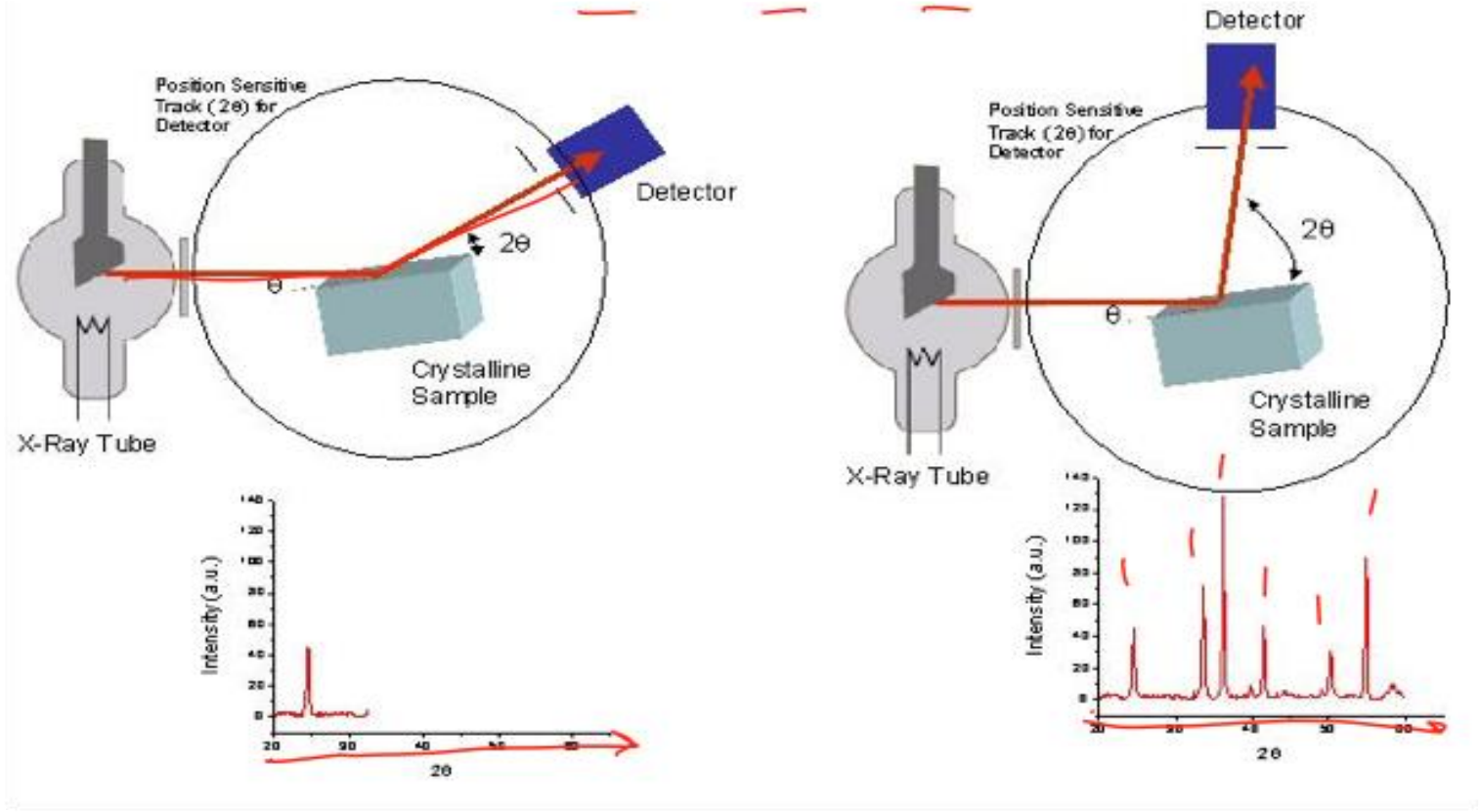
X-ray Diffraction in Crystalline Solids



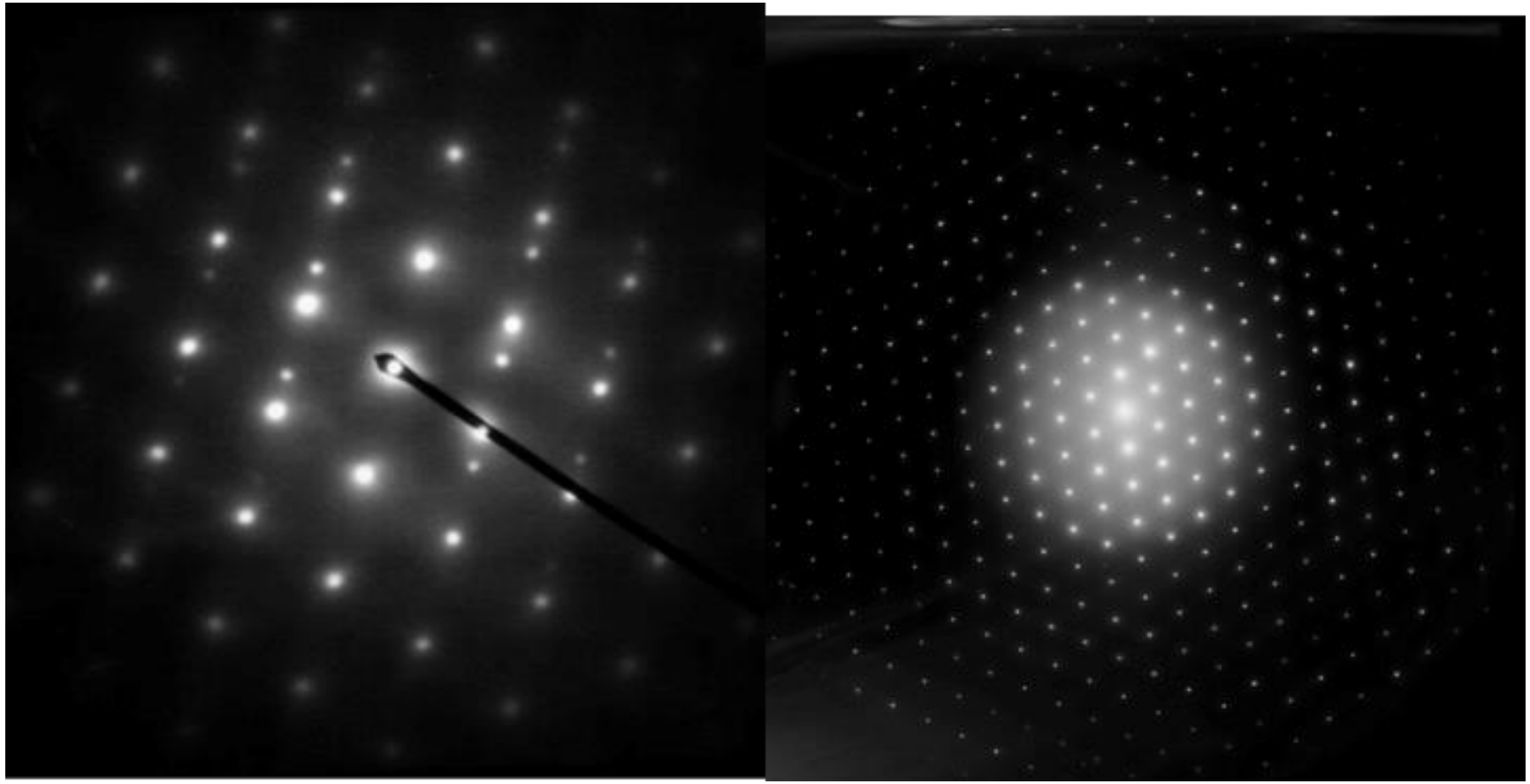


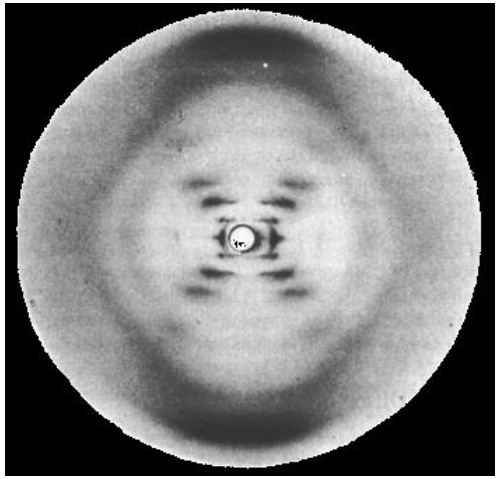
