Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

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Chapter 1: Introduction to Materials Science & Engineering

ISSUES TO ADDRESS...

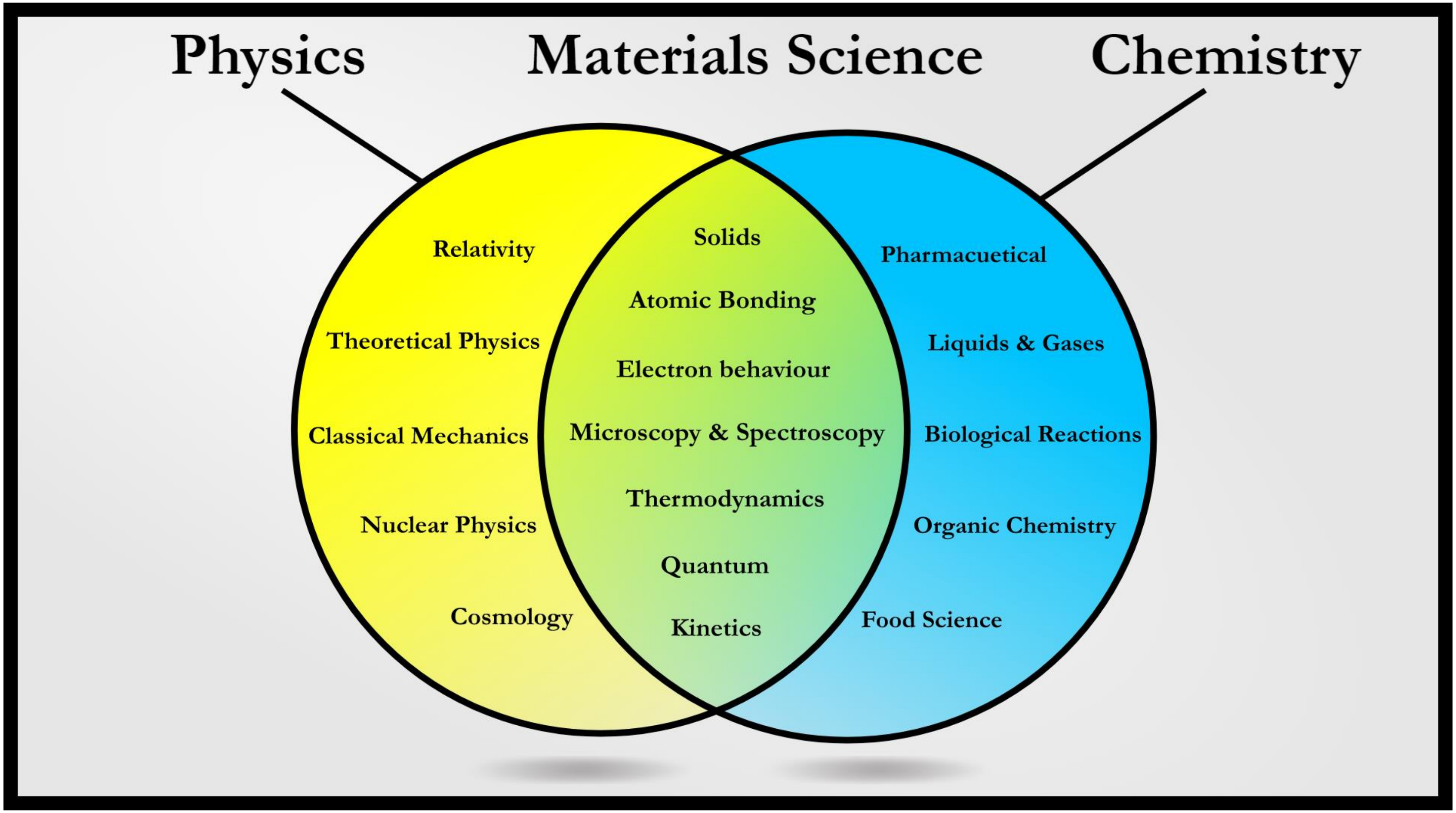
- What is **materials science** and **engineering**?
- Why are materials important?
- Why is it important for engineers to understand materials?

- Typical **material types**.
- Typical **material properties**.
- The **structure-property** correlation.

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

What is Materials Science & Engineering?

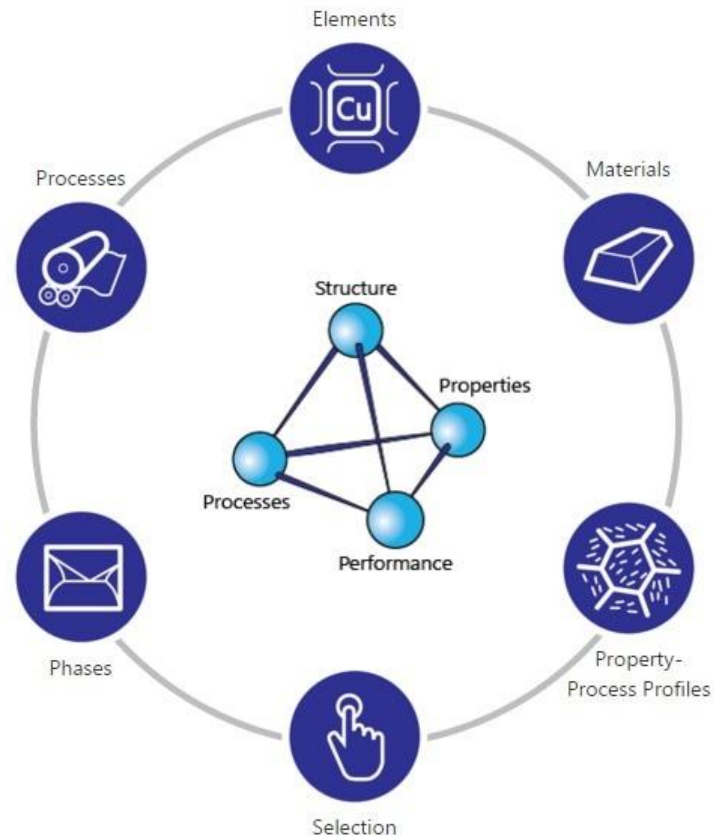
www.menti.com and use code **“1708 0257”** to describe



