Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

Prof. Junhe Lian
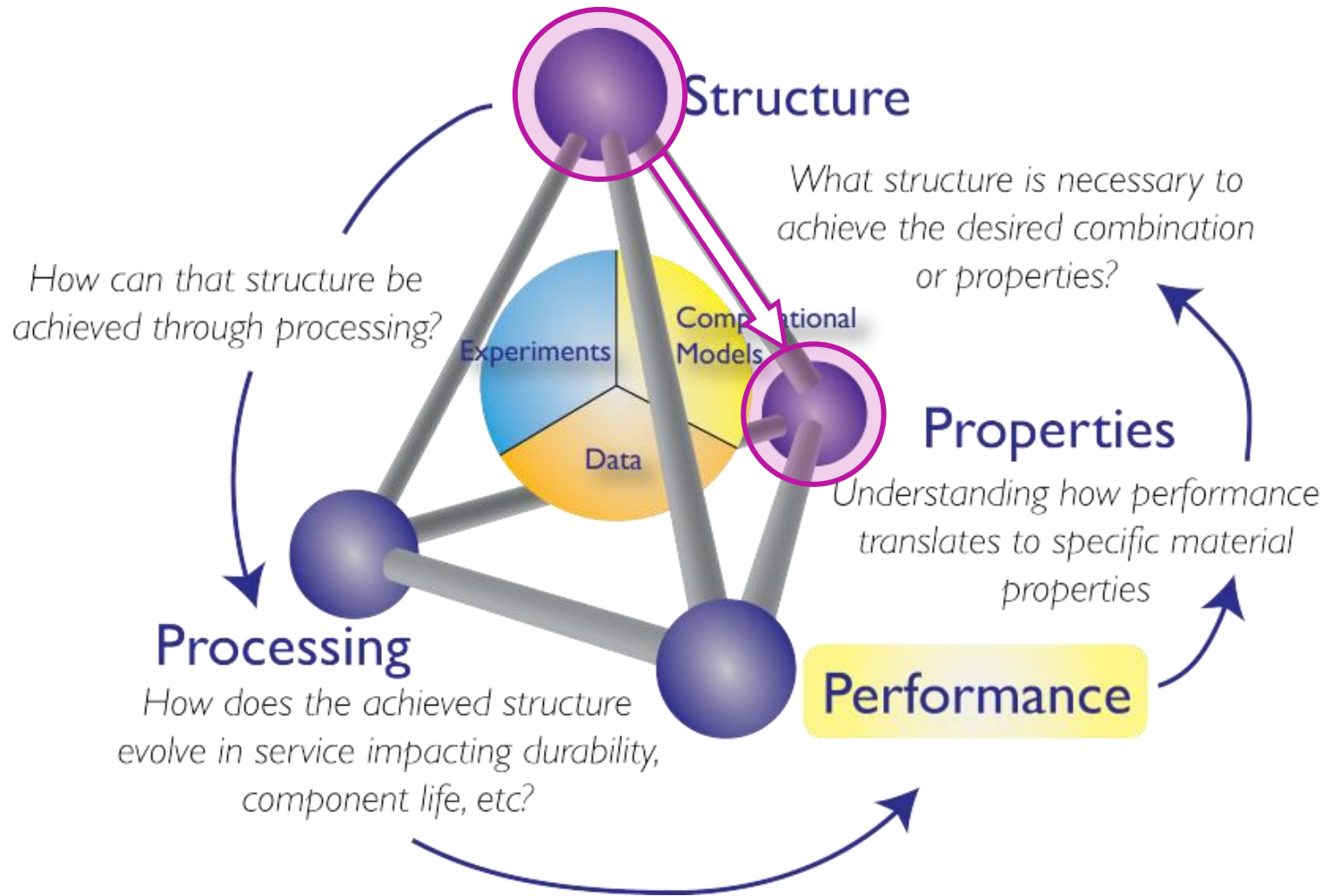*Wenqi Liu (Primary Teaching Assistant)*
Rongfei Juan and Sayoojya Prasad (Teaching Assistants)

Updates:

- Get familiar with MyCourses

- Active participation is very much appreciated

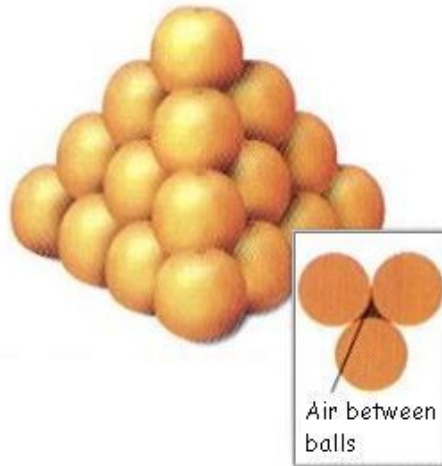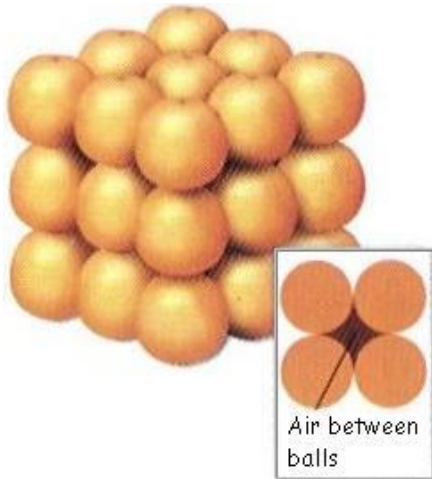- Get some paper and pen. Let's calculate.

Previouly

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provided by Callister & Rethwisch on Wiley

How to best stack oranges?

Air between balls

Air between balls

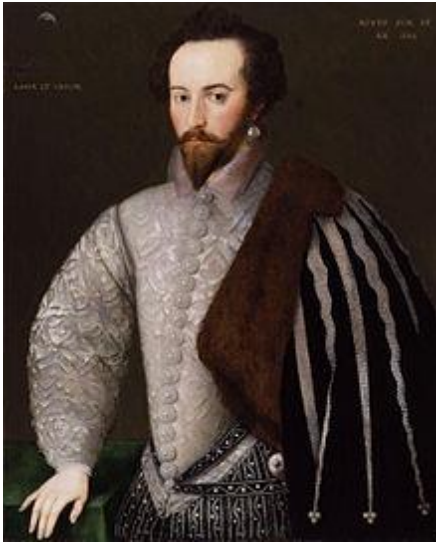**Aalto University**
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A 400-year mathematical story
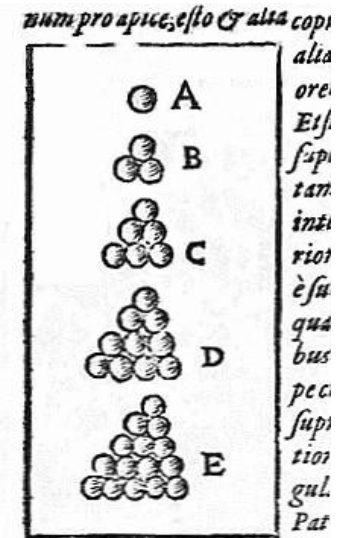

Walter Raleigh
https://en.wikipedia.org/wiki/Walter_Raleigh

Thomas Harriot
https://en.wikipedia.org/wiki/Thomas_Harriot

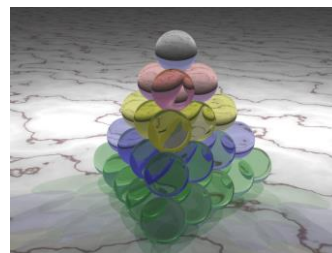## Johannes Kepler
https://en.wikipedia.org/wiki/Johannes_Kepler

A New Year's Gift of Hexagonal Snow (1611)

http://www.math.sunysb.edu/~tony/whatsnew/column/pennies-1200/cass1.html

https://pixabay.com/zh/photos/cannon-balls-balls-iron-metal-hard-187243/

https://commons.wikimedia.org/wiki/File:Pyramid_of_35_spheres_animation_original.gif

Kepler conjecture

It states that no arrangement of equally sized spheres filling space has a greater average density than that of the cubic close packing (face-centered cubic) and hexagonal close packing arrangements. The density of these arrangements is around 74.05%.

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A 400-year mathematical story

Carl Friedrich Gauss

https://en.wikipedia.org/wiki/Carl_Friedrich_Gauss

David Hilbert

https://en.wikipedia.org/wiki/David_Hilbert

László Fejes Tóth

https://en.wikipedia.org/wiki/L%C3%A1szl%C3%B3_Fejes_T%C3%B3th

Carl Gauss (1831) proved that the Kepler conjecture is true if the spheres have to be arranged in a regular lattice.

In 1900 David Hilbert included it in his list of twenty three unsolved problems of mathematics— it forms part of Hilbert's eighteenth problem.

Fejes Tóth (1953) showed that the problem of determining the maximum density of all arrangements (regular and irregular) could be reduced to a finite (but very large) number of calculations. This meant that a proof by exhaustion was, in principle, possible. As Fejes Tóth realised, a fast enough computer could turn this theoretical result into a practical approach to the problem.

Atom Packing

- Non dense, random packing
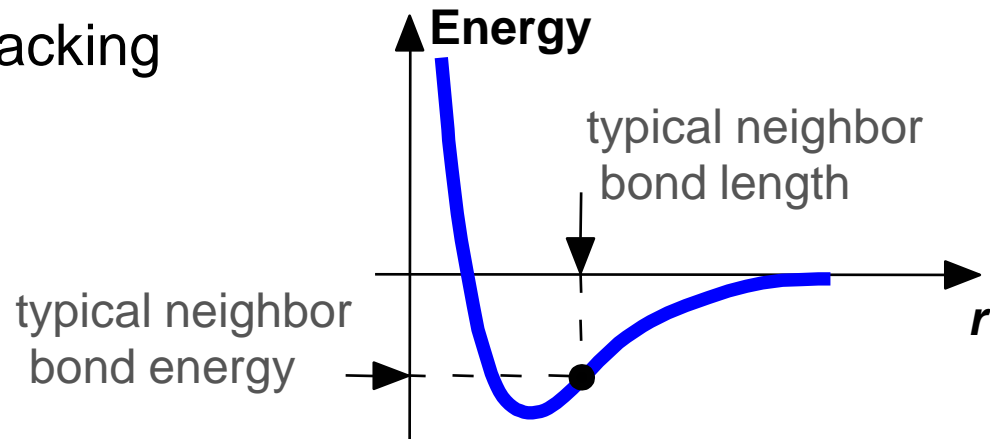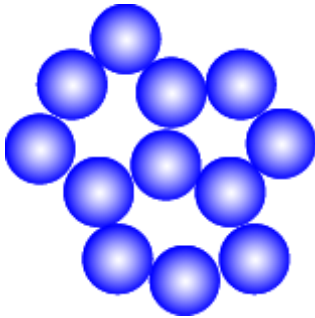
- Dense, ordered packing
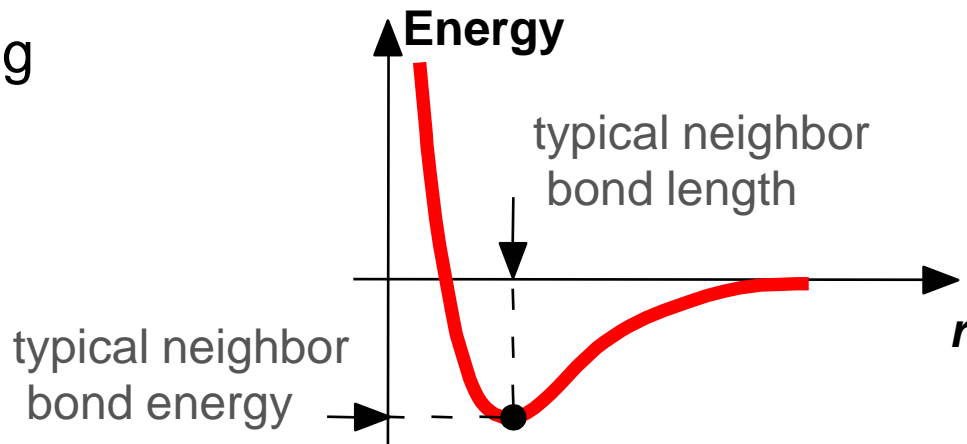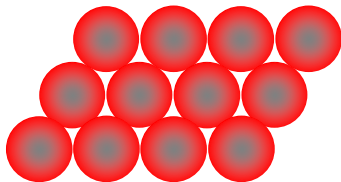
Ordered structures tend to be nearer the minimum in bonding energy and are more stable.

Chapter 3: The Structure of Crystalline Solids

ISSUES TO ADDRESS...

- What is the difference in atomic arrangement between **crystalline** and **noncrystalline** solids?

- What are the **crystal structures** of metals?

- What are the **characteristics** of crystal structures?

- How are crystallographic **points**, **directions**, and **planes** specified?

- What characteristics of a material's atomic structure determine its **density**?

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Materials and Atomic Arrangements

Crystalline materials...

- atoms arranged in periodic, 3D arrays
- typical of: -metals
                 -many ceramics
                 -some polymers
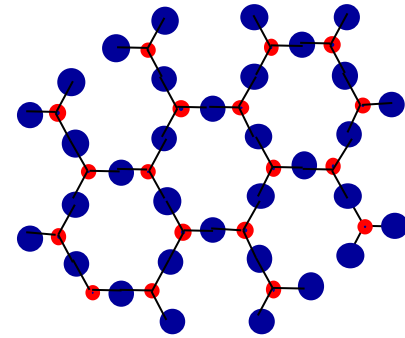
crystalline SiO_2
Adapted from Fig. 3.24(a),
Callister & Rethwisch 10e.

•Si   ● Oxygen

Noncrystalline materials...

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

"Amorphous" = Noncrystalline
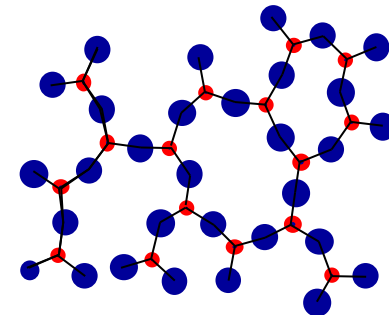
noncrystalline SiO_2
Adapted from Fig. 3.24(b),
Callister & Rethwisch 10e.

The slides are developed based on the recourses
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Metallic Crystal Structures: Atomic Packing

• Dense atomic packing for crystal structures of metals.

Reasons for dense packing:

- Bonds between metal atoms are nondirectional.
- Nearest neighbor distances tend to be small in order to lower bond energy.
- High degree of shielding (of ion cores) provided by free electron cloud.

• Crystal structures for metals simpler than structures for ceramics and polymers.

We will examine **three** such structures for metals...