Bragg's Law

$$n \cdot \lambda = 2 \cdot d \cdot \sin\theta$$



Diffraction Patterns

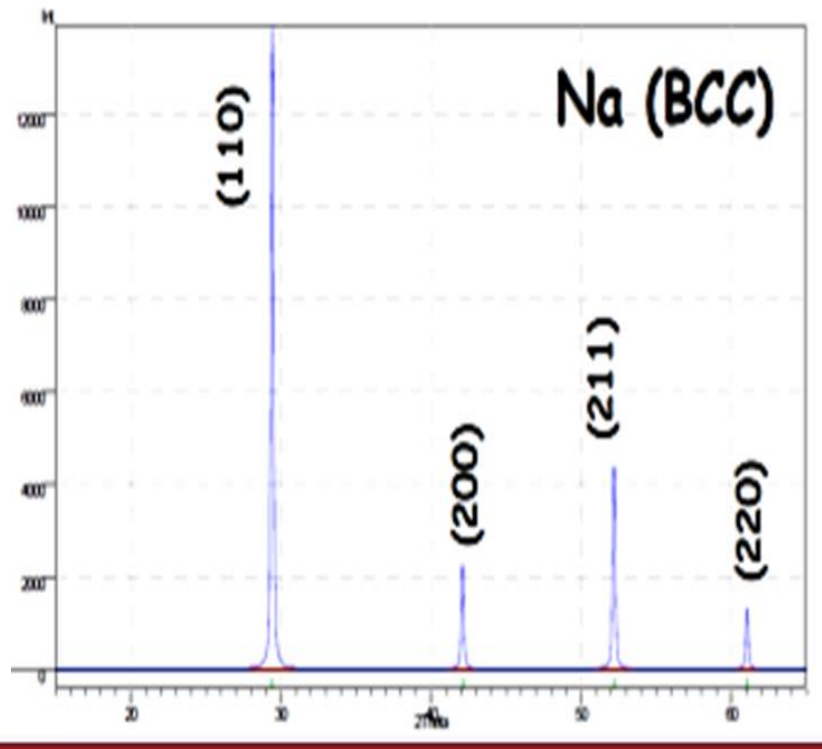