https://msestudent.com/13-reasons-why-you-should-study-materials-science-and-engineering/

What is Materials Science & Engineering?

- Materials science
  - Investigate relationships between structures and properties of materials
  - Design/develop new materials
- Materials engineering
  - Create products from existing materials
  - Develop materials processing techniques



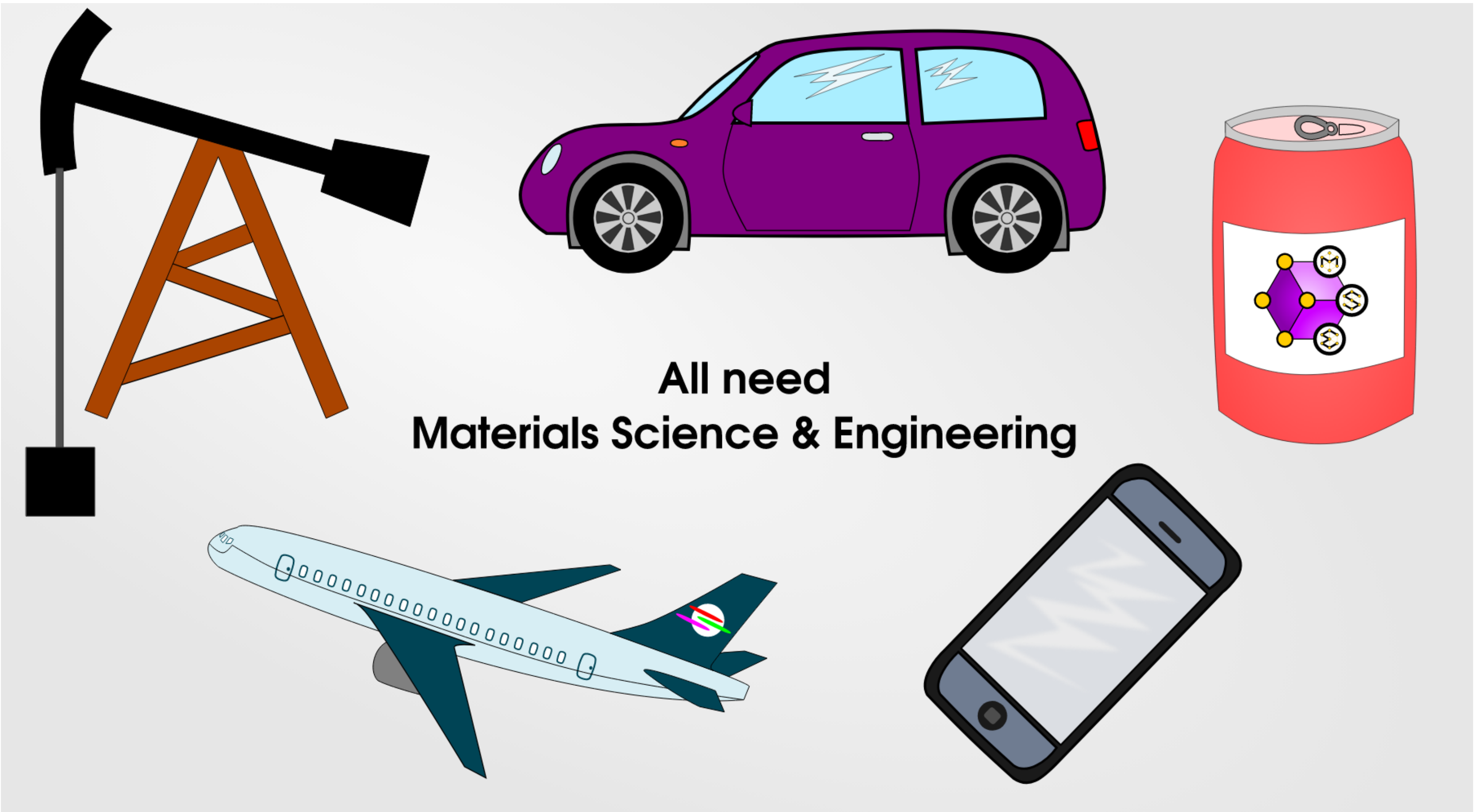
http://www.stemclopedia.com/Matsci.html

Why Are Materials Important?

- Materials drive advancements in our society
  - Stone Age
  - Bronze Age
  - Iron Age

- What is today's material age?
  - Silicon (Electronic Materials) Age?
  - Nanomaterials Age?
  - Polymer Age?

Why is it Important for Engineers to Understand Materials?