Crystal structures of metals

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Simple Cubic (SC) Crystal Structure

- Centers of atoms located at the eight corners of a cube
- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.
- Coordination # = 6 (# nearest neighbors)

ex: Po

Lattice points
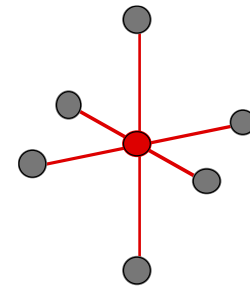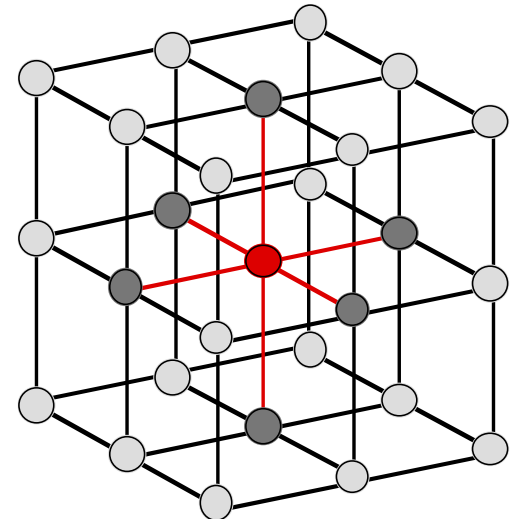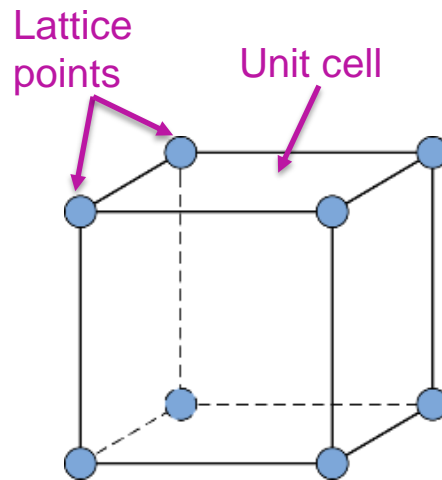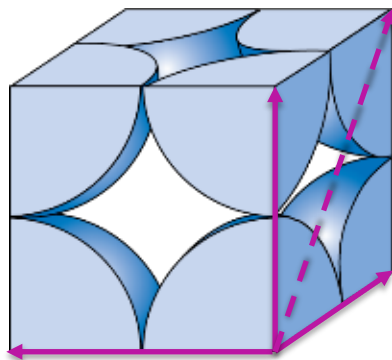
Unit cell

Adapted from Fig. 3.3, *Callister & Rethwisch 10e.*

- ❑ **Lattice**: atomic arrangement can be described to a network of lines in 3D.
- ❑ **Unit cell**: smallest repeating entity of the atomic structure. The basic building block of the crystal structure.

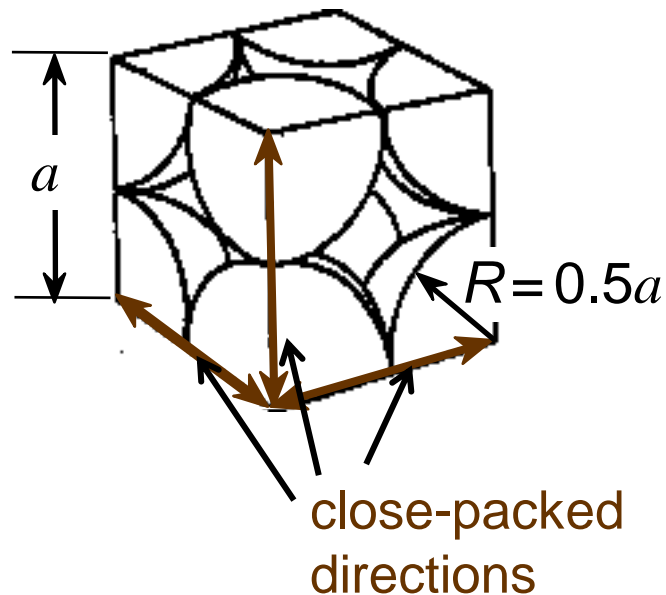# Definitions

Coordination Number

> Coordination Number = number of **nearest**-neighbor or touching atoms

Atomic Packing Factor (APF)

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

*assume hard spheres

Atomic Packing Factor (APF) for Simple Cubic

$R = 0.5a$

close-packed directions

$$\text{APF} = \frac{\overbrace{1}^{\frac{\text{atoms}}{\text{unit cell}}} \cdot \overbrace{\frac{4}{3} \pi (0.5a)^3}^{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}} = 0.52$$

Unit cell contains 1 atom = 8 x 1/8 = 1 atom/unit cell
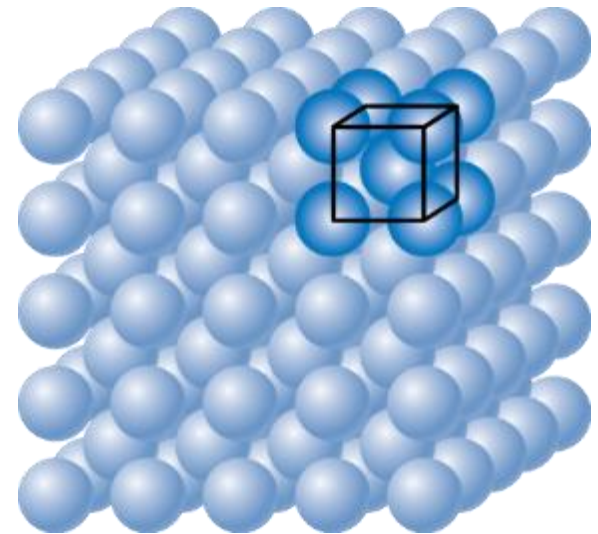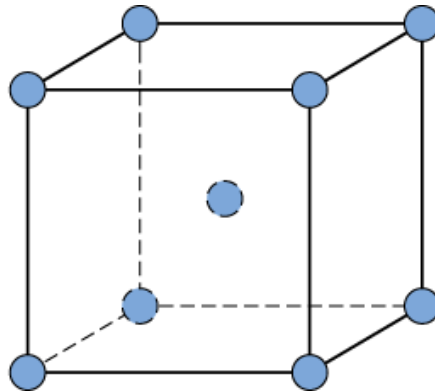
Body-Centered Cubic Structure (BCC)

- Atoms located at 8 cube corners with a single atom at cube center.

  Note: All atoms in the animation are identical; the center atom is shaded differently for ease of viewing.

- Coordination # = 8

ex: Cr, W, Fe (α), Ta, Mo

Adapted from Fig. 3.2, *Callister & Rethwisch 10e.*

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

Atomic Packing Factor: BCC

$4R = \sqrt{3}\,a$

a

$\sqrt{2}\,a$

For close-packed directions

$R = \sqrt{3}\,a/4$

$$\text{APF} = \dfrac{2\;\dfrac{4}{3}\pi\,(\sqrt{3}a/4)^3}{a^3} = \dfrac{8}{3}\pi\left(\dfrac{\sqrt{3}}{4}\right)^3 = 0.68$$

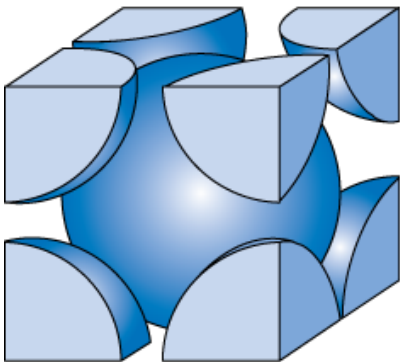atoms / unit cell

volume / atom

volume / unit cell

Face-Centered Cubic Structure (FCC)

- Atoms located at 8 cube corners and at the centers of the 6 faces.

Note: All atoms in the animation are identical; the face-centered atoms are shaded differently for ease of viewing.
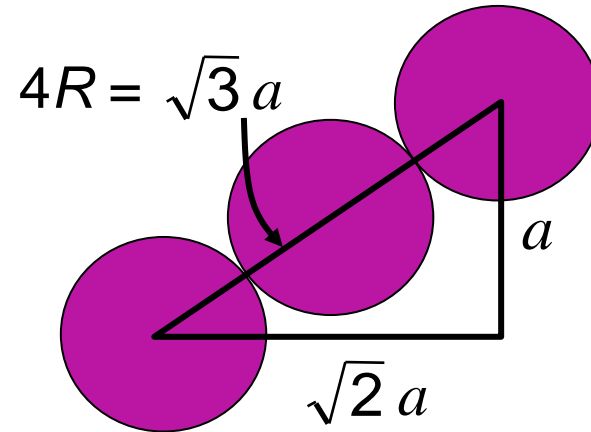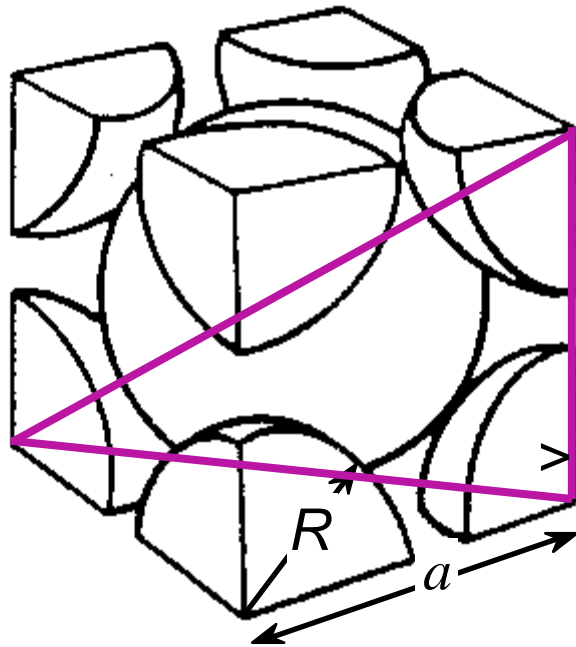
- Coordination # = 12

ex: Al, Cu, Au, Pb, Ni, Pt, Ag
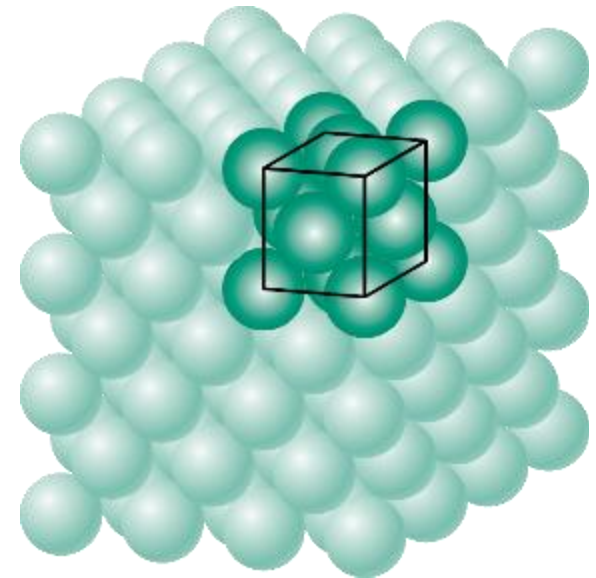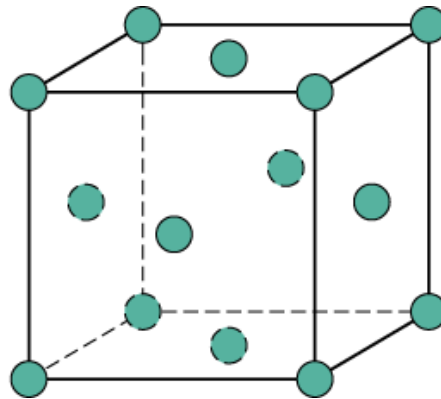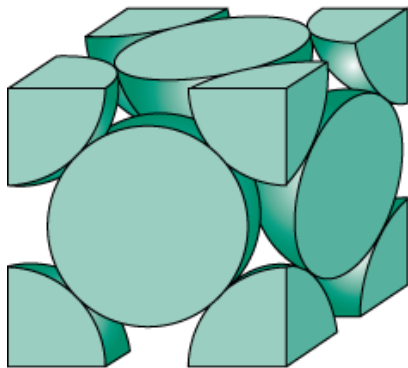
Adapted from Fig. 3.1, *Callister & Rethwisch 10e.*

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

Atomic Packing Factor: FCC
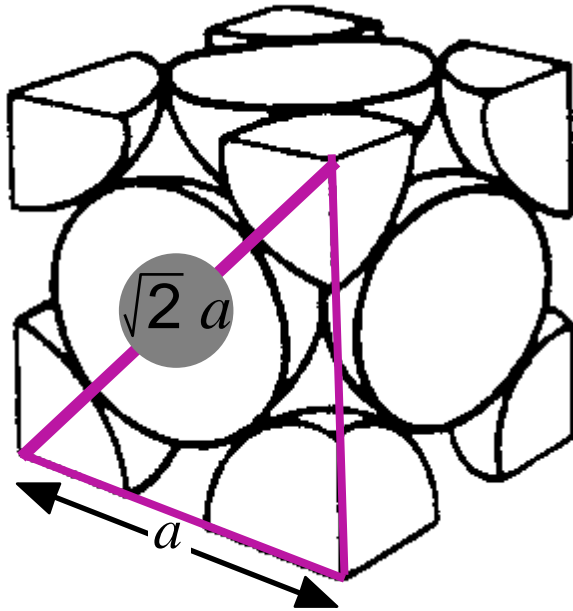
maximum achievable APF

For close-packed directions:

$$4R = 2\sqrt{a} \qquad \left(\text{i.e., } R = \frac{\sqrt{2}a}{4} \right)$$

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

$$\text{APF} = \frac{4 \cdot \frac{4}{3}\pi(\sqrt{2}a/4)^3}{a^3} = 0.74$$

atoms / unit cell

volume / atom

volume / unit cell

FCC Plane Stacking Sequence

- Stacking Sequence–Close-Packed Planes of Atoms
- 2D Projection

ABCABC...