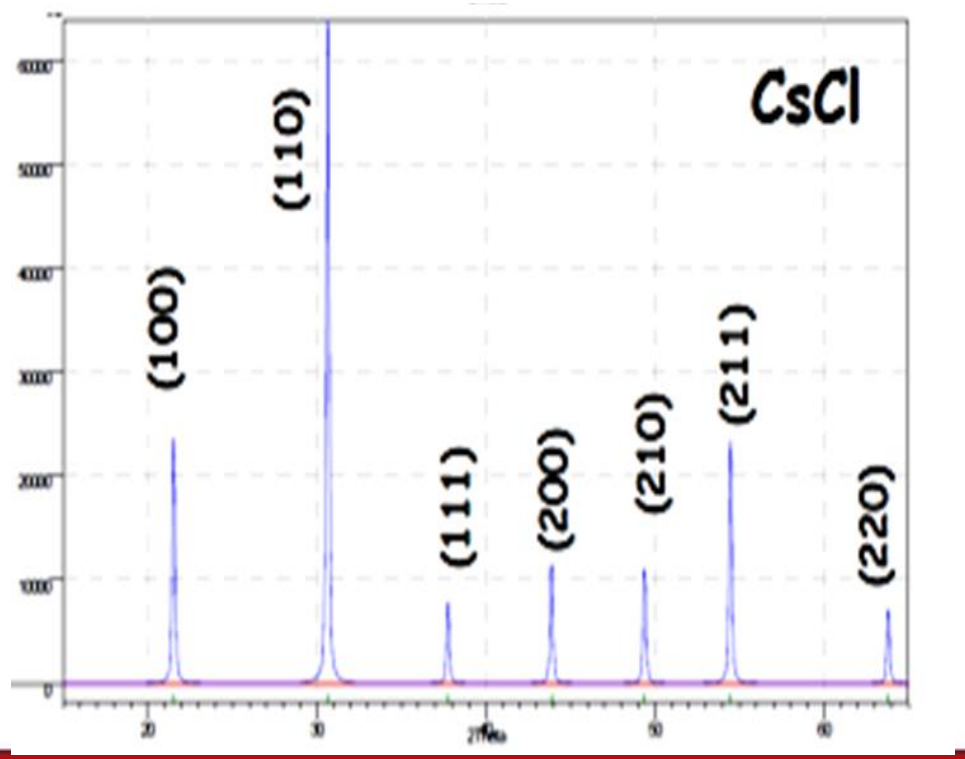


Common X-Ray Wavelengths

Target	$K\alpha_1$ (nm)
Fe	0.193604
Co	0.178897
Ni	0.165791
Cu	**0.154056**
Zr	0.078593
Mo	0.070930