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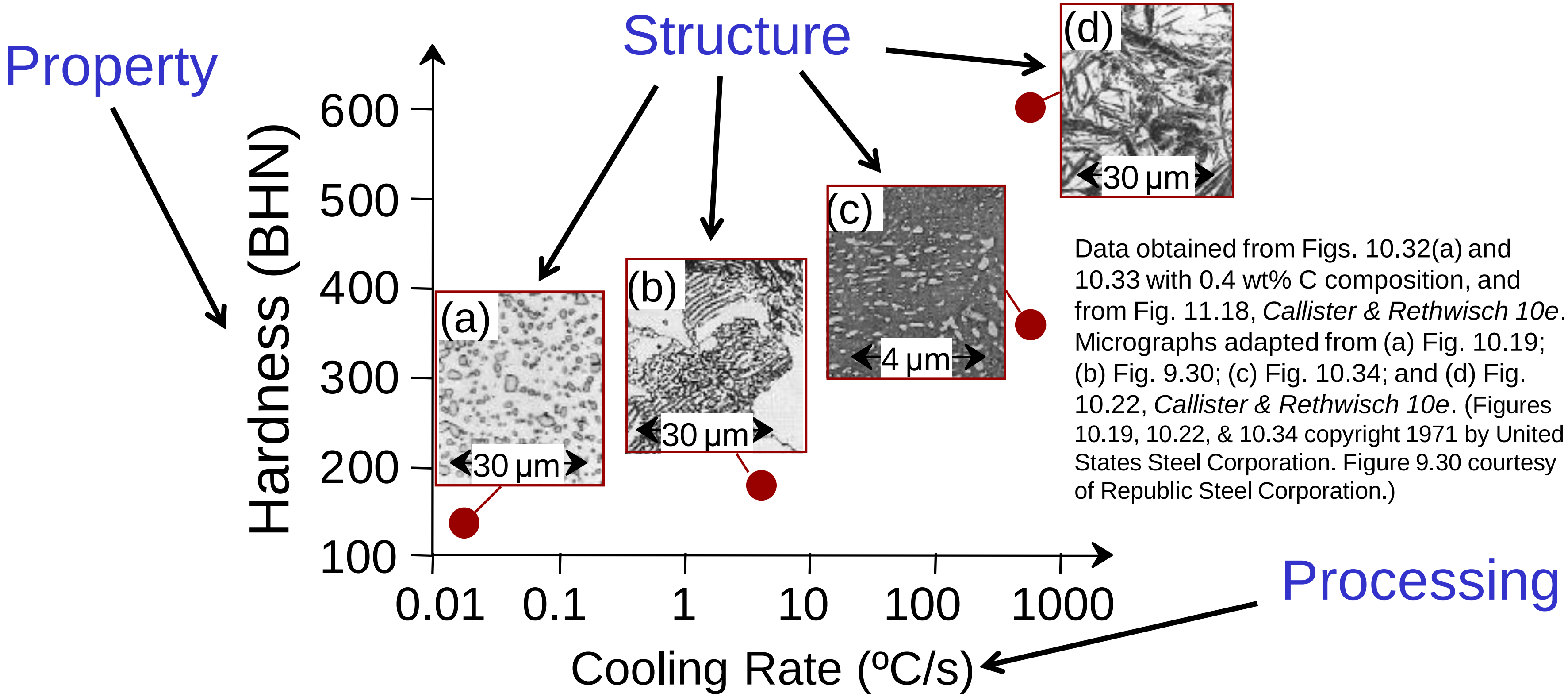
Why is it Important for Engineers to Understand Materials? (cont.)

- Products/devices/components that engineers design are all made of materials

- To select appropriate materials and processing techniques for specific applications engineers must
  - have knowledge of material properties and
  - understand the structure-property relationships

Relationships Among Processing, Structure, & Properties

- Processing (e.g., cooling rate of steel from high temperature) affects structure (microstructure)
- Structure in turn effects hardness



Data obtained from Figs. 10.32(a) and 10.33 with 0.4 wt% C composition, and from Fig. 11.18, *Callister & Rethwisch 10e*. Micrographs adapted from (a) Fig. 10.19; (b) Fig. 9.30; (c) Fig. 10.34; and (d) Fig. 10.22, *Callister & Rethwisch 10e*. (Figures 10.19, 10.22, & 10.34 copyright 1971 by United States Steel Corporation. Figure 9.30 courtesy of Republic Steel Corporation.)

Types of Materials

- Metals:
  - Strong, ductile
  - High thermal & electrical conductivities
  - Opaque, reflective

- Polymers/plastics: compounds of non-metallic elements
  - Soft, ductile, low strengths, low densities
  - Low thermal & electrical conductivities
  - Opaque, translucent or transparent

- Ceramics: compounds of metallic & non-metallic elements (oxides, carbides, nitrides, sulfides)
  - Hard, Brittle
  - Low thermal & electrical conductivities
  - Opaque, translucent, or transparent

Material Property Types

Properties of materials fall into six categories as follows:

- Mechanical
- Electrical
- Thermal
- Magnetic
- Optical
- Deteriorative

Mechanical Properties

Affect of carbon content on the hardness of a common steel:

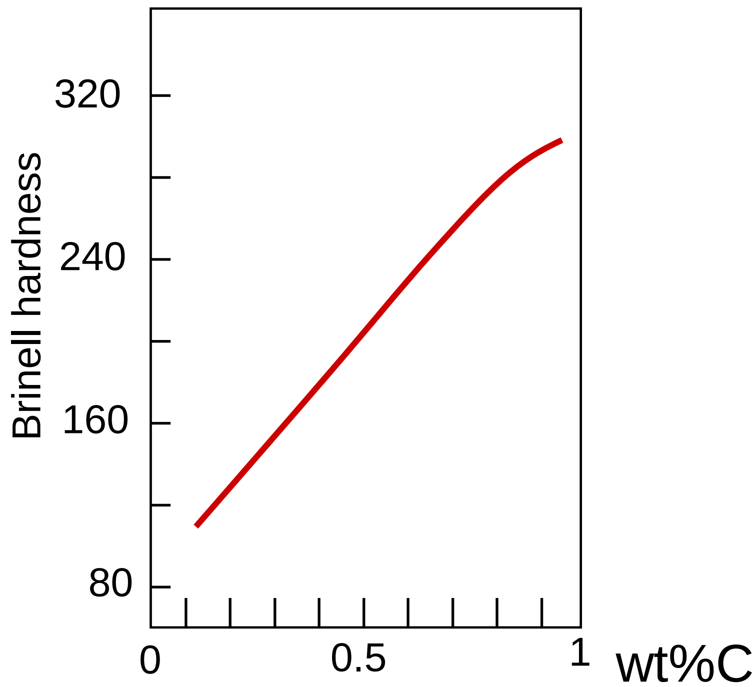


Fig. 10.31, *Callister & Rethwisch 10e.* [Data taken from *Metals Handbook: Heat Treating*, Vol. 4, 9th edition, V. Masseria (Managing Editor), 1981. Reproduced by permission of ASM International, Materials Park, OH.]

- Increasing carbon content increases hardness of steel.

Electrical Properties

Factors that affect electrical resistivity – for copper:

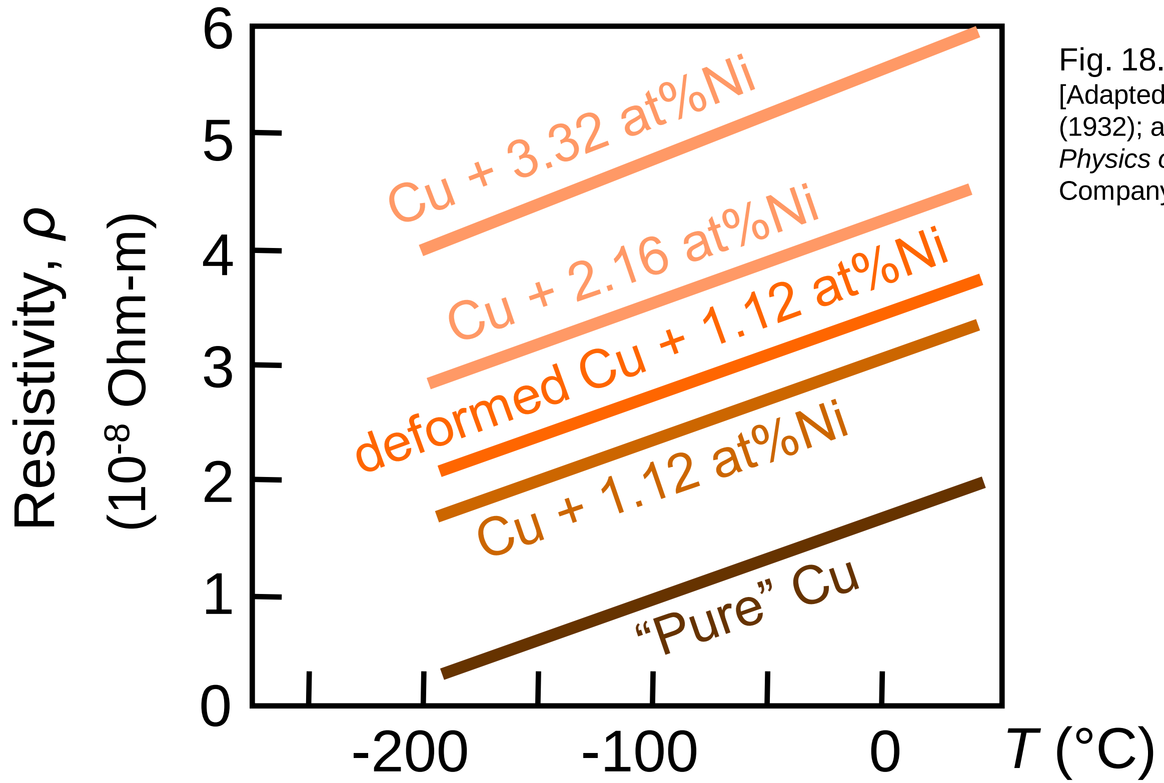


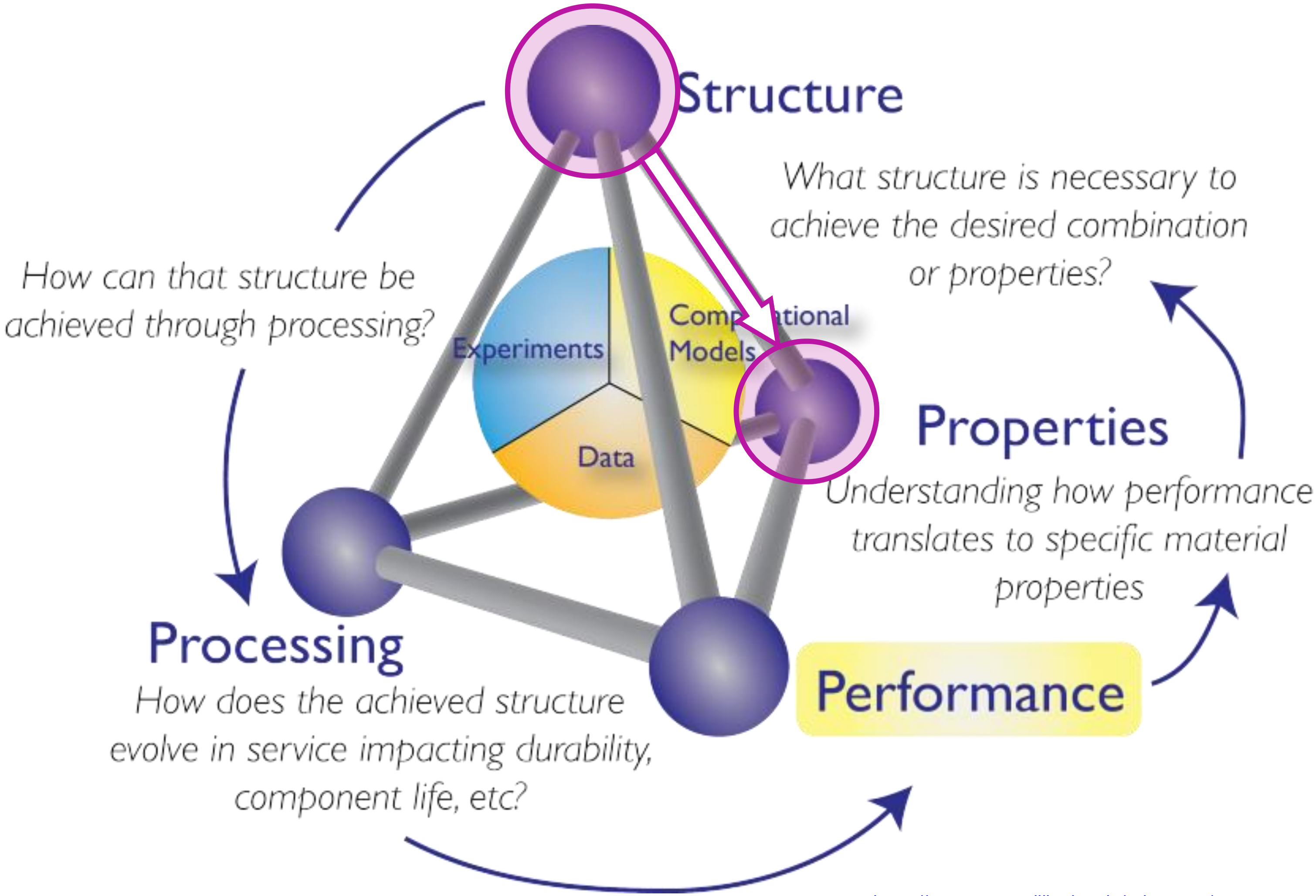
Fig. 18.8, *Callister & Rethwisch 9e.*
[Adapted from: J.O. Linde, *Ann Physik* **5**, 219 (1932); and C.A. Wert and R.M. Thomson, *Physics of Solids*, 2nd edition, McGraw-Hill Company, New York, 1970.]

- Increasing temperature increases resistivity.
- Increasing impurity content (e.g., Ni) increases resistivity.
- Deformation increases resistivity.

Summary so far

- Appropriate materials and processing decisions require engineers to understand **materials** and their **properties**.
- Materials' properties depend on their **structures**; structures are determined by how materials are **processed.**
- In terms of chemistry the three classifications of materials are *metals*, *ceramics*, and *polymers*
- Most properties of materials fall into the following six categories: *mechanical, electrical, thermal, magnetic, optical*, and *deteriorative.*

Outlook of the course



https://gems.matse.illinois.edu/educators/

Chapter 2: Atomic Structure & Interatomic Bonding

ISSUES TO ADDRESS...

- What is the structure of atoms?
- What characteristics of atoms/molecules promote interatomic/intermolecular bonding?
- What types of interatomic/intermolecular bonds exist?
- What properties of materials depend on the magnitude of interatomic/intermolecular bonds?

Atomic Structure – Basics

- Atom – electrons – 9.11×10^{-31} kg

  protons, neutrons $\}$ 1.67×10^{-27} kg

- Atomic number = # of protons in nucleus of atom
  = # of electrons in neutral species