A sites

B sites

C sites
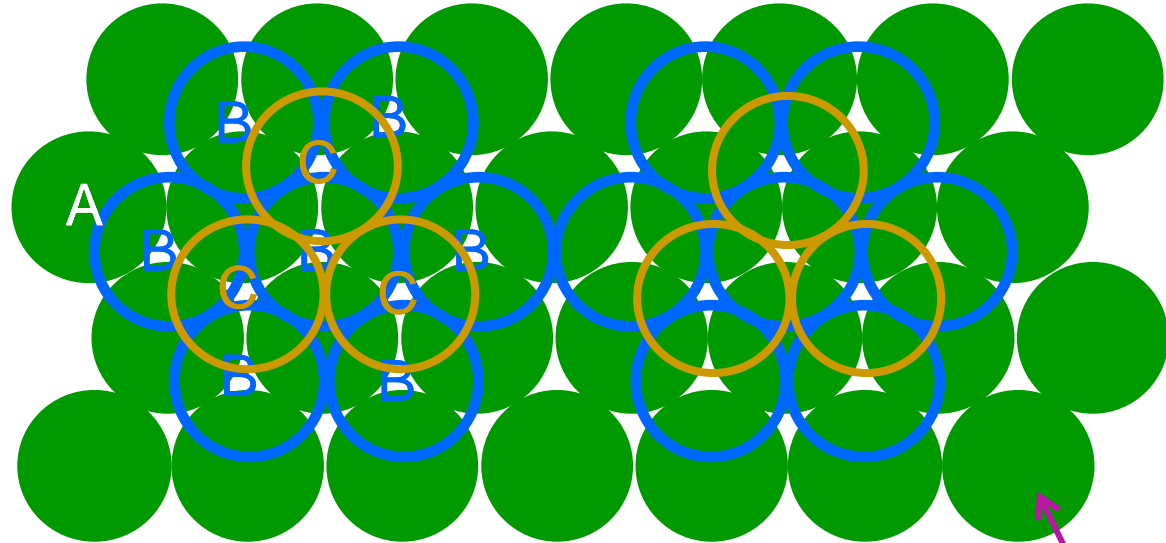
- Stacking Sequence Referenced to an FCC Unit Cell.
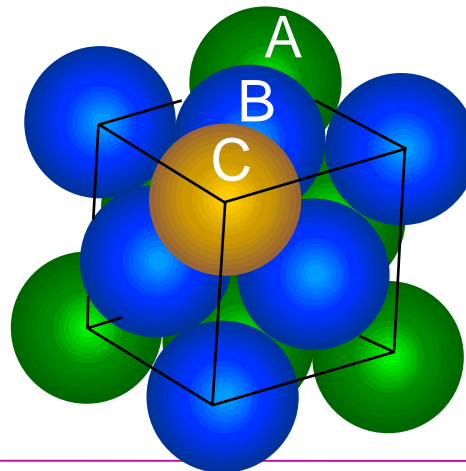
Close-Packed Plane

Hexagonal Close-Packed Structure (HCP)

- Stacking Sequence–Close-Packed Planes of Atoms

- 3D Projection

A sites

B sites

A sites

c

a

- 2D Projection

Top layer

Middle layer

Bottom layer

ABAB...

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

- Coordination # = 12

- APF = 0.74

- Ideal c/a = 1.633

Theoretical Density for Metals, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}} = \frac{(nA/N_A)}{V_C}$$

$$\rho = \frac{nA}{V_C N_A}$$

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
= 6.022×10^{23} atoms/mol

Theoretical Density Computation for Chromium

❑ Cr has BCC crystal structure

A = 52.00 g/mol

R = 0.125 nm

n = 2 atoms/unit cell

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

$V_C = a^3$ = 2.406 x 10^{-23} cm^3

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

$$\rho = \frac{n \quad A}{V_C \quad N_A} = \frac{2 \quad 52.00}{2.406 \times 10^{-23} \quad 6.022 \times 10^{23}} = 7.19 \text{ g/cm}^3$$

$\frac{\text{atoms}}{\text{unit cell}}$ → 2

52.00 ← $\frac{\text{g}}{\text{mol}}$

$\frac{\text{volume}}{\text{unit cell}}$ → 2.406 x 10^{-23}

6.022 x 10^{23} ← $\frac{\text{atoms}}{\text{mol}}$

Densities Comparison for Four Material Types

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

Why?

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

Ceramics have...
- often lighter elements

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

Composites have...
- moderate to low densities

ρ (g/cm^3)

Metals/Alloys: Platinum, Gold, W, Tantalum, Silver, Mo, Cu,Ni, Steels, Tin, Zinc, Titanium, Aluminum, Magnesium

Graphite/Ceramics/Semicond: Zirconia, Al oxide, Diamond, Si nitride, Glass -soda, Concrete, Silicon, Graphite

Polymers: PTFE, Silicone, PVC, PET, PS, PE

Composites/fibers: Glass fibers, GFRE*, Carbon fibers, CFRE*, Aramid fibers, AFRE*, Wood

Based on data in Table B1, Callister
*GFRE, CFRE, & AFRE are Glass, Carbon, & Aramid Fiber-Reinforced Epoxy composites (values based on 60% volume fraction of aligned fibers in an epoxy matrix).

Anisotropy

- Anisotropy — Property value depends on crystallographic direction of measurement.

  - Observed in a crystal.

  - Example: modulus of elasticity (E) in BCC iron

  E(edge) ≠ E(diagonal)

E (diagonal) = 273 GPa
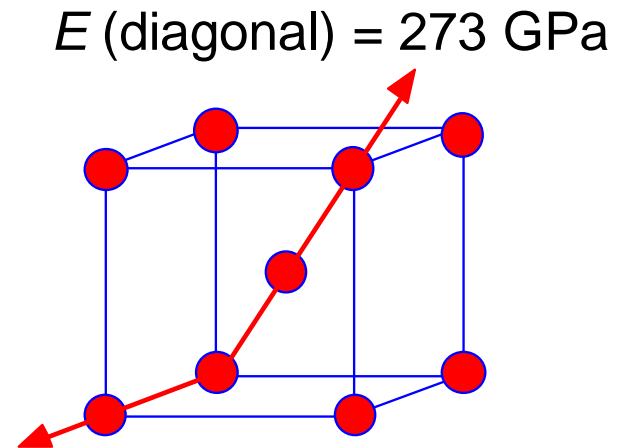
E (edge) = 125 GPa

Unit cell of BCC iron

Single Crystals

• When the periodic arrangement of atoms (crystal structure) extends without interruption throughout the entire specimen.

-- diamond single crystals for abrasives
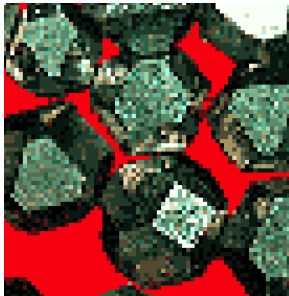
(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

-- Quartz single crystal

(Courtesy P.M. Anderson)

-- single crystal for turbine blade

Fig. 8.35(c), *Callister & Rethwisch 10e.*
(courtesy of Pratt and Whitney)

Characterization of crystal structures

Point Coordinates

A point coordinate is a lattice position in a unit cell

Determined as fractional multiples of a, b, and c unit cell edge lengths

Example: Unit cell upper corner

1. Lattice position is

$$a, b, c$$

2. Divide by unit cell edge lengths (a, b, and c) and remove commas

$$\frac{a}{a} \quad \frac{b}{b} \quad \frac{c}{c} = 111$$

a,1b,1c
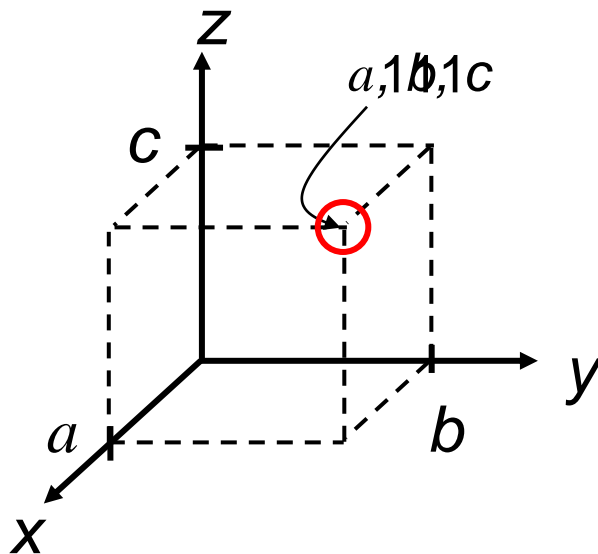
3. Point coordinates for unit cell corner are   111

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Crystallographic Directions I.

Example Problem I

Algorithm – determine direction indices

1. Determine coordinates of vector tail, pt. 1: x_1, y_1, & z_1; and vector head, pt. 2: x_2, y_2, & z_2.
2. Tail point coordinates subtracted from head point coordinates.
3. Normalize coordinate differences in terms of lattice parameters a, b, and c:

$$\frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}$$

4. Reduce to smallest integer values
5. Enclose indices in square brackets, no commas   [uvw]   Miller Indices

ex:

pt. 1 $x_1 = 0$, $y_1 = 0$, $z_1 = 0$
pt. 2 $x_2 = a$, $y_2 = 0$, $z_2 = c/2$

$$\frac{a - 0}{a} \quad \frac{0 - 0}{b} \quad \frac{c/2 - 0}{c}$$

=> 1, 0, 1/2   => 2, 0, 1

=> [201]

Crystallographic Directions II:

z

pt. 2 head

pt. 1: tail

x

y
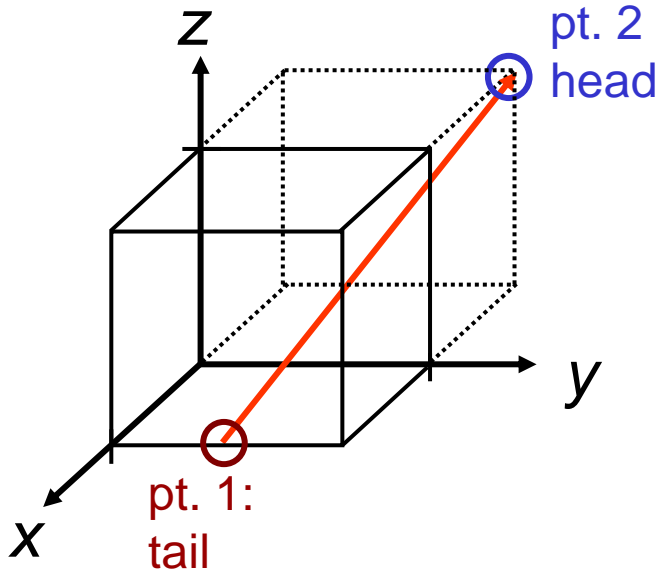
1. Point coordinates of tail and head

tail   pt. 1 $x_1 = a,\ \ y_1 = b/2,\ \ z_1 = 0$

head   pt. 2 $x_2 = -a,\ \ y_2 = b,\ \ \ \ z_2 = c$

2 & 3. Subtract and normalize

$$\frac{-a - a}{a} = -2;\quad \frac{b - b/2}{b} = 1/2;\quad \frac{c - 0}{c} = 1$$

=>   -2, 1/2, 1

4 & 5. Multiply by 2 to eliminate the fraction, then place in square brackets (no commas)

-4, 1, 2   => $[\overline{4}12]$ where the overbar represents a negative index

Family of directions – all directions that are crystallographically equivalent (have the same atomic spacing) – indicated by indices in angle brackets

Ex: <100> = [100], [010], [001], [$\overline{1}$00], [0$\overline{1}$0], [00$\overline{1}$]

Common Crystallographic Directions

Adapted from Fig. 3.7, *Callister & Rethwisch 10e.*
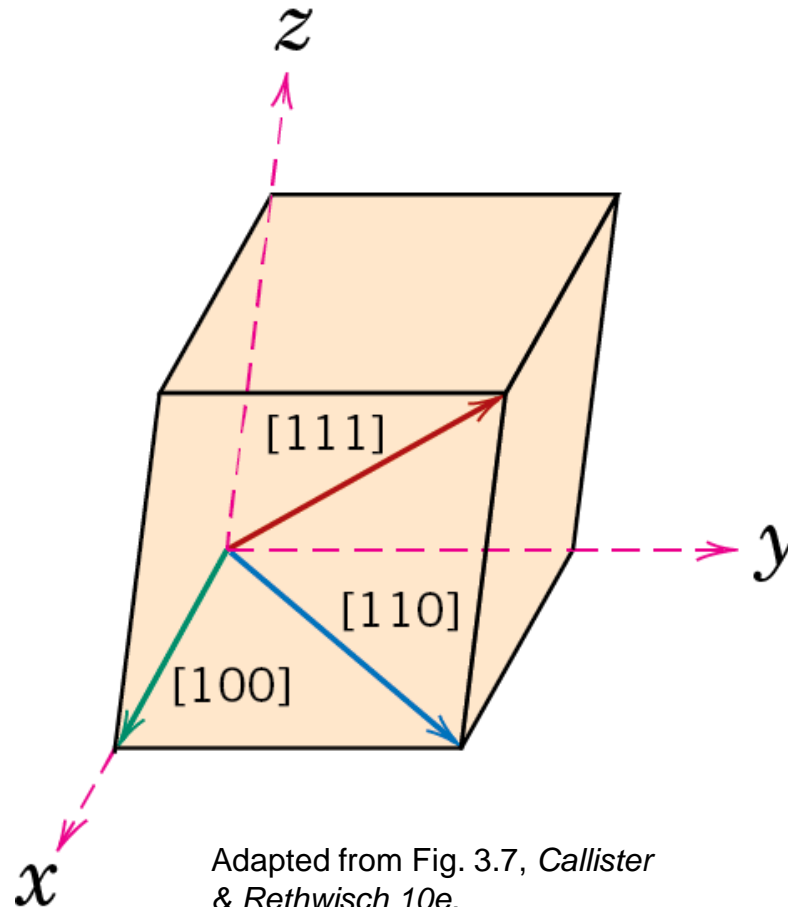
Crystallographic Planes

Algorithm for determining the Miller Indices of a plane

1. If plane passes through selected origin, establish a new origin in another unit cell
2. Read off values of intercepts of plane (designated A, B, C) with x, y, and z axes in terms of a, b, c
3. Take reciprocals of intercepts
4. Normalize reciprocals of intercepts by multiplying by lattice parameters a, b, and c
5. Reduce to smallest integer values
6. Enclose resulting Miller Indices in parentheses, no commas i.e., (*hkl*)

Crystallographic Planes

Example Problem I

		x	y	z
1.	Relocate origin – not needed			
2.	Intercepts	a	b	∞c
3.	Reciprocals	$1/a$	$1/b$	$1/\infty c$
4.	Normalize	a/a	b/b	$c/\infty c$
		1	1	0
5.	Reduction	1	1	0
6.	Miller Indices	(110)		
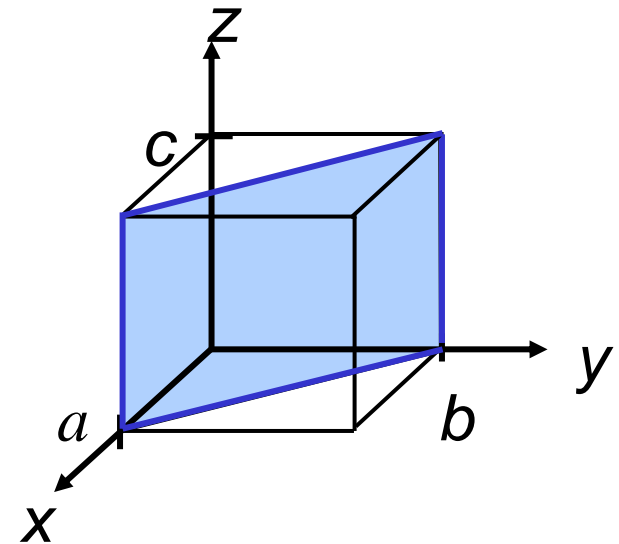
Crystallographic Planes