X-Ray Powder Diffraction Patterns





Miller Indices

Understanding crystal orientation

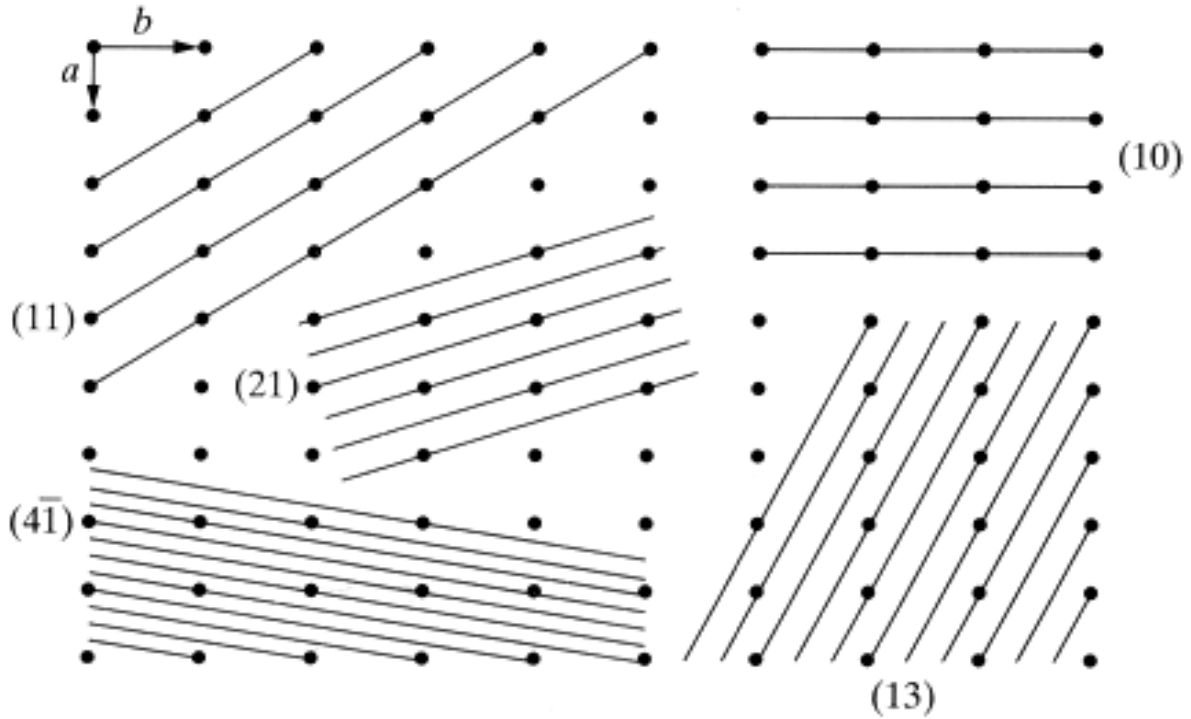


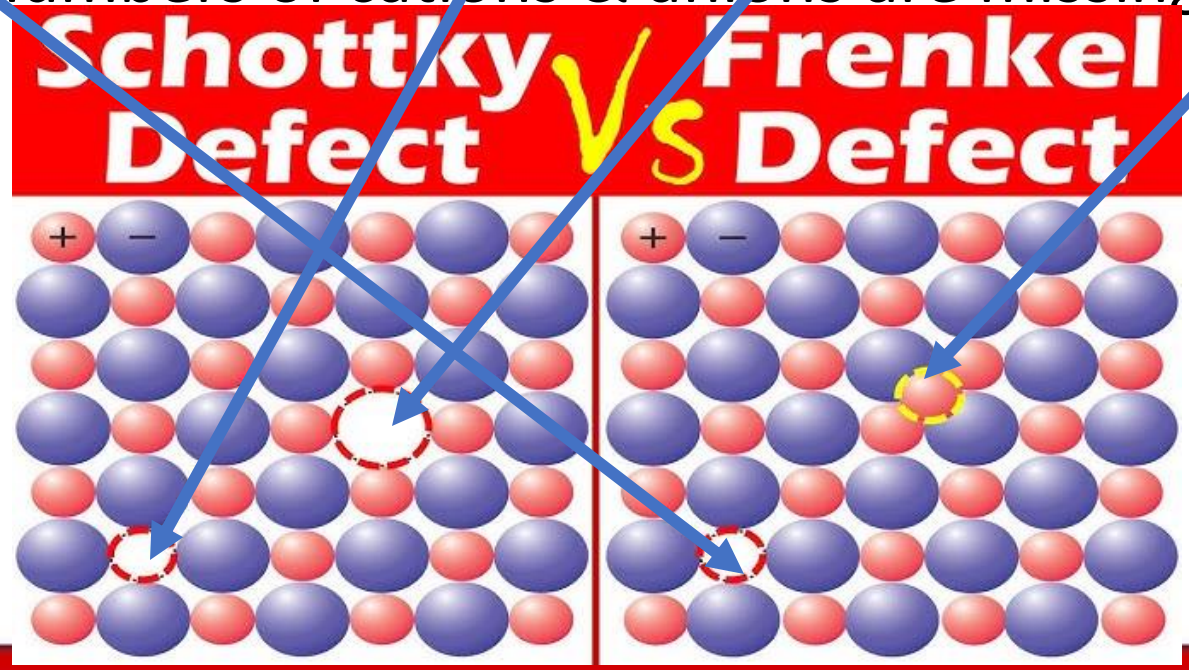
Figure 2-6 Two-dimensional lattice, showing that lines of lowest indices have the greatest spacing and the greatest density of lattice points.

Imperfections

- Types of Imperfections
- Line Defects – involve an entire row of lattice points. Considered one dimensional – grain boundaries
- Point Defects – considered zero dimensional-interstitial cations & anions
- Volume Defects – 3-dimensional defect – voids or empty spaces, foreign particles
- Surface Defects – imperfections at the surface

Point Defects

- Interstitial Cations and Anions same as Frenkel defects
- Frenkel – occurs when an ion tries to fit somewhere it doesn't belong
- Leaves a hole somewhere else in structure where it has moved from
- Schottky – equal numbers of cations & anions are missing from crystal structure

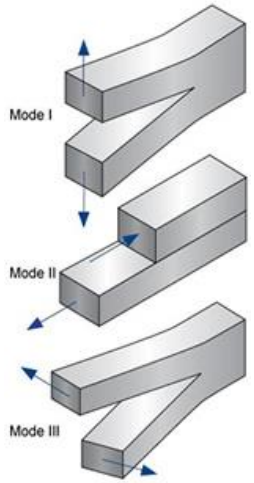


Brittle Fracture

- A type of fracture that occurs when a material fails catastrophically with out much if any plastic deformation
- Occurs typically in materials like glasses and ceramics, but may also occur in metals and some polymers
- It is always sudden and extremely fast
- Occurs in materials with high yield strengths, giving no way for stresses to be relieved
- Actually breaks atomic bonds apart.
- Break occurs so fast, it exceeds sound barrier, which accounts for sound