- Atomic mass unit = amu = 1/12 mass of ^{12}C

  Atomic wt = A = wt of 6.022×10^{23} molecules or atoms

  1 amu/atom = 1 g/mol

- Avogadro constant = $N_A = 6.022 \times 10^{23}\ \mathrm{mol}^{-1}$

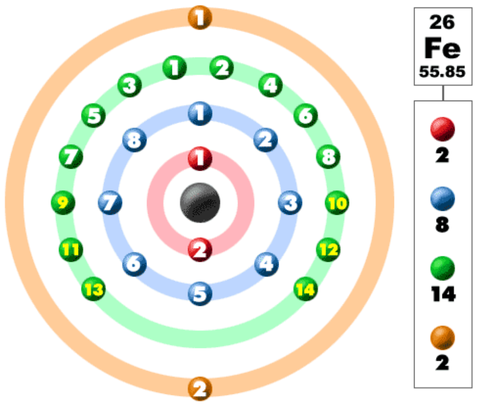
Electronic Structure

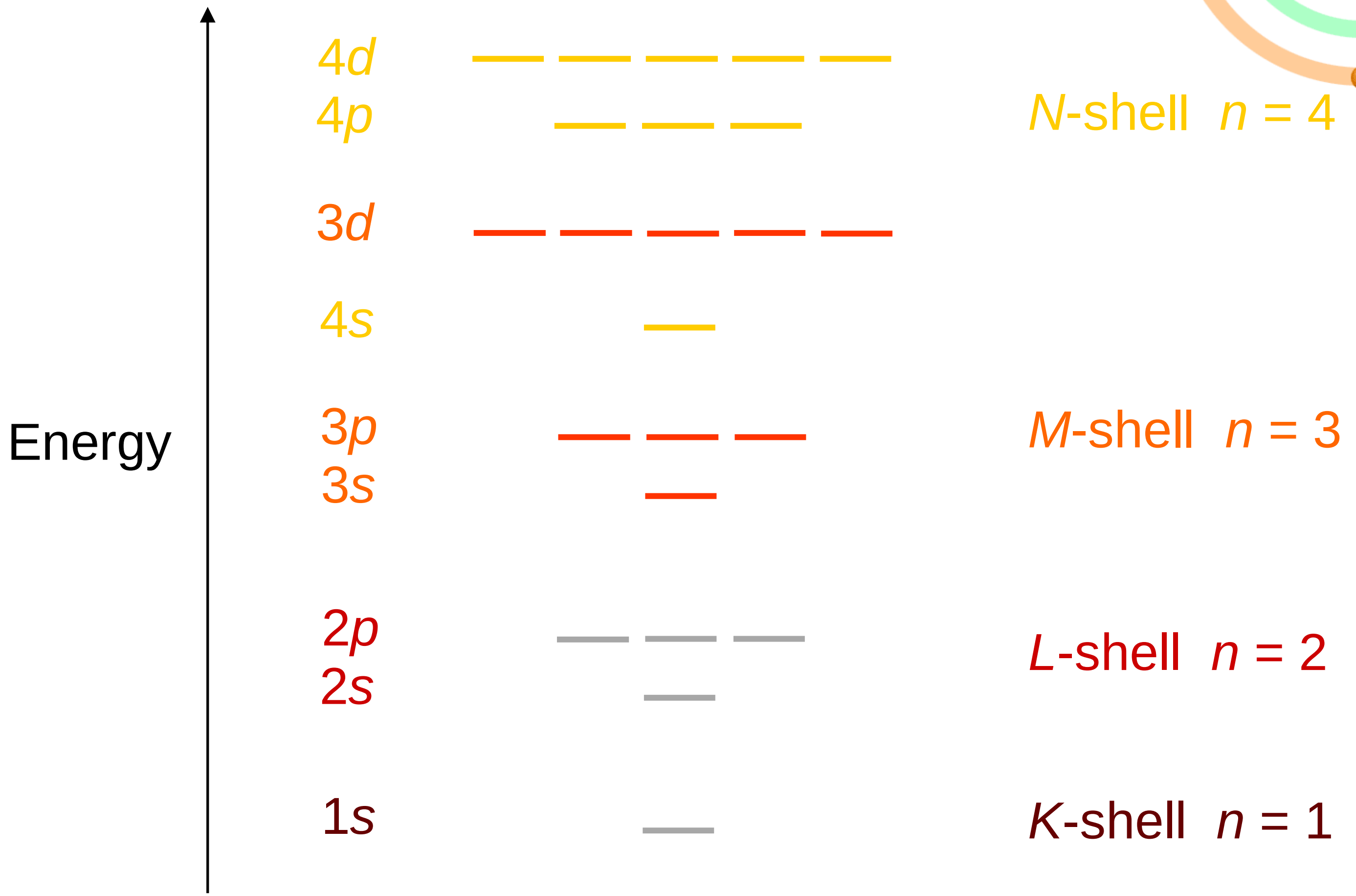
- Electrons have wave-like and particle-like characteristics.
- Two wave-like characteristics are
  - Electron position in terms of probability density
  - Shape, size, orientation of probability density determined by quantum numbers

Quantum #	Designation/Values
n = principal (shell)	*K*, *L*, *M*, *N*, *O* (1, 2, 3, 4, etc.)
ℓ = azimuthal (subshell)	*s*, *p*, *d*, *f* (0, 1, 2, 3,…, n-1)
m_ℓ = magnetic (no. of orbitals)	1, 3, 5, 7 ($-\ell$ to $+\ell$)
m_s = spin	½, -½

Electron Energy States

- have discrete energy values
- tend to occupy lowest available energy sta





Survey of Elements

- Most elements: Electron configurations not stable.

Element	Atomic #	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$	
...		...	
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$	(stable)
...	...	...	
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$	(stable)

- Why not stable? Valence (outer) shell usually not completely filled.

Electron Configurations

- Valence electrons – those in outer unfilled shells
- Filled shells are more stable – require more energy to gain or lose electrons
- Valence electrons available for bonding and tend to determine an atom's chemical properties