Example Problem II

		x	y	z
1.	Relocate origin – not needed			
2.	Intercepts	$a/2$	∞b	∞c
3.	Reciprocals	$2/a$	$1/\infty b$	$1/\infty c$
4.	Normalize	$2a/a$	$b/\infty b$	$c/\infty c$
		2	0	0
5.	Reduction	2	0	0
6.	Miller Indices	(200)		
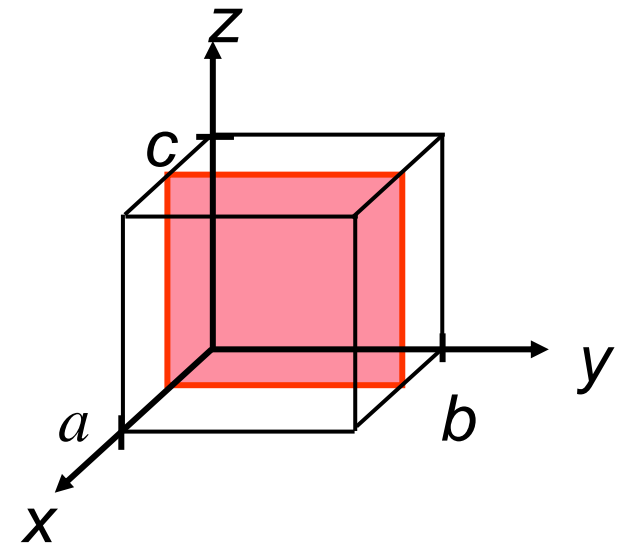
Crystallographic Planes

Example Problem III

		x	y	z
1.	Relocate origin – not needed			
2.	Intercepts	$a/2$	b	$3c/4$
3.	Reciprocals	$2/a$	$1/b$	$4/3c$
4.	Normalize	$2a/a$	b/b	$4c/3c$
		2	1	4/3
5.	Reduction (x3)	6	3	4
6.	Miller Indices	(634)		
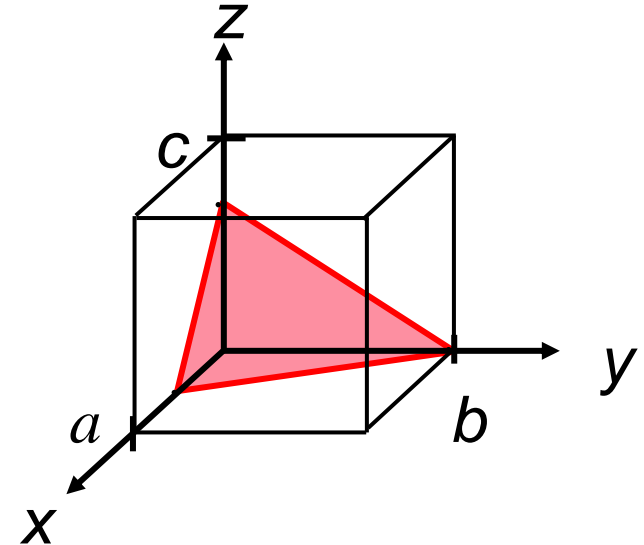
Family of planes – all planes that are crystallographically equivalent (have the same atomic packing) – indicated by indices in braces

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

Common Crystallographic Planes

(001) Plane referenced to the origin at point O

Other equivalent (001) planes

(a)

(110) Plane referenced to the origin at point O

Other equivalent (110) planes

(b)

(111) Plane referenced to the origin at point O

Other equivalent (111) planes

(c)
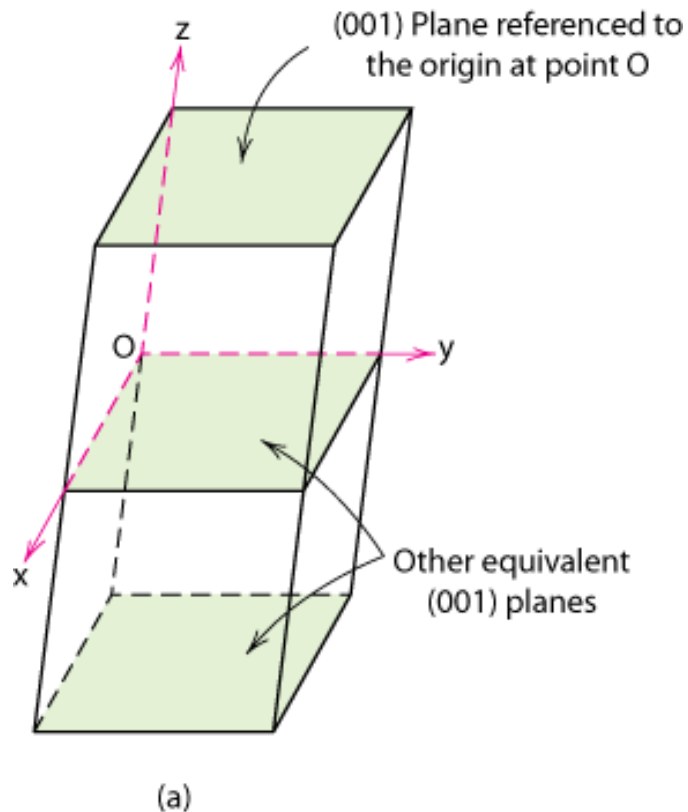
Adapted from Fig. 3.11,
Callister & Rethwisch 9e.

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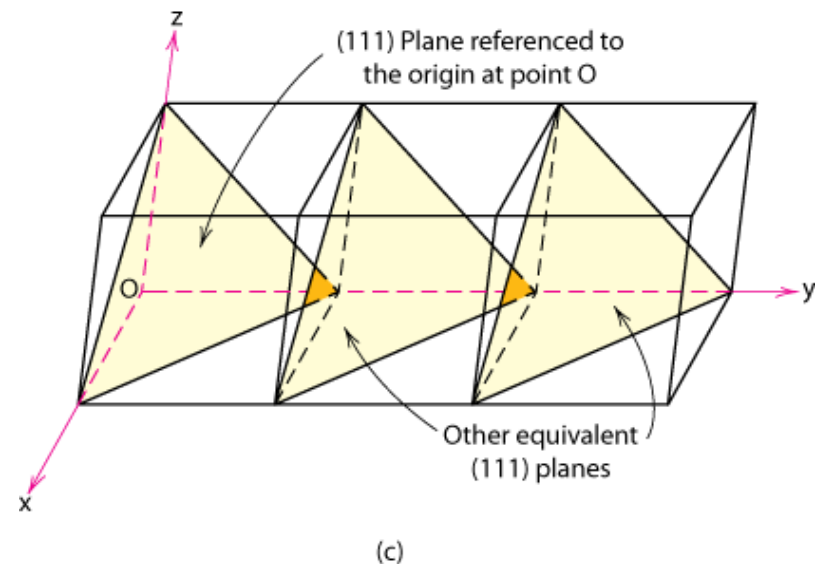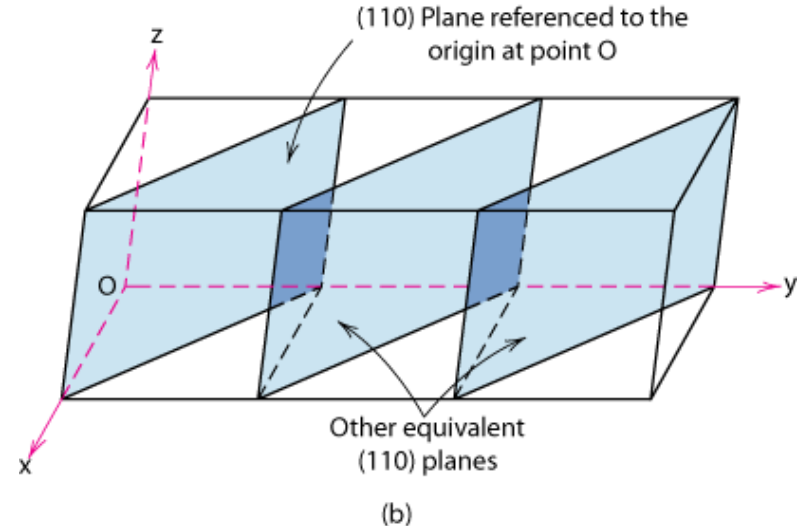
Summary so far

❑ Atoms may assemble into **crystalline** (ordered) or **amorphous** (disordered) structures.

❑ Common *metallic* crystal structures are **FCC**, **BCC**, and **HCP**. Coordination number and atomic packing factor are the same for both FCC and HCP crystal structures.

❑ Crystallographic points, directions and planes may be specified in terms of indexing schemes, e.g. **Miller index**.

❑ The crystal structure determines the properties of materials, e.g. **density** and **anisotropy** in elasticity.

Break

Issues with the theoretical Density of Chromium
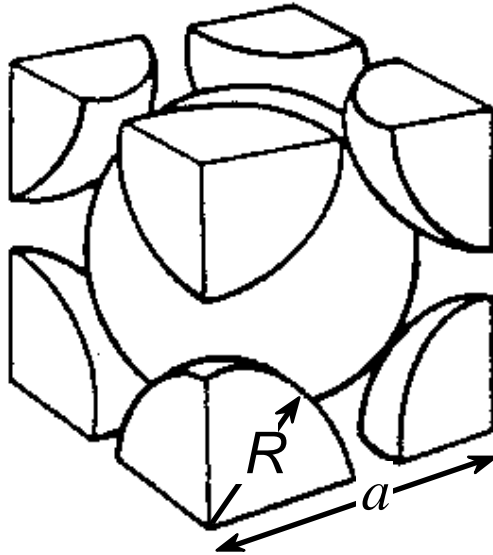
❏ Cr has BCC crystal structure

A = 52.00 g/mol

R = 0.125 nm

n = 2 atoms/unit cell

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

$V_C = a^3 = 2.406 \times 10^{-23}$ cm^3

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

$$\rho = \frac{n \; A}{V_C \; N_A} = \frac{2 \cdot 52.00}{2.406 \times 10^{-23} \cdot 6.022 \times 10^{23}} = 7.19 \text{ g/cm}^3$$

$\dfrac{\text{atoms}}{\text{unit cell}}$ → 2

52.00 ← $\dfrac{\text{g}}{\text{mol}}$

$\dfrac{\text{volume}}{\text{unit cell}}$ → 2.406 x 10^{-23}

6.022 x 10^{23} ← $\dfrac{\text{atoms}}{\text{mol}}$

ρ_{actual} = 7.15 g/cm^3

Chapter 4: Imperfections in Solids

ISSUES TO ADDRESS...

- What types of **defects** exist in solid materials?

- How does the number of vacancies depend on **temperature**?

- What are the two types of **solid solutions**?

- What are the three types of **dislocations**?

- What **properties** will be influenced by defects?

Imperfections in Solids

There is no such thing as a perfect crystal. Crystalline imperfections (or defects) are always present.

❑ Many of the properties of materials are sensitive to the presence of imperfections.

❑ Crystalline defect refers to a lattice irregularity with dimensions on the order of an atomic diameter.

❑ What kinds of crystalline imperfections exist in solids?

Types of Imperfections

- Vacancies
- Interstitial atoms
- Substitutional impurity atoms

Point defects
(0-Dimensional)

- Dislocations

Linear defects
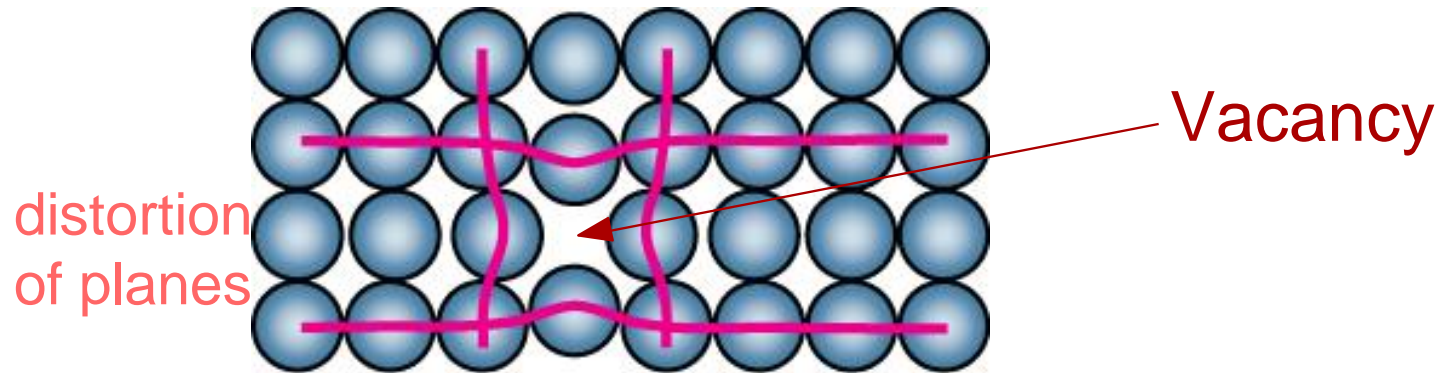(1-Dimensional)

- Grain Boundaries (twin boundaries)
- Stacking faults

Interfacial defects
(2-Dimensional)

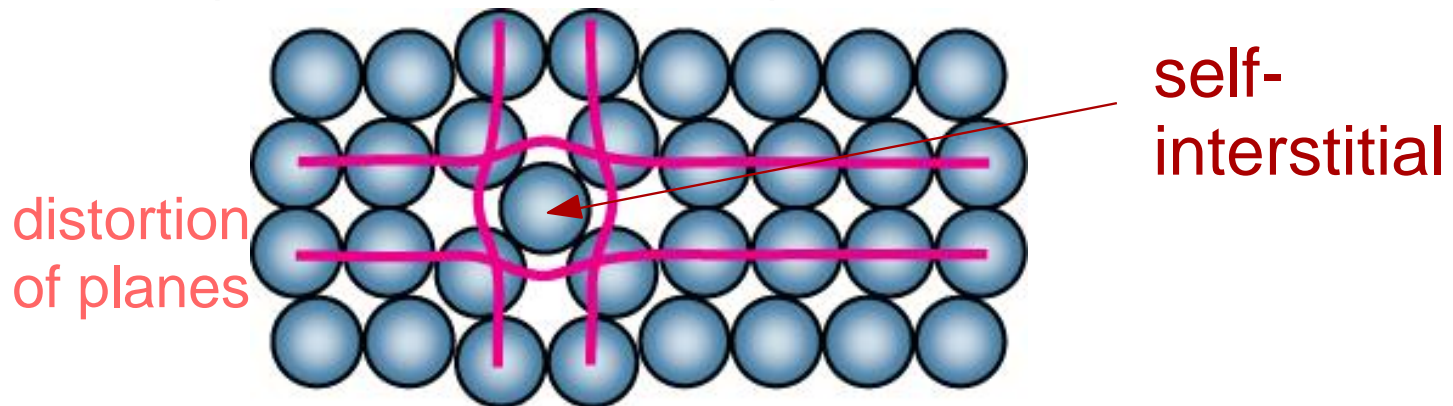# Point Defects

Point Defects in Metals

- Vacancies:

  -vacant atomic sites.

distortion of planes

Vacancy

- Self-Interstitials:

  -Host atoms positioned in interstitial positions between atoms.

distortion of planes

self-interstitial

Vacancies – Computation of Equilibrium Concentration

- Equilibrium concentration varies with temperature!