Fracture Toughness

- Fracture toughness is a measure of how much force you have to exert to propagate an existing fracture.
- Fractures inherently exist in everything.
- There are several ways stress can be applied
- $K_1 = \sigma\sqrt{\pi\alpha\beta}$



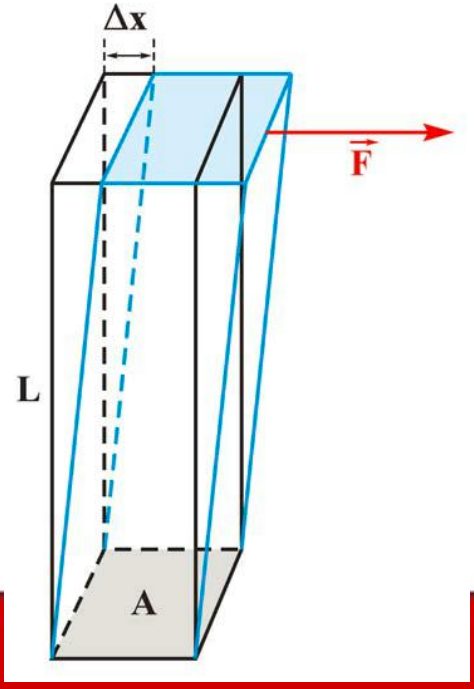
K_1	**is the fracture toughness**
σ	is the applied stress
α	is the crack length
β	is a crack length and component geometry factor that is different for each specimen and is dimensionless.

Fracture Toughness

- Fracture toughness is a measure of how much force you have to exert to propagate an existing fracture
- Fractures inherently exist in everything
- There are several ways stress can be applied
- $K_1=\sigma\sqrt{\pi\alpha\beta}$

Shear Modulus

- The deformation that takes place when a force is applied parallel to one face while an adjacent face is held steady
- $S = \frac{Shear\ Stress}{Shear\ strain} = \frac{\frac{F}{A}}{\frac{\Delta x}{L}} = \frac{FL}{A\Delta x}$



Sheer Force

- Form the Play Dough into a thin rectangular box
- Note the dimensions of the box.
- Put the smallest side of the box on the table and plant it there
- Use the cup and spring scale to apply a force on the top of the box, making sure the bottom does not move
- Note the force applied & how far top moved over
- Sheer Force = $(F*L)/(A*\Delta x)$

Calculating Flexural Strength

- **The formula for flexural strength, σ, under a three-point load is equal to $3FL/2bd^2$, where:**

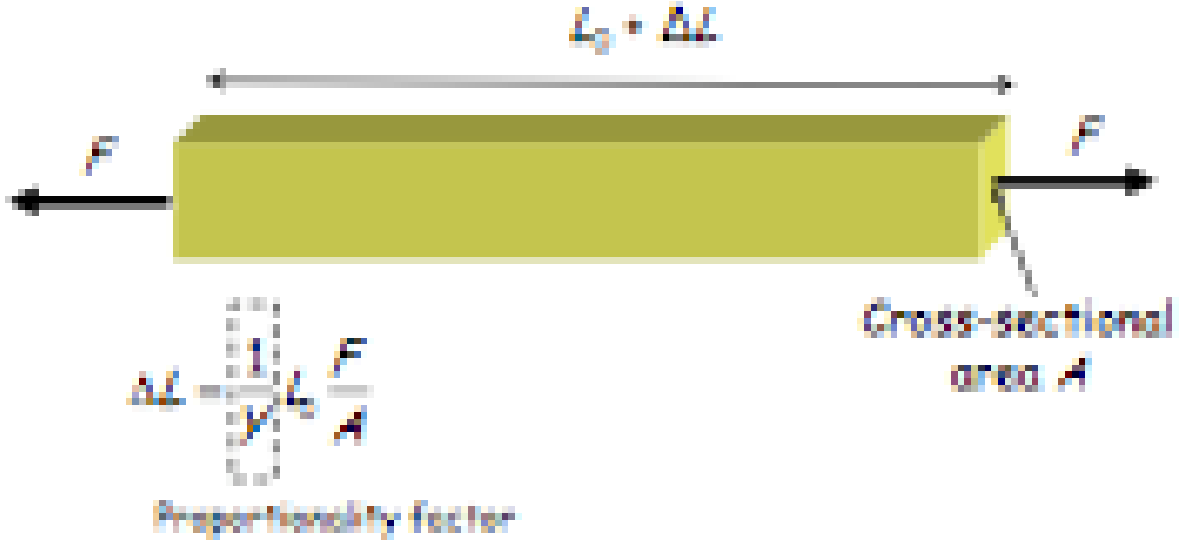
1. F = force at fracture point.
2. L = support span length.
3. b = width of sample.
4. d = thickness of sample.