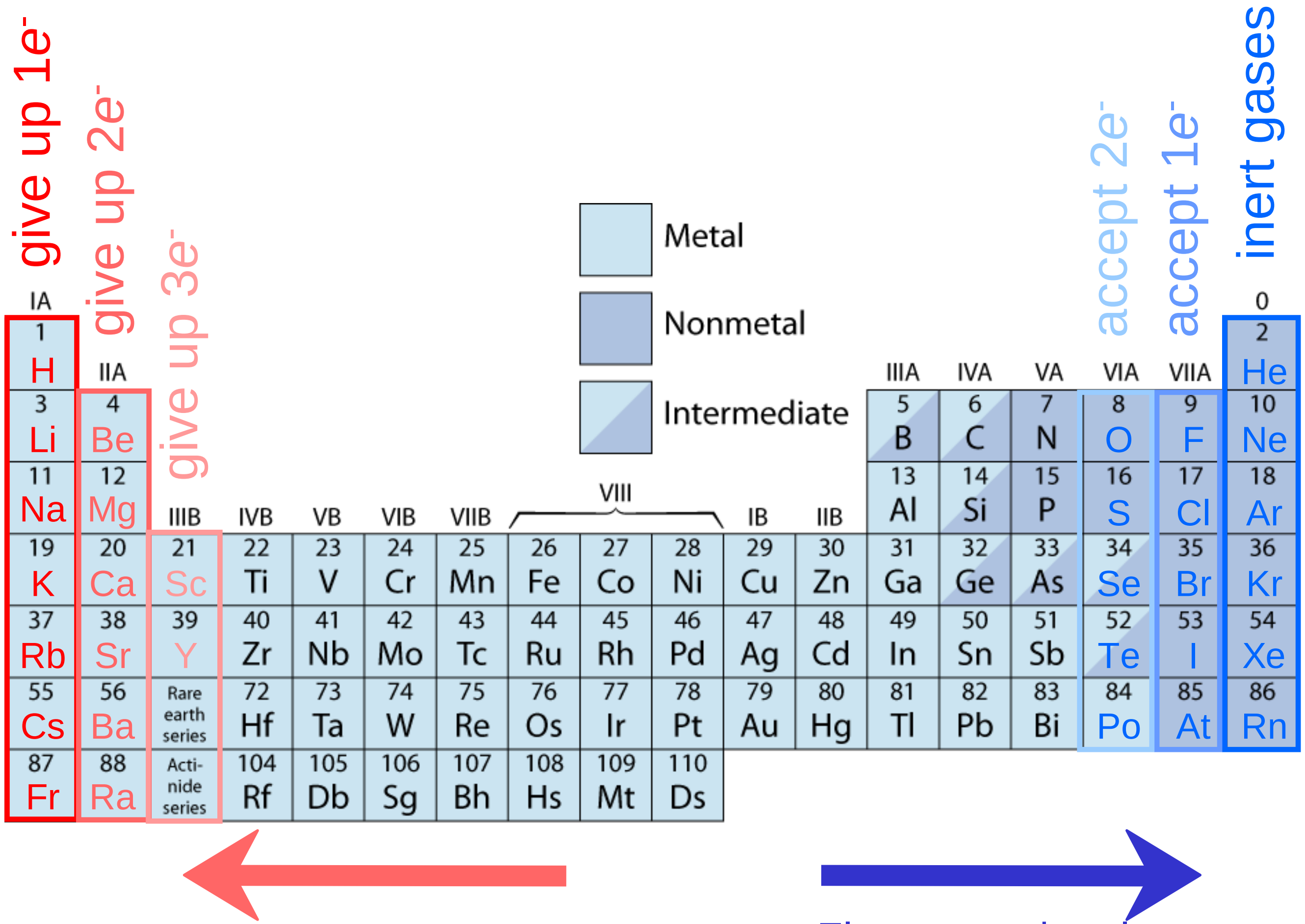
  - example: C (atomic number = 6)

$1s^2 \; \boxed{2s^2 \, 2p^2}$

valence electrons

The Periodic Table

- Elements in each column: Similar valence electron structure



Electropositive elements:
Readily give up electrons to become + ions.

Electronegative elements:
Readily acquire electrons to become - ions.

Electronegativity

- Ranges from 0.7 to 4.0
- Large values: tendency to acquire electrons.

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Smaller electronegativity

Larger electronegativity

Ionization Process

metal atom + nonmetal atom

donates electrons

accepts electrons

Dissimilar electronegativities

ex: MgO

Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$

[Ne] $3s^2$

O $1s^2\ 2s^2\ 2p^4$

Mg^{2+} $1s^2\ 2s^2\ 2p^6$

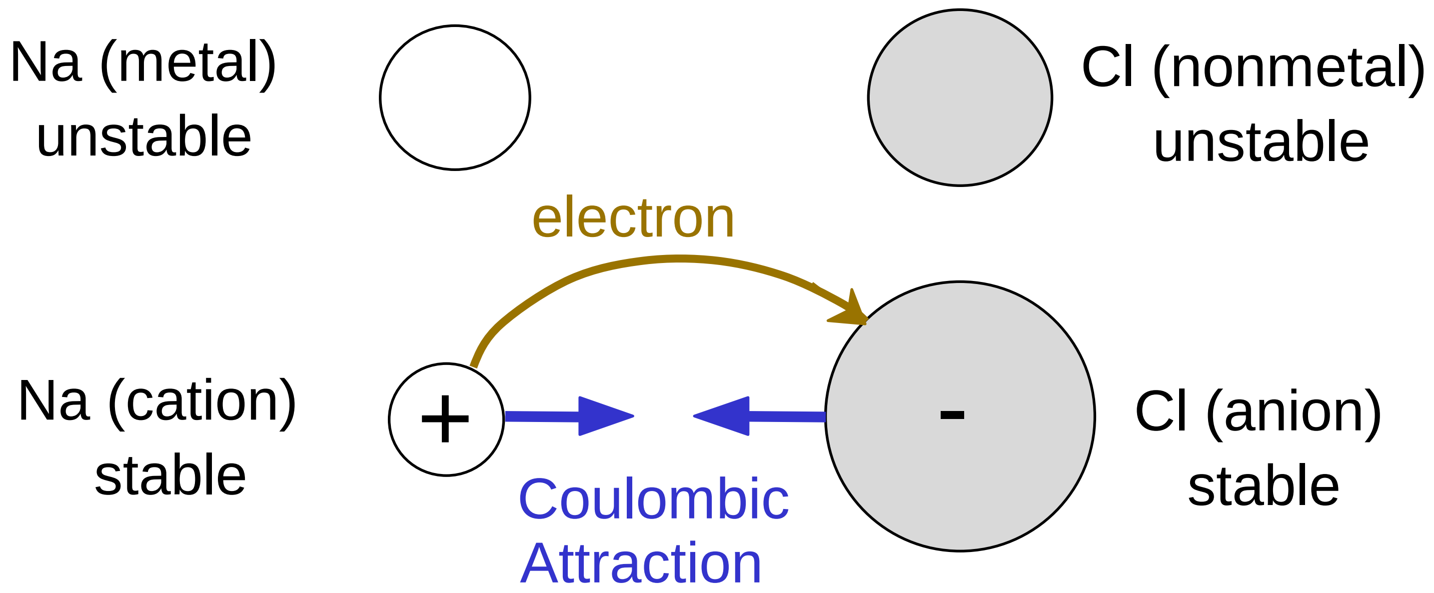
[Ne]