Number of vacancies

Activation energy

Total number of lattice sites

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

Temperature

Boltzmann's constant

$(1.38 \times 10^{-23}$ J/atom-K$)$

$(8.62 \times 10^{-5}$ eV/atom-K$)$
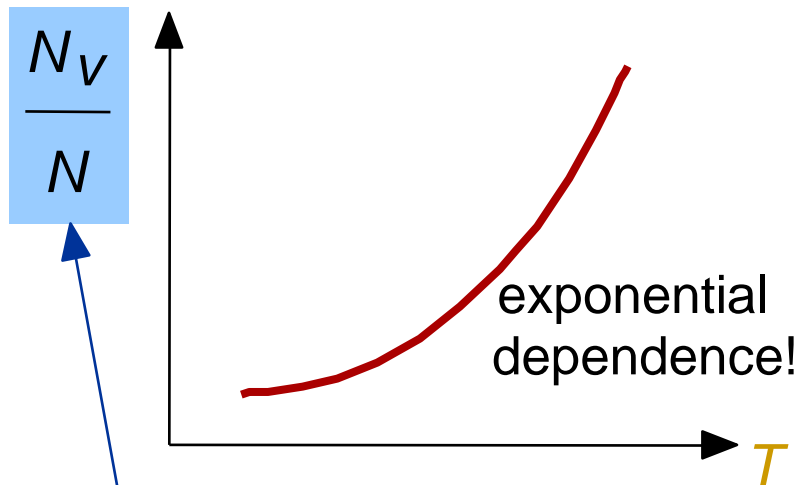
Note: Each lattice site is a potential vacancy.

Determination of Activation Energy for Vacancy Formation

- Q_v can be determined experimentally.
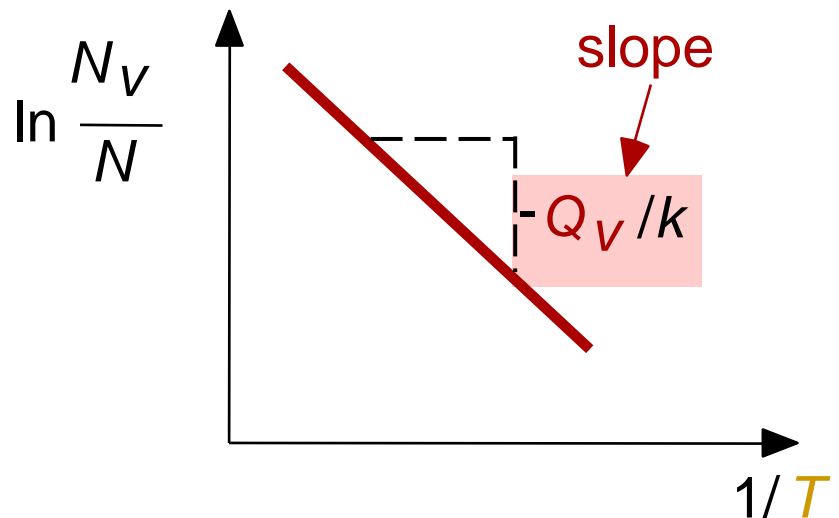
$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

- Data may be plotted as...

- Replot data as follows...

$\dfrac{N_v}{N}$

exponential dependence!

T

defect concentration

$\ln \dfrac{N_v}{N}$

slope

$-Q_v/k$

$1/T$

Computation of Equilibrium Vacancy Concentration

- Find the equilibrium number of vacancies in 1 m^3 of Cu at 1000°C.

- Given:

$$\rho = 8.4 \text{ g /cm}^3 \qquad A_{Cu} = 63.5 \text{ g/mol}$$

$$Q_V = 0.9 \text{ eV/atom} \qquad N_A = 6.022 \times 10^{23} \text{ atoms/mol}$$

Solution: The first step is to determine the total number of lattice sites N using Equation

$$N = \frac{N_A \rho}{A_{Cu}} = \frac{(6.022 \times 10^{23} \text{ sites/mol})(8.4 \text{ g/cm}^3)}{63.5 \text{ g/mol}} \left(\frac{10^6 \text{ cm}^3}{m^3} \right)$$

$$= 8.0 \times 10^{28} \text{ sites/m}^3$$

Computation of Equilibrium Vacancy Concentration (cont.)

The second step is to determine the equilibrium vacancy concentration N_V using Equation.

$$N_V = N \exp\left(\frac{-Q_V}{kT}\right) = N \exp\left(\frac{-0.9 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/atom-K})(1273 \text{ K})}\right)$$

$$= (2.7 \times 10^{-4})\, N$$
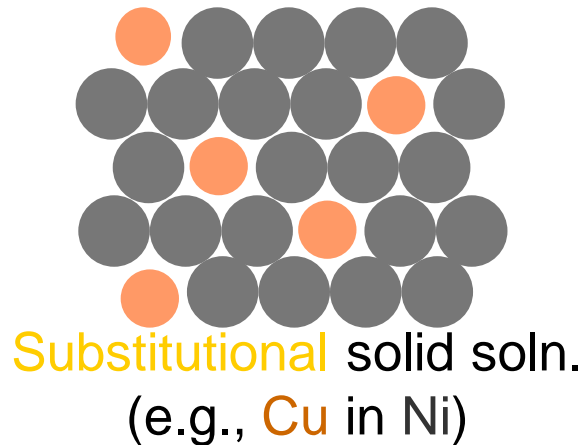
- Answer:

$$N_V = (2.7 \times 10^{-4})(8.0 \times 10^{28}) \text{ sites/m}^3$$

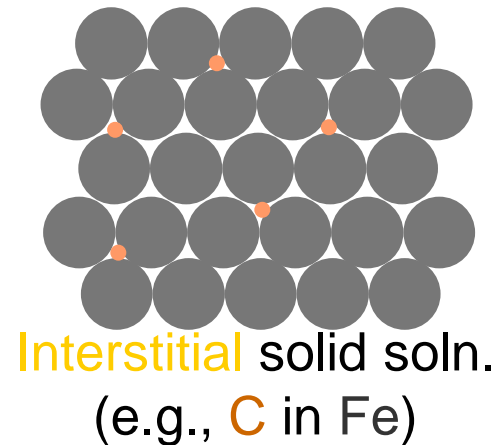$$= 2.2 \times 10^{25} \text{ vacancies/m}^3$$

The slides are developed based on the recourses provided by Callister & Rethwisch on Wiley

Impurities in Metals

Two outcomes if impurity B atoms are added to a solid composed of host A atoms:

- Solid solution of B in A (i.e., random dist. of B atoms)

OR

Substitutional solid soln.
(e.g., Cu in Ni)

Interstitial solid soln.
(e.g., C in Fe)

- Solid solution of B in A, plus particles of a new phase (usually for larger concentrations of B)
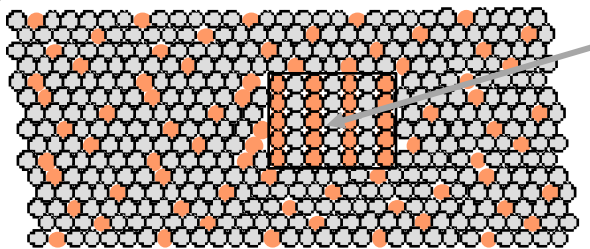
Second phase particle
-- different composition
-- often different structure.

Specification of Composition

☐ weight percent

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

m_1 = mass of component 1

☐ atom percent

$$C_1^{'} = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

n_{m1} = number of moles of component 1

Line Defects

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Linear Defects—Dislocations

- ❑ **Dislocations**
  - ❑ Are one-dimensional defects around which atoms are misaligned
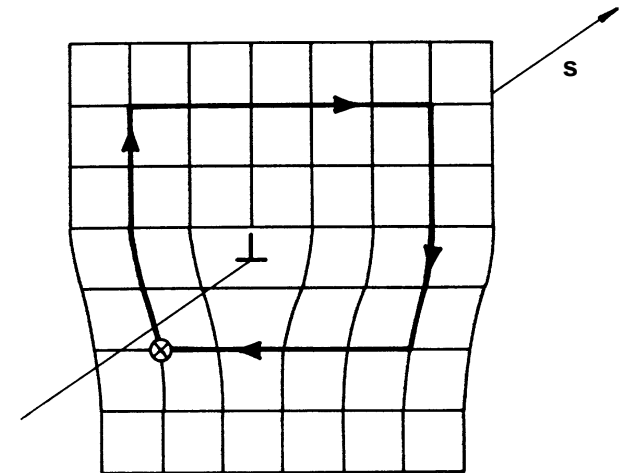
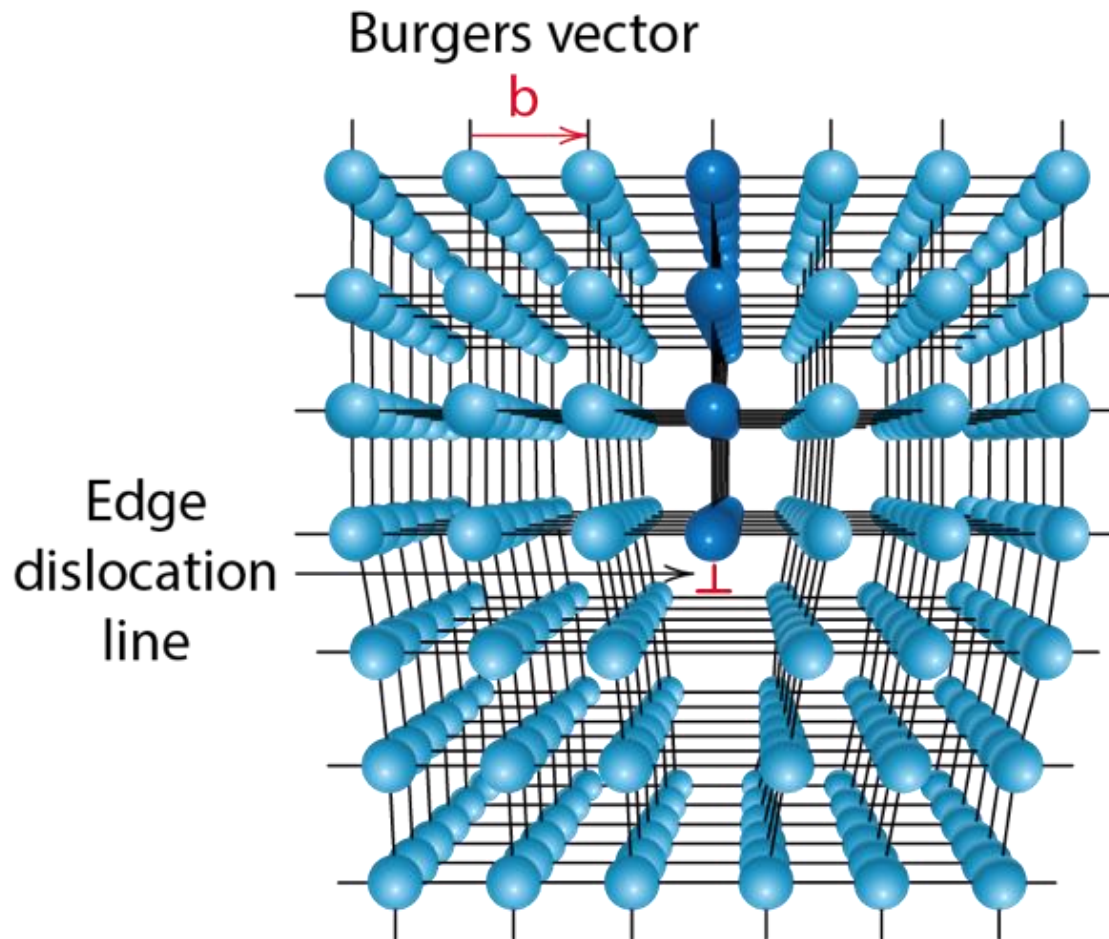- ❑ **Edge dislocation:**
  - ❑ extra half-plane of atoms inserted in a crystal structure
  - ❑ **b** perpendicular ($\perp$) to dislocation line
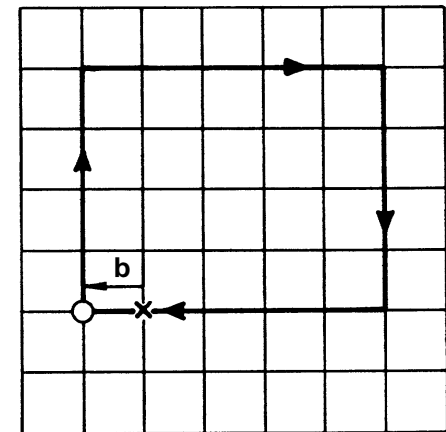
- ❑ **Screw dislocation:**
  - ❑ spiral planar ramp resulting from shear deformation
  - ❑ **b** parallel ($\parallel$) to dislocation line