Young's Modulus – Elastic Modulus

- $E = \sigma/\varepsilon = (F/A_o)/(\Delta L/L_o)$
- Where
- E = Young's Modulus
- σ = Stress
- ε = Strain
- F = Force
- A_o = Initial cross section of material
- ΔL = Change in length of material
- L_o = Initial length of material

Linear Deformation–Stress & Strain

Stress - force applied over a given area. Units of lbs/in^2 or Gigapascals



Strain - Deformation of material as a change in dimension from initial. *Unitless

Young's modulus

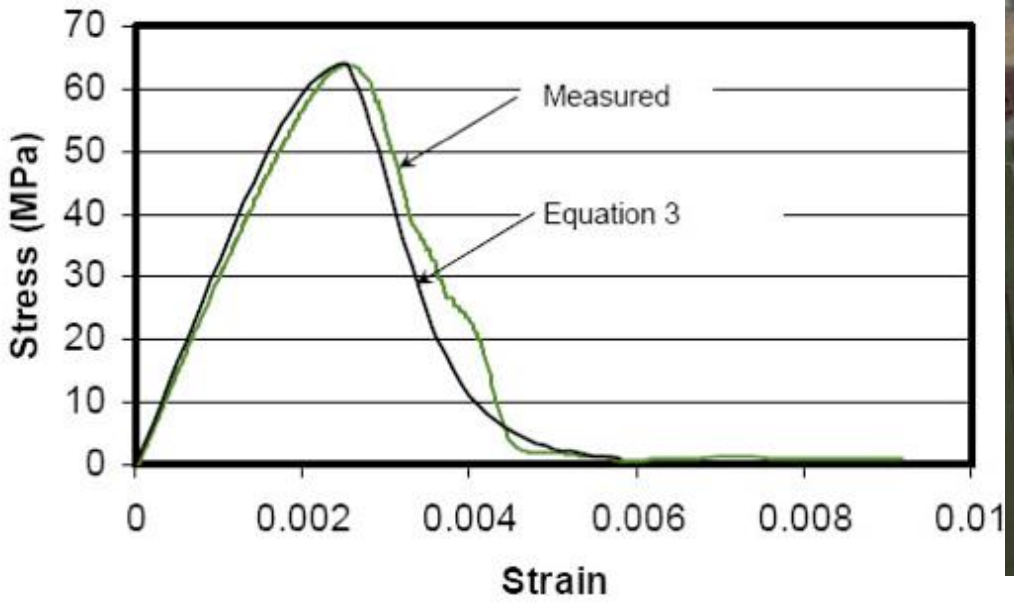
$$Y = \frac{F/A}{\Delta L/L_0}$$

stress

strain (deformation)

Materials Performance

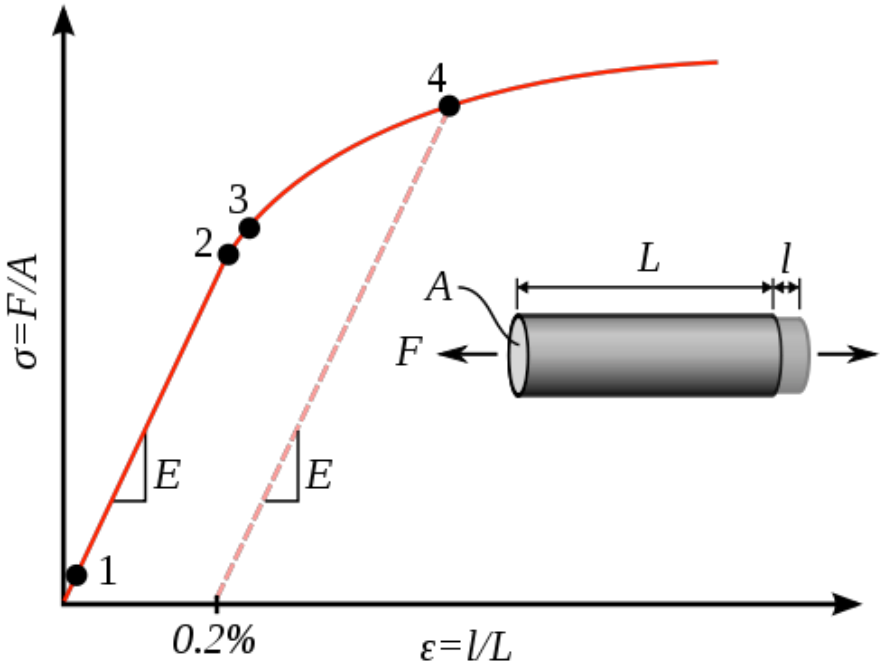
- Stress Vs. Strain relationship



Stress, Strain, & Young's Modulus

- **Young's Modulus**
- **- a measure of material "stiffness"**
- **- $E = \sigma/\varepsilon$**
  $= F/A$
  l/L