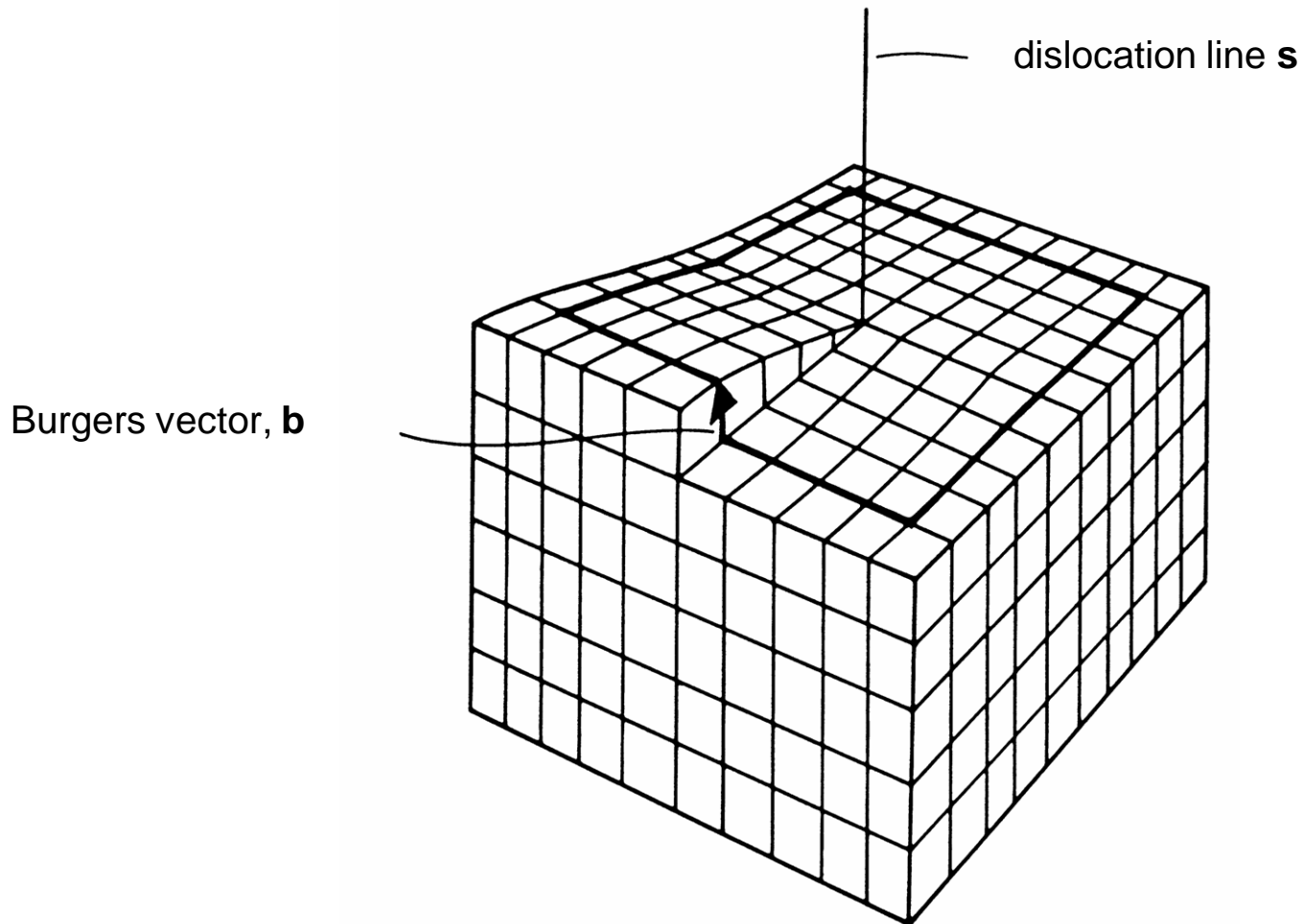 Burger's vector, **b**: measure of lattice distortion

Edge Dislocation

Burgers vector

b

Edge dislocation line

(a)

b

(b)

Fig. 4.4, *Callister & Rethwisch 10e.*

Screw Dislocation

dislocation line **s**

Burgers vector, **b**

Screw Dislocation

(a) Schematic of screw dislocation in a crystal

(b) Top view of screw dislocation in (a)

Dislocation line

Burgers vector b

(a)

(b)
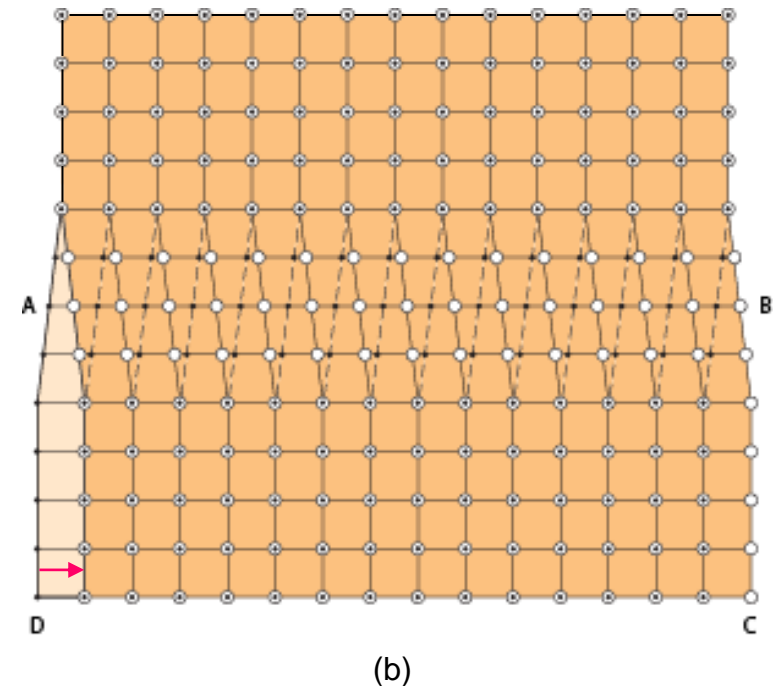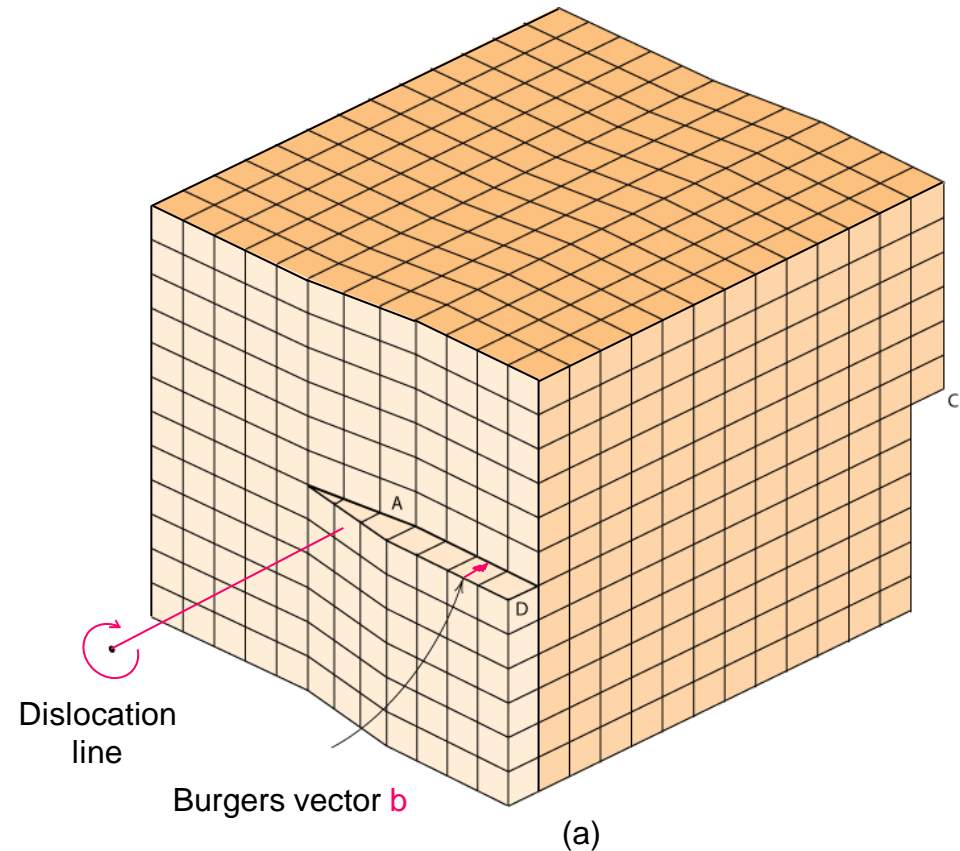
Adapted from Fig. 4.5, *Callister & Rethwisch 10e.*
[Figure (b) from W. T. Read, Jr.,Dislocations in Crystals, McGraw-Hill Book Company, New York, NY, 1953.]

Edge, Screw, and Mixed Dislocations

Mixed

Edge

Screw

Adapted from Fig. 4.6, *Callister & Rethwisch 10e.*
[Figure (b) from W. T. Read, Jr., Dislocations in Crystals,
McGraw-Hill Book Company, New York, NY, 1953.]
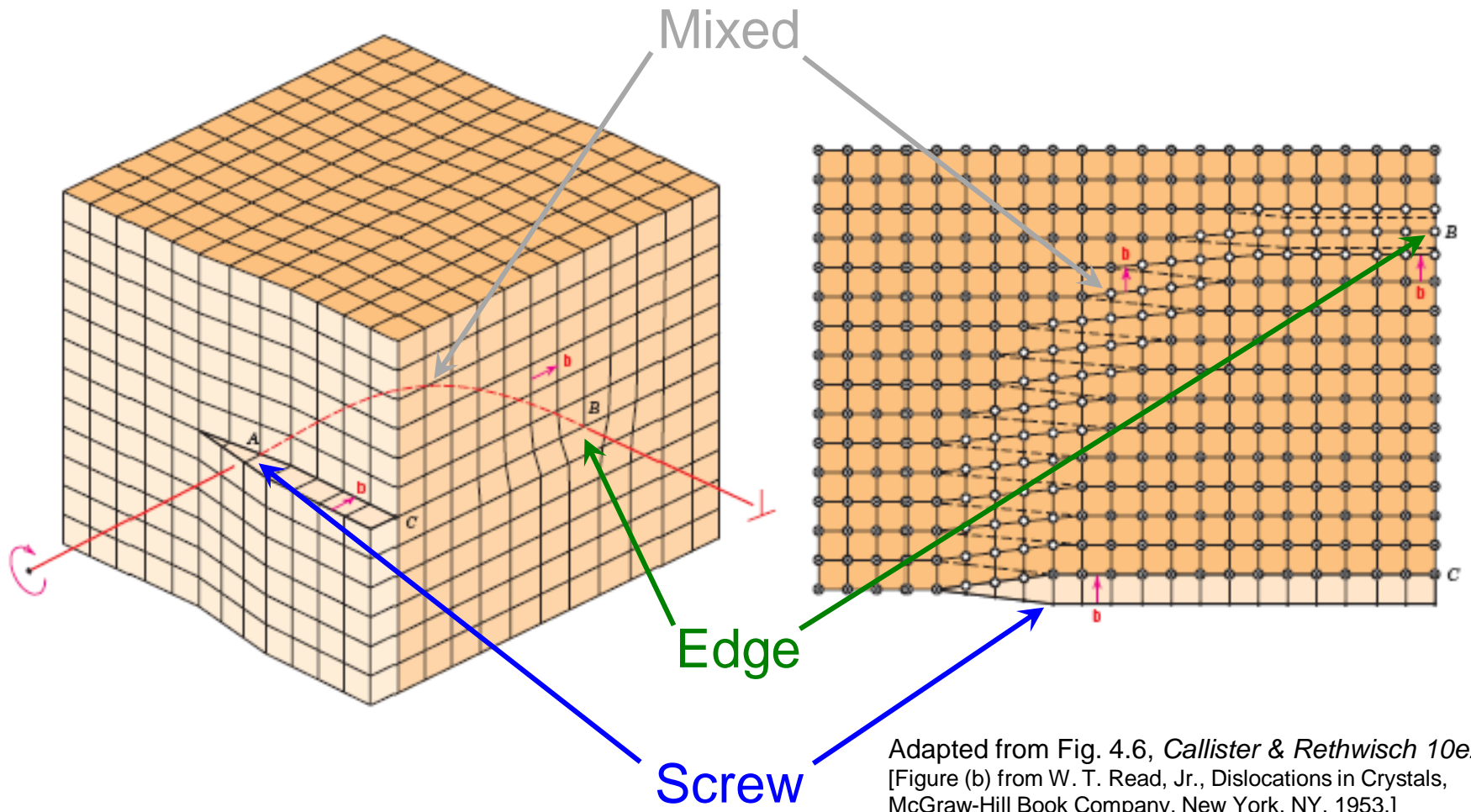
Observation of Dislocations

Dislocations appear as dark lines
in this electron micrograph
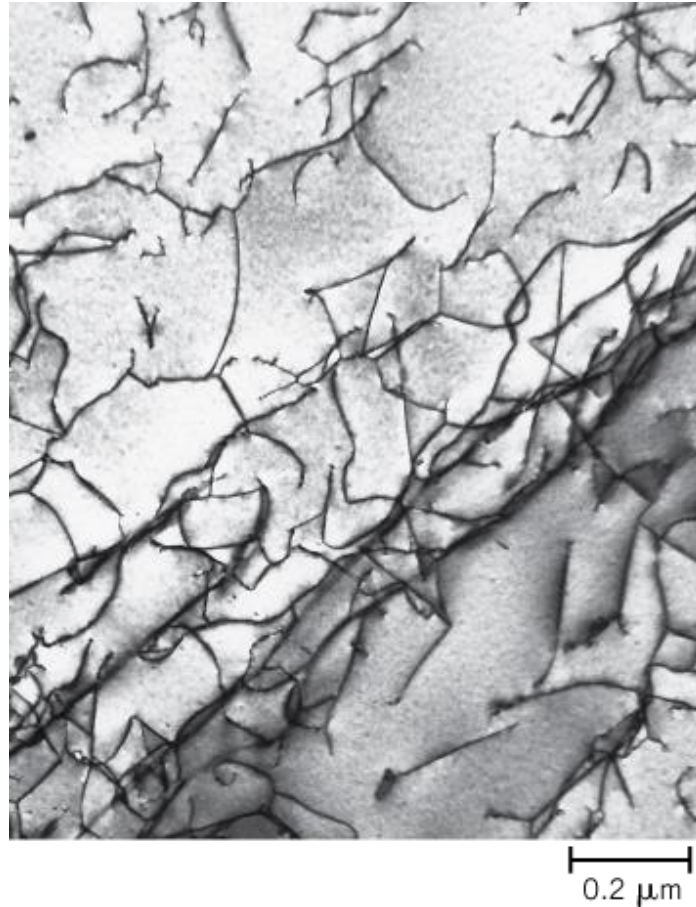
Fig. 4.7, *Callister & Rethwisch 10e.*
(Courtesy of M. R. Plichta, Michigan
Technological University.)

0.2 μm

Linear Defects—Dislocations

Dislocations:

- move when stresses are applied,
- permanent (plastic) deformation results from dislocation motion.

Schematic of a single crystal metal

- unstressed (undeformed)

- after tensile elongation (after plastic deformation)
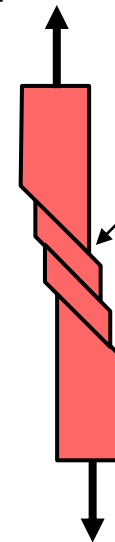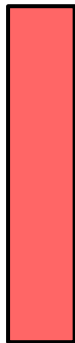
Steps correspond to plastic deformation: each step is produced by dislocations that have moved to the crystal surface.

Interfacial Defects

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Interfacial (Planar) Defects

boundary

$b \perp$

$D = b/\Theta$

grain 1 — — grain 2

Θ

https://www.springer.com/gp/book/9783540401391

grain boundary

grain boundary

https://www.springer.com/gp/book/9783540401391
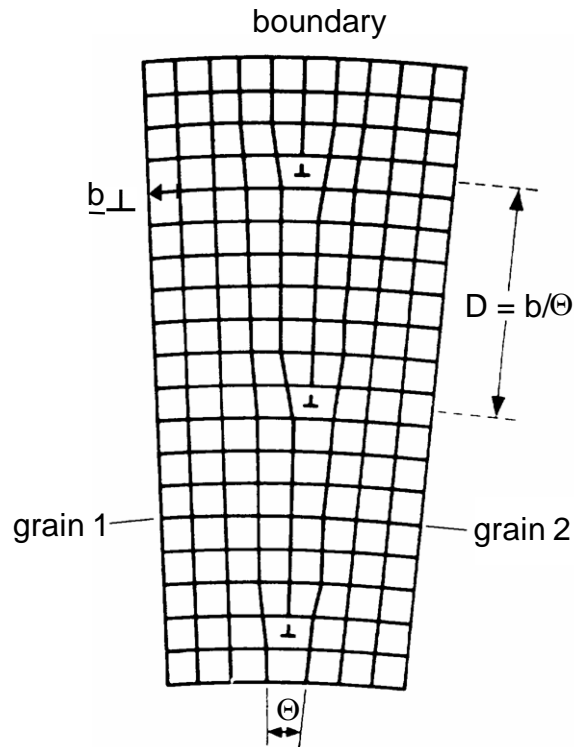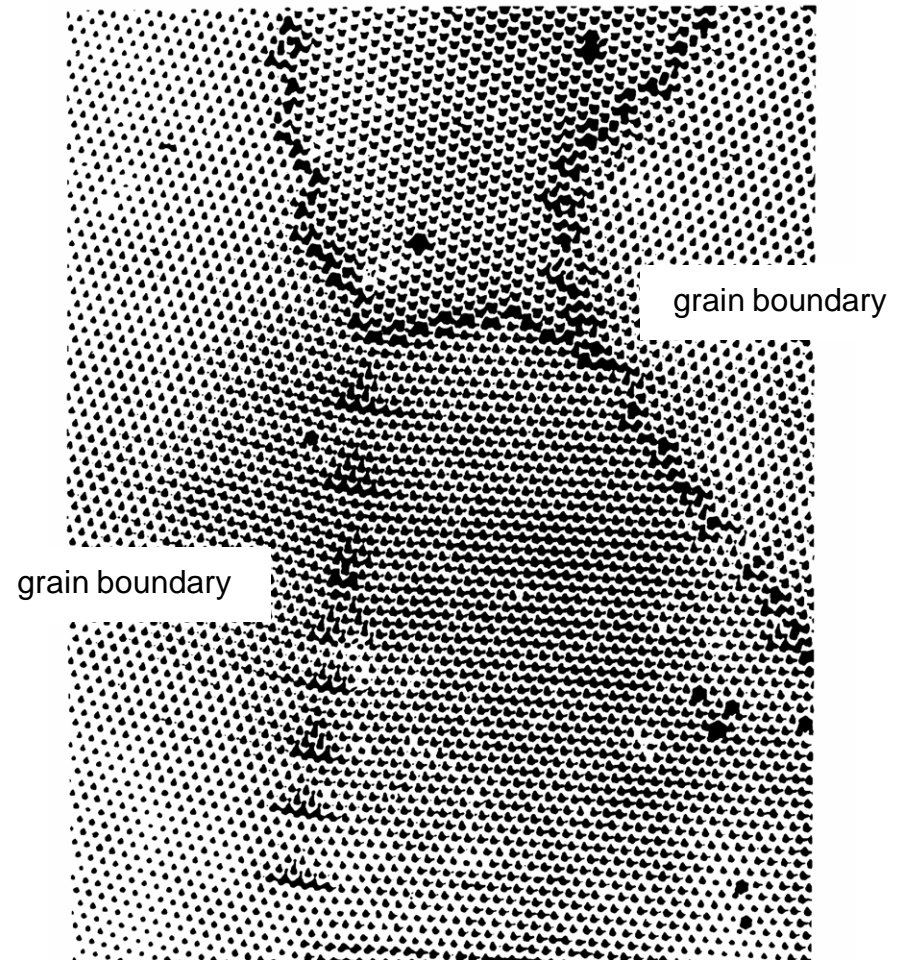
Grains and Grain Boundaries

Grain Boundaries

❑ regions between grains (crystals)

❑ crystallographic misalignment across a grain boundary

❑ Slight atomic disorder
   ❑ high atomic mobility
   ❑ high chemical reactivity

Fig. 4.8, *Callister & Rethwisch 10e.*

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Polycrystalline Materials
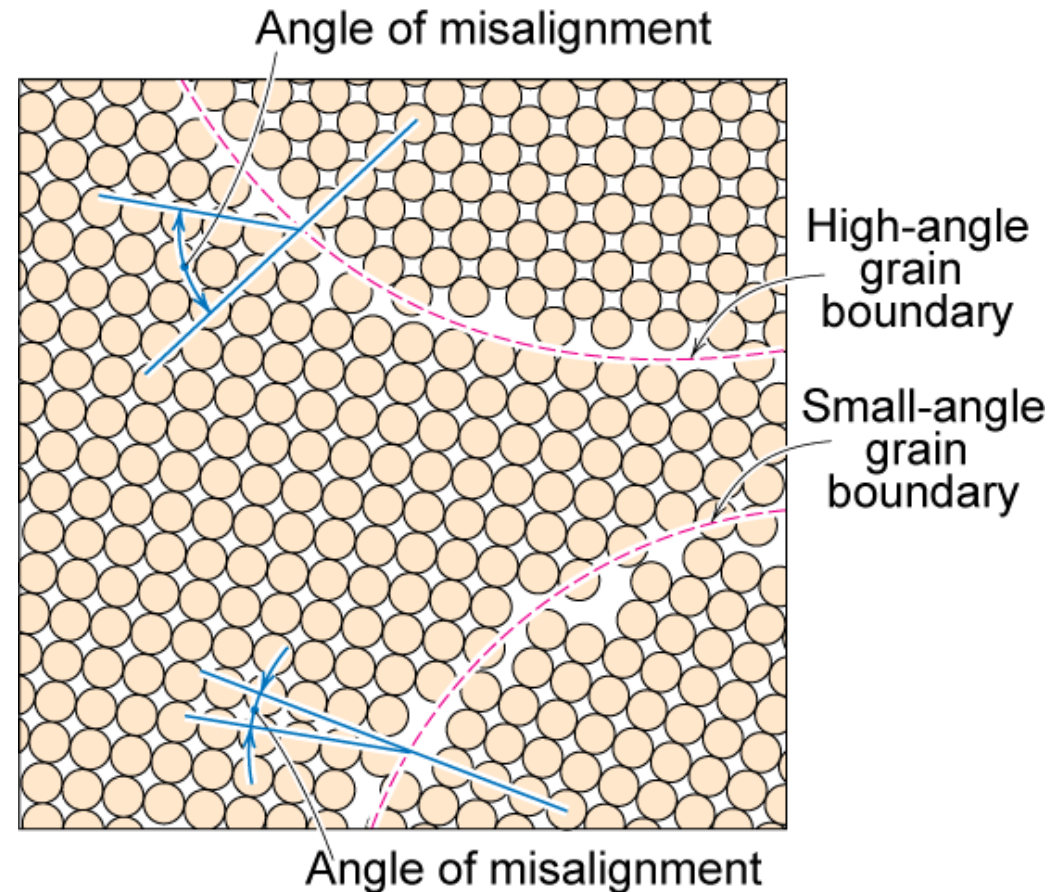
- Most engineering materials are composed of many small, single crystals (i.e., are *polycrystalline*).

Courtesy of Paul E. Danielson, Teledyne Wah Chang Albany

1 mm

large grain

small grain

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- Grain sizes typically range from 1 nm to 2 cm
  (i.e., from a few to millions of atomic layers).

Isotropy & Anisotropy

For Polycrystals

- *If properties are equal in all directions, a material is termed as 'Isotropic'.*

- *If the properties tend to be greater or diminished in any direction, a material is termed as 'Anisotropic'.*

- In an isotropic polycrystalline material, grain orientations are random.

- Many/most materials are anisotropic.

- Anisotropy results from preferred orientations or 'Texture'.
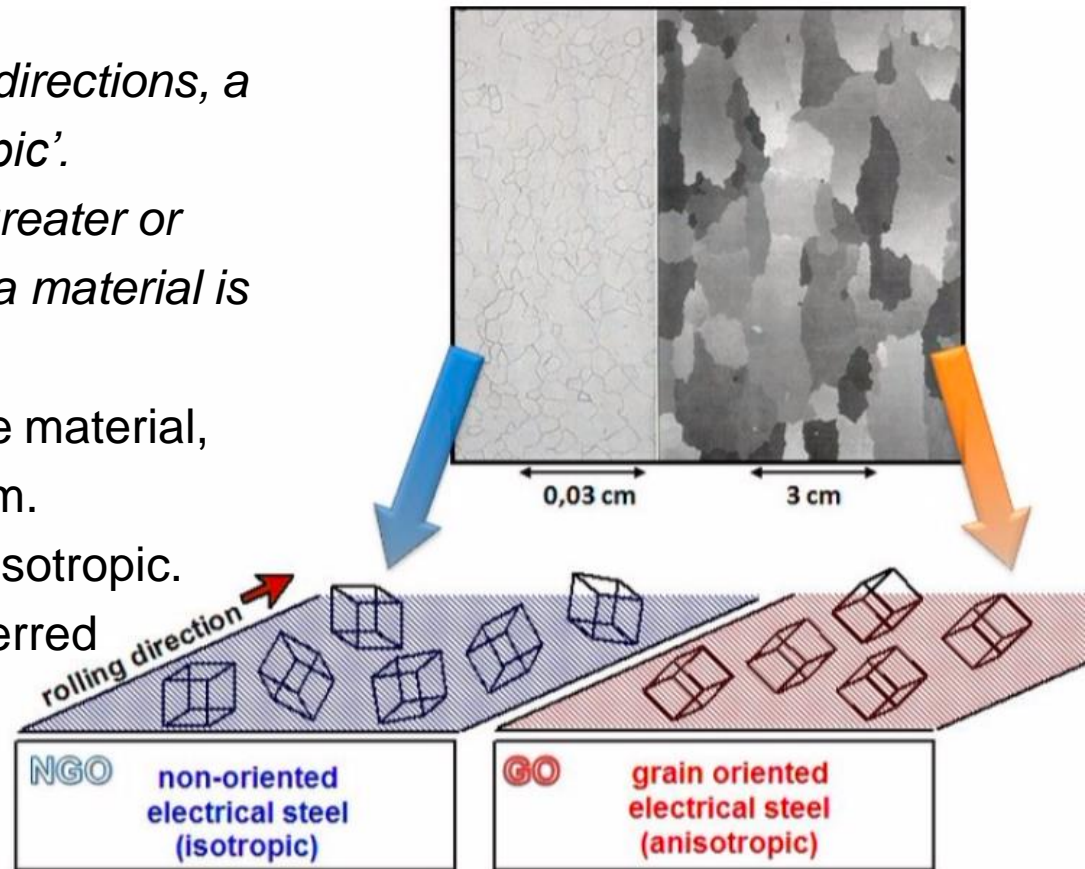
Texture

- *preferred orientations in a polycrystal.*

- Texture may range from slight to highly developed.

0,03 cm   3 cm

rolling direction

NGO non-oriented electrical steel (isotropic)

GO grain oriented electrical steel (anisotropic)

http://www.dierk-raabe.com/electrical-steels-fe-3-si/

Crystallographic orientation

ND: Normal Direction

RD: Rolling Direction

TD: Transverse Direction

Cold rolled sheet steel

https://images.app.goo.gl/eSLBdrEBpMiqqqpr5

BD: Building Direction

TD: Transverse Direction

SD: Scanning Direction
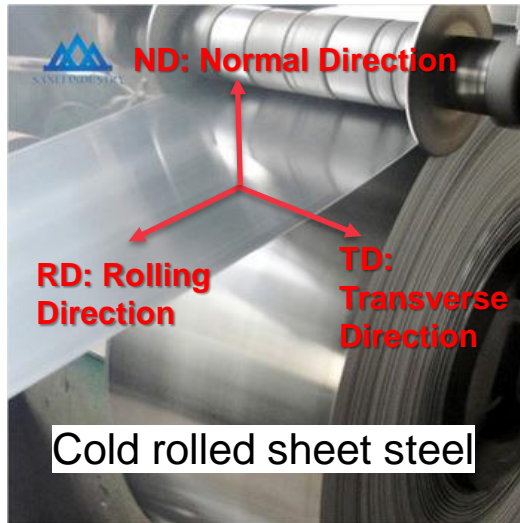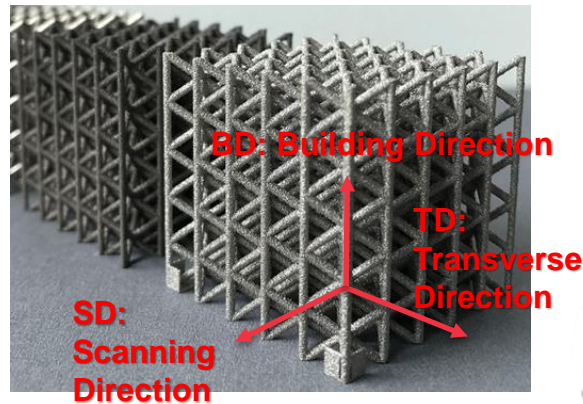
Additive manufacturing material

https://images.app.goo.gl/aJJ1R8R2953RKM5Z9

Crystallographic orientation:

*Rotation **g** to transform the sample frame **{S}** into the crystal frame **{C}**: **{C}** = **g** · **{S}***

g : 3x3 rotation matrix

$$g = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} cos\alpha_1 & cos\beta_1 & cos\gamma_1 \\ cos\alpha_2 & cos\beta_2 & cos\gamma_2 \\ cos\alpha_3 & cos\beta_3 & cos\gamma_3 \end{pmatrix}$$

External axes

ND
TD
RD

Crystal axes

[001]
[010]
[100]
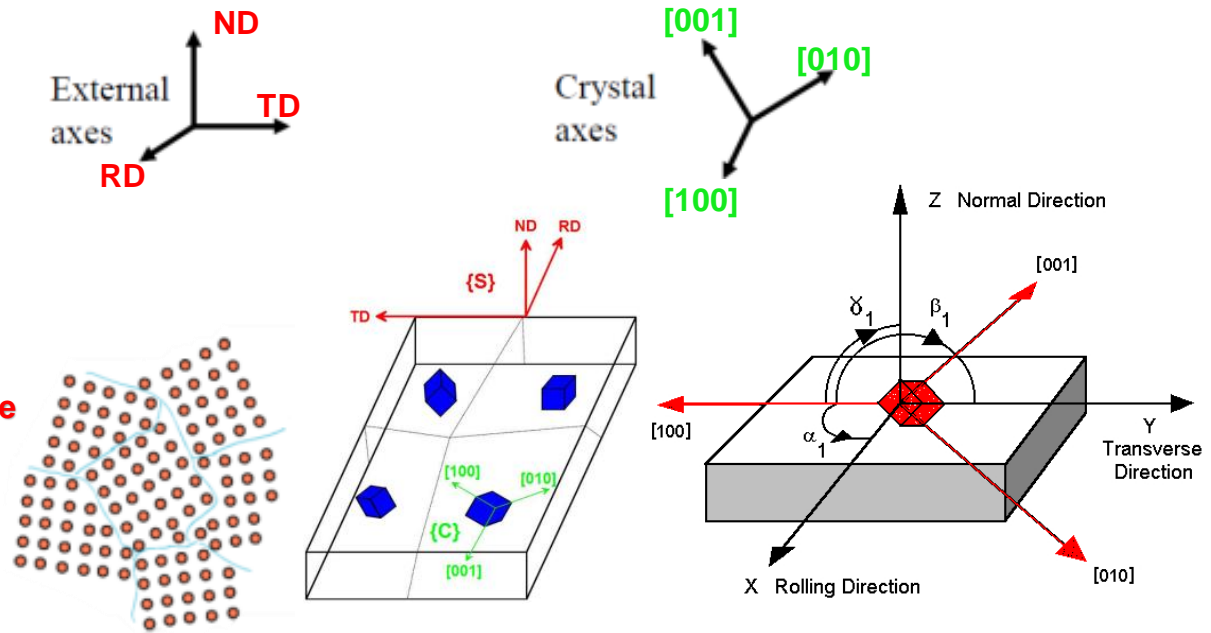
Olaf Engler (Hydro Aluminium): Introduction to Texture Analysis: Macrotexture, Microtexture, Orientation Microscopy