Hooke's Law: $F = k * \Delta x$
spring constant: k = $F/\Delta x$



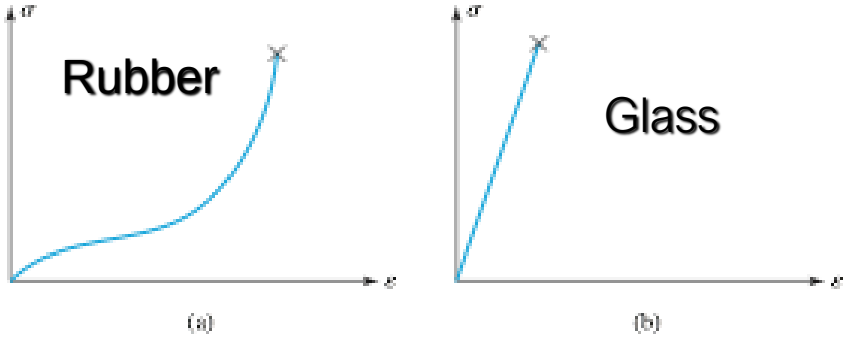
Young’s Modulus

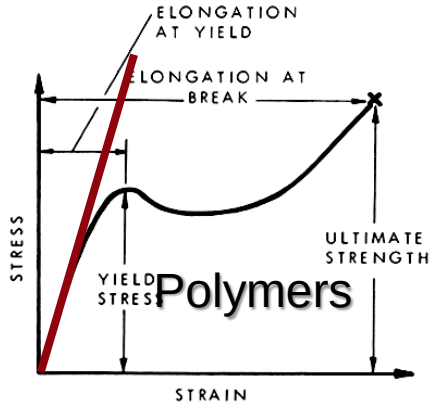
- Determine Young’s modulus of the dough
- $E=(F*L)/(\Delta L*A)$

Young's Modulus Continued

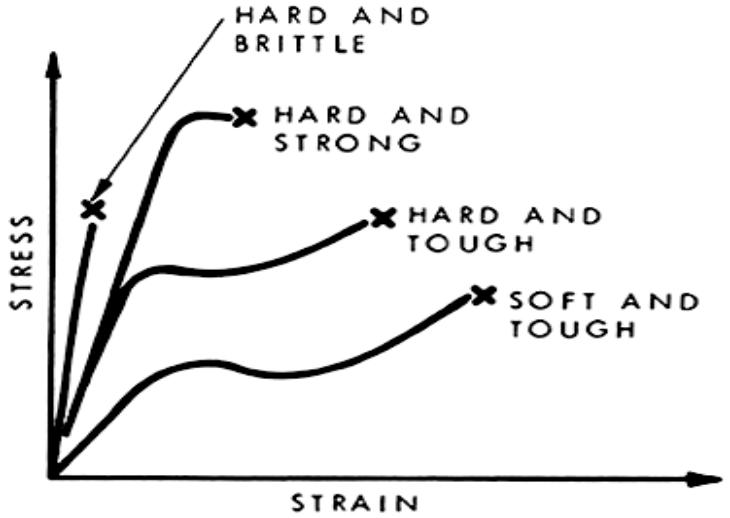
- Stress = Force/$Area_0$
  - Determine the Force
  - Determine the initial area of the cylinder
  - Divide
- Strain = $\Delta L/L_0$
  - Determine the difference in the heights
  - Divide the difference by the original height
- Young's Modulus
  - Divide Stress by Strain

Yield Strength





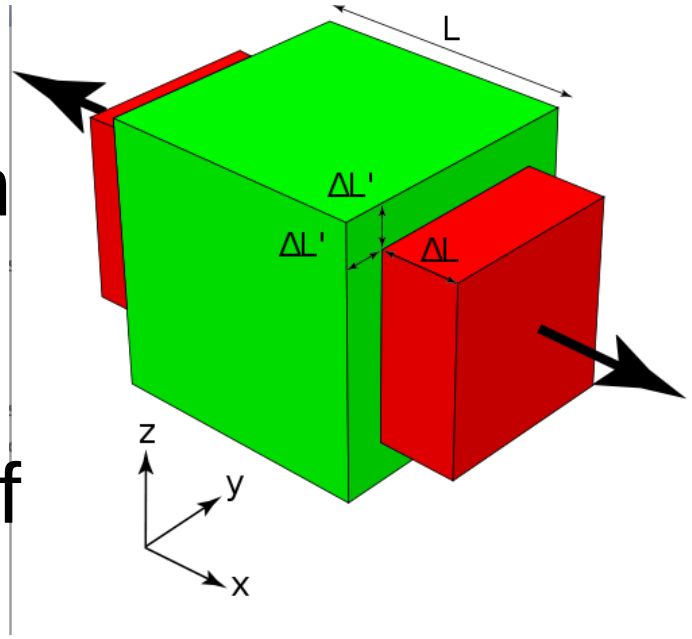
True Elastic Behavior vs. Elastic Region



Vable, M. Mechanics of Materials: Mechanical properties of Materials. Sept. 2011

Poisson's Ratio

- $\nu = -\varepsilon_{trans}/\varepsilon_{axial}$
- Where
- ν = Poisson's Ratio
- ε_{trans} = Transverse Strain
- ε_{axial} = Axial Strain
- $\varepsilon = \Delta L/L_o$
- ΔL = Change in length of material
- L_o = Initial length of material



Resources

- Miller Indices
  - http://www.doitpoms.ac.uk/tlplib/miller_indices/printall.php
- Stress, Strain, etc.
  - http://www.ndt-ed.org/EducationResources/CommunityCollege/Materials/Mechanical/Mechanical.htm

Resources Continued

- YouTube.
  - LOTS of nice videos on stress, strain, Young's Modulus, etc.
- Polymer Database
  - http://polymerdatabase.com/index.html

Questions?