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Grain size
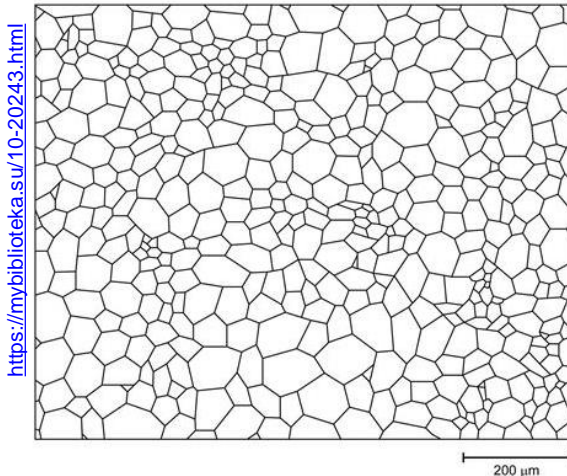
Idea: Fit a circle to the points making up a grain based on the equivalent area criterion.

log-normal distribution
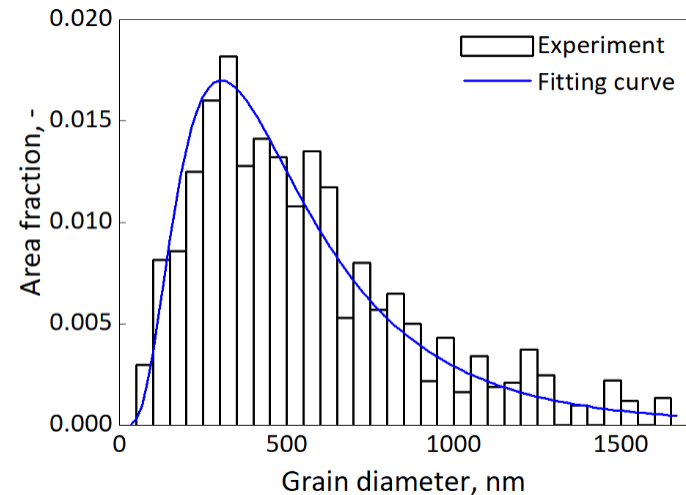
$$\text{mean}(d) = \exp(\mu + \sigma^2/2)$$

Equivalent grain diameter d

grain area

equivalent circle

grain equivalent diameter

$$f(d; \mu, \sigma)\mathrm{d}y = \frac{1}{d\sigma\sqrt{2\pi}} \exp\left(-\frac{(\ln d - \mu)^2}{2\sigma^2}\right) \mathrm{d}y,$$

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Grain shape

grain area | fitted ellipse | Major axis | θ | horizontal direction | Minor axis
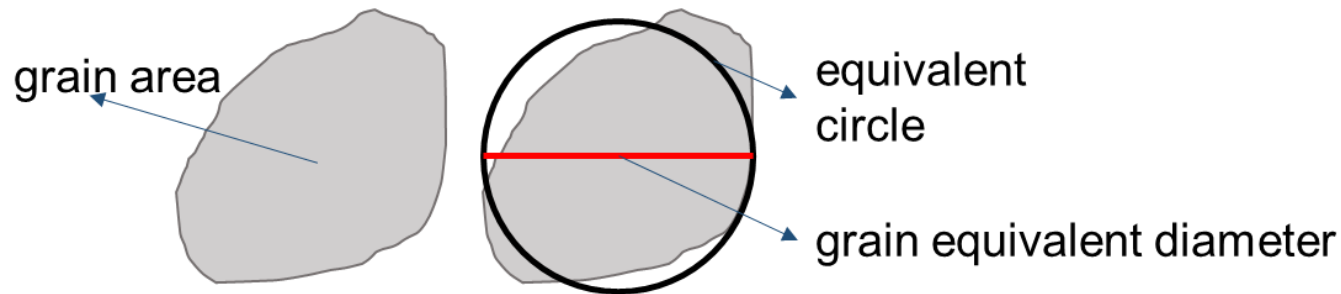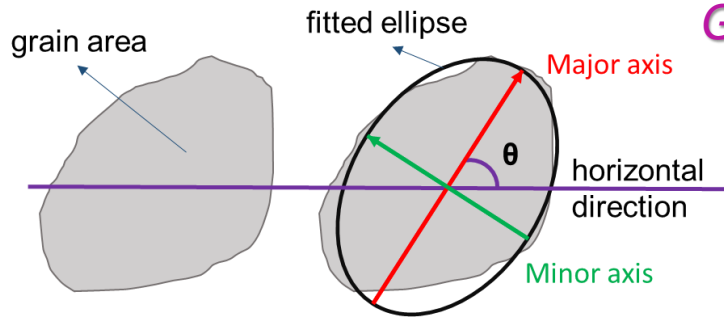
Idea: Fit an ellipse to the points making up a grain based on the equivalent area criterion.

Grain shape factor: Equivalent grain aspect ratio

$$Aspect\ ratio = \frac{Length\ of\ the\ minor\ axis}{Length\ of\ the\ major\ axis}$$

Examples:
1:1:1 refers to equiaxed grains,
1:0.1 to cold-rolled grains,
ranges from 0 to 1.

Grain shape angle/ orientation θ

The angle between the major axis direction of a fitted ellipse the horizontal direction.

Beta distribution

$$f(x; \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

$$B(\alpha, \beta) = \int_0^1 x^{\alpha-1}(1-x)^{\beta-1}\ \mathrm{d}t$$

$$mean(x) = \frac{1}{1 + \frac{\beta}{\alpha}}$$

Summary

❑ Point, Linear, and Interfacial defects exist in solids.

- Point defects
    - Vacancies
    - Interstitial atoms
    - Substitutional impurity atoms

- Linear defects
    - Dislocations
- Interfacial defects
    - Grain boundaries
    - Twin boundaries
    - Stacking Faults

❑ The equilibrium number vacancy defects depends on **temperature**.

❑ Dislocation types include **edge**, **screw**, and **mixed**.

❑ Polycrystals might result in **isotropic** properties.

Announcements

Reading: Textbook Ch. 3-4

Assignment: Open today; DL: 18:00 Sunday

Q&A time: Tuesday 16:30

Exercise: Thursday 10:15 – 12:00

Preparation of your computational environment is needed before the exercise sessions.

SOFTWARE for exercise and assignment

Matlab: Aalto software download service Download.aalto.fi (Aalto user credentials log in is needed).

**MTEX toolbox:** open-sourced software https://mtex-toolbox.github.io/

Aalto VDI system: **mfavdi.aalto.fi**, or VMware Horizon Client **vdi.aalto.fi**, for more information, please refer to Remote access to Windows classroom computers.

IMPORTANT! Please remember to do '**Sign Out**' after the session (NOT Disconnect). Click your username in Start and click 'Sign Out'.
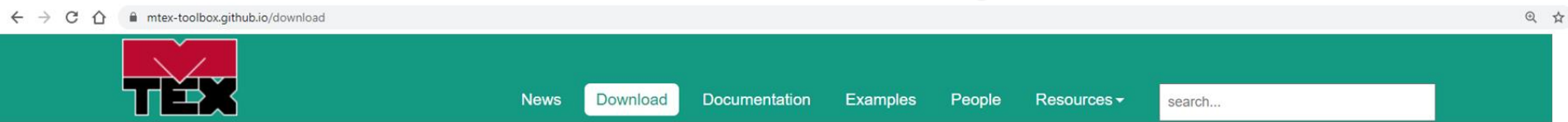
Basic Rule: Please use DOT as the decimal separator, NO COMMA!

IMPORTANT! Please download and extract the zip file of **MTEX 5.4.0**. Copy it to your Matlab work direction or add it to the Matlab work path.

Please also download the 'EBSDdata.ctf' file as input. (in MyCourses Exercise1)

SOFTWARE for exercise and assignment
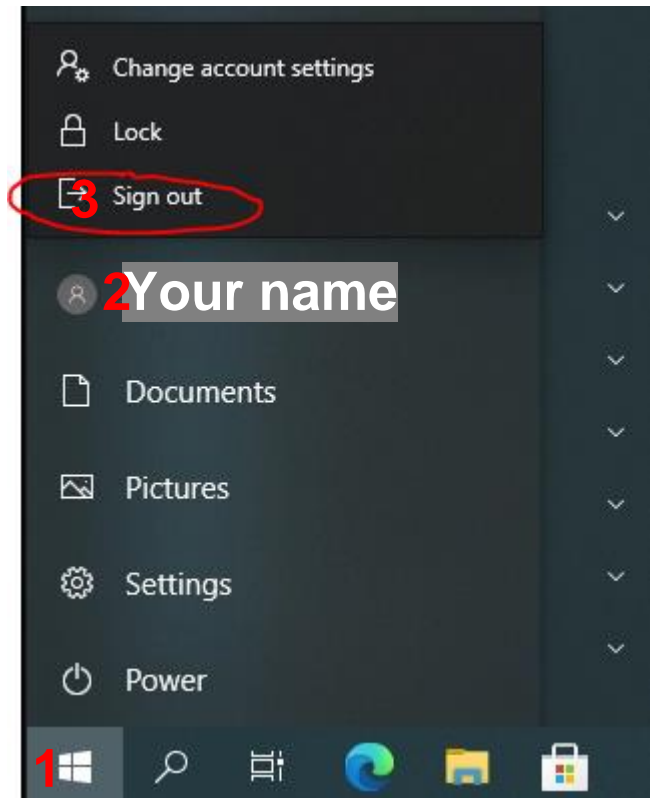
https://mtex-toolbox.github.io/download

Mtex Download

Download

Installation

1. download and extract the zip file to an arbitrary folder
2. start Matlab (version 2016b or newer required - older versions have not been tested)
3. change the current folder in Matlab to the folder where MTEX is installed
4. type `startup_mtex` into the command window
5. click one of the menu items to import data or to consult the documentation

In case you experience any problems, especiall on Mac OSX, have a look at our trouble shooting page

Downloads

File Name	Release Date	Comments	Downloads
mtex-5.7.0.zip	May 2021	improved parent grain reconstruction, changelog	4.5k
mtex-5.6.1.zip	March 2021	bug fix release, changelog	1.5k
mtex-5.6.0.zip	January 2021	simplified parent grain reconstruction, changelog	2.4k
mtex-5.5.2.zip		**1. Download 'mtex-5.4.0.zip' to your Matlab work folder.**	
mtex-5.4.0.zip	July 2020	parent grain reconstruction, changelog	2767
mtex-5.3.1.zip	June 2020	bug fixes, boundary curvature, changelog	1051
mtex-5.3.zip	April 2020	performance updates, changelog	2118

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SOFTWARE for exercise and assignment

2. Run Matlab, set the path to your work folder.

3. Find the download .zip file. Double click to extract.

A 400-year mathematical story – Finale
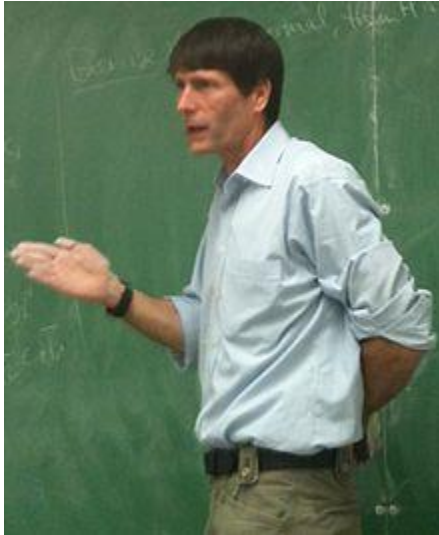
Thomas Callister Hales

Thomas Hales, then at the University of Michigan, determined that the maximum density of all arrangements could be found by minimizing a function with 150 variables.

1 of 121 pages

Annals of Mathematics, 162 (2005), 1065–1185

A proof of the Kepler conjecture

By THOMAS C. HALES*

To the memory of László Fejes Tóth

Contents
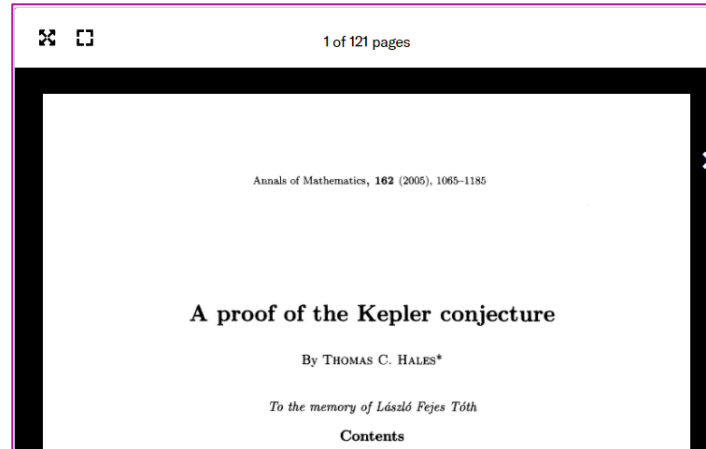
1998
- 250 pages
- 3 GB data
- 99% correct

2015
- 11 years of work
- 21 collaborators

CrossMark

1

A FORMAL PROOF OF THE KEPLER CONJECTURE

THOMAS HALES[1], MARK ADAMS[2,3], GERTRUD BAUER[4],
TAT DAT DANG[5], JOHN HARRISON[6], LE TRUONG HOANG[7],
CEZARY KALISZYK[8], VICTOR MAGRON[9], SEAN MCLAUGHLIN[10],
TAT THANG NGUYEN[7], QUANG TRUONG NGUYEN[1],
TOBIAS NIPKOW[11], STEVEN OBUA[12], JOSEPH PLESO[13], JASON RUTE[14],
ALEXEY SOLOVYEV[15], THI HOAI AN TA[7], NAM TRUNG TRAN[7],
THI DIEP TRIEU[16], JOSEF URBAN[17], KY VU[18] and
ROLAND ZUMKELLER[19]
[1] University of Pittsburgh, USA;

Questions?