- Thank you
- Time to play!

Optical Properties

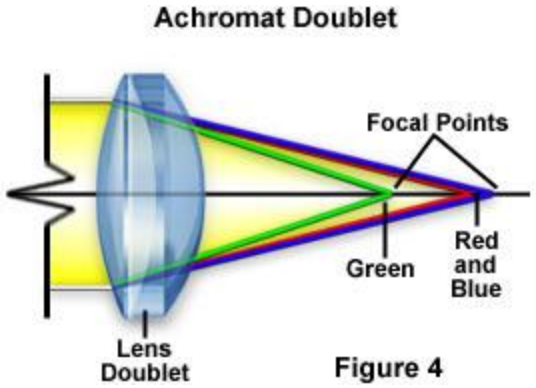
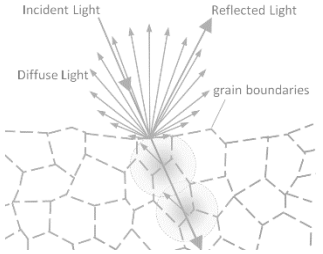


Figure 4

- Polarization
- UV-most common polymers clear because they do not absorb light in the visible spectrum
- Transmittance-ratio of light passing through to light recieved
- Dispersion-scattered light
- Gloss-how well a surface reflects light
- Transparency-both absorption & scattering negligible
- Opaque- High Scattering – almost no tranmisttance



Optical Properties

- Clarity-little light scattering
- Haze-due to light scattering on grain boundaries in crystal polymers
- Color-most common polymers colorless because they do not selectively absorb light in the visible spectrum
- Refractive index- velocity of light in a vacuum relative to the velocity of light in the polymer-changes @ glass transition pt
- Reflectivity-if reflectance is~0, the surface is matt, if smooth, shiny
- Translucence- <90% transmittance

Casting

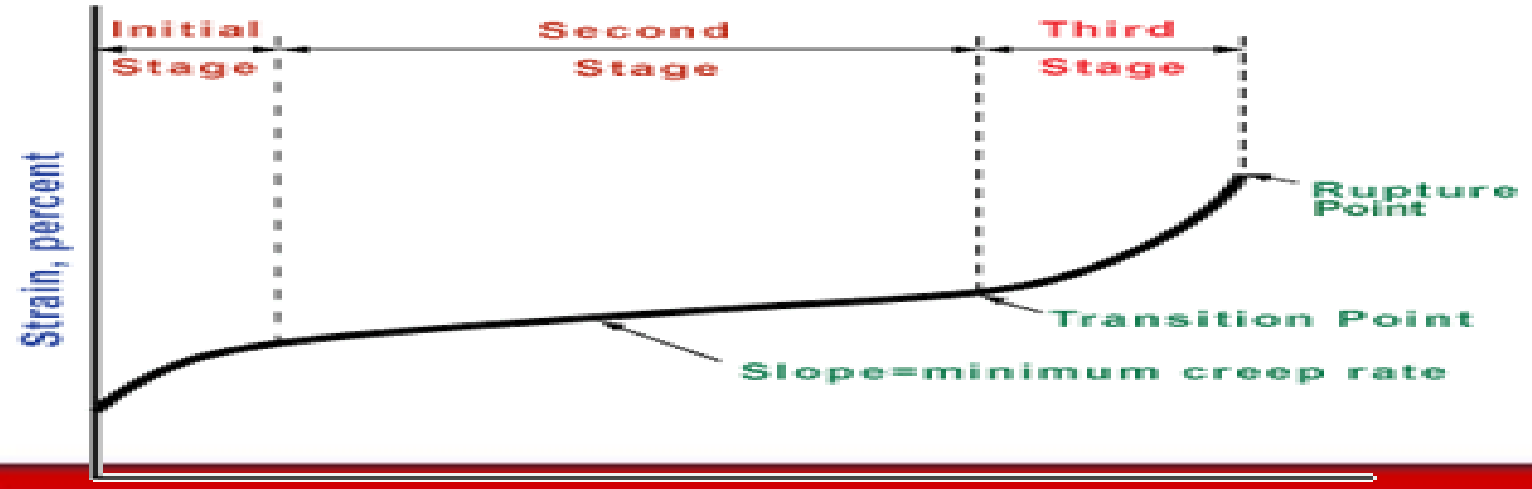
- The liquid or semi-liquid material goes into the molds under just gravity.
- Some type of finishing is generally required after the material solidifies.

Coatings

- A coating is something applied to a substrate
- It is often used to protect the substrate
- Consideration in coatings is thickness of the material
- Uniformity in applying

Creep Rate-State & National

- Creep is the movement of material under stress over time usually at higher temperatures
- Creep ends when the material breaks



Density

- Density = $\frac{Mass}{Volume}$
- Can be found by direct measurement
- Can use differential Density Materials
  - Two liquids, whose density is known are used to bracket the density of the polymer by determining when the polymer sinks or floats