O^{2-} $1s^2\ 2s^2\ 2p^6$

[Ne]

Ionic Bonding

- Occurs between + and - ions.
- Requires electron transfer.
- Large difference in electronegativity required.
- Example: NaCl



Ionic Bonding (cont.)

- Energy – minimum energy most stable
  - Net energy = sum of attractive and repulsive energies
  - Equilibrium separation when net energy is a minimum

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$$

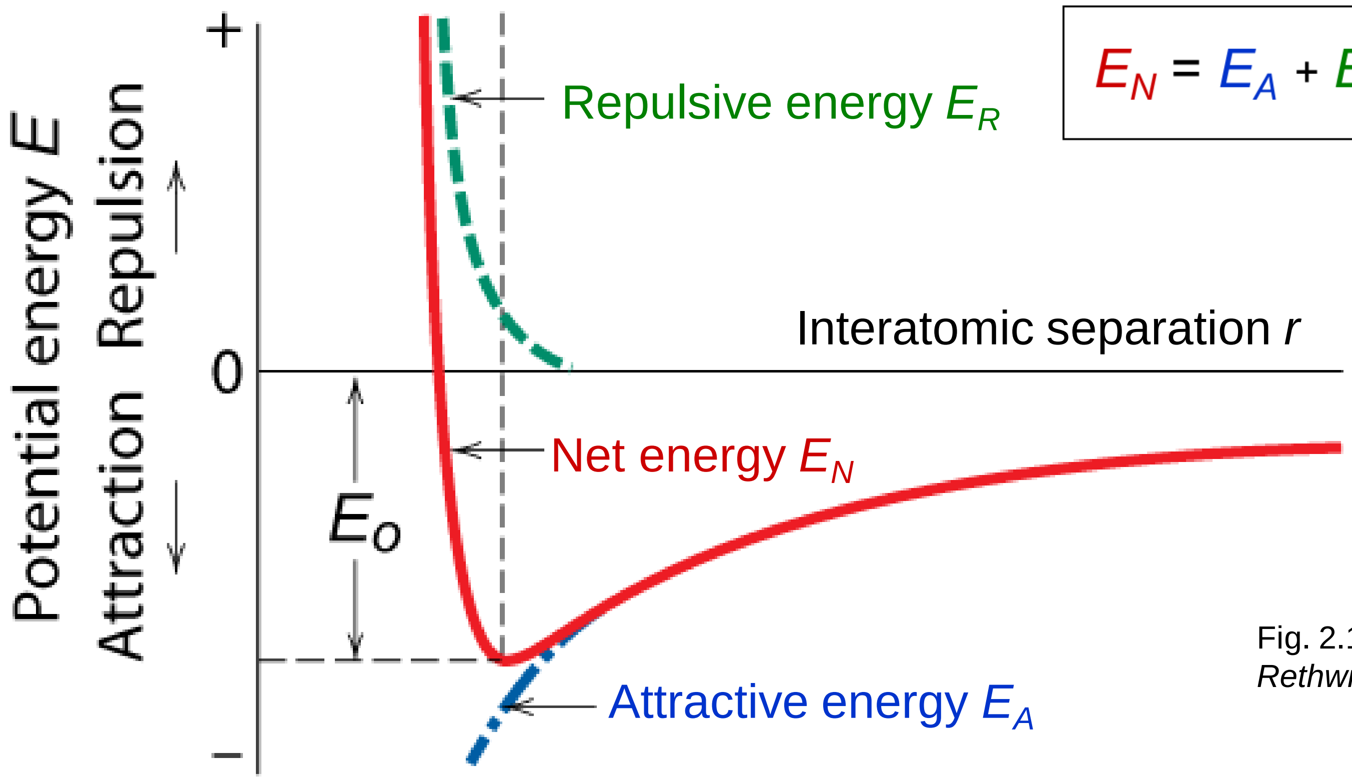


Fig. 2.10(b), *Callister & Rethwisch 10e.*

Ionic Bonding (cont.)

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$$

In this expressions, A, B, and n are constants whose values depend on the particular ionic system. The value of n is approximately 8, and the B is the fitting constant

A represents lattice energy

$$A = \frac{1}{4\pi\epsilon_0}(|Z_1 e|)(|Z_2 e|)$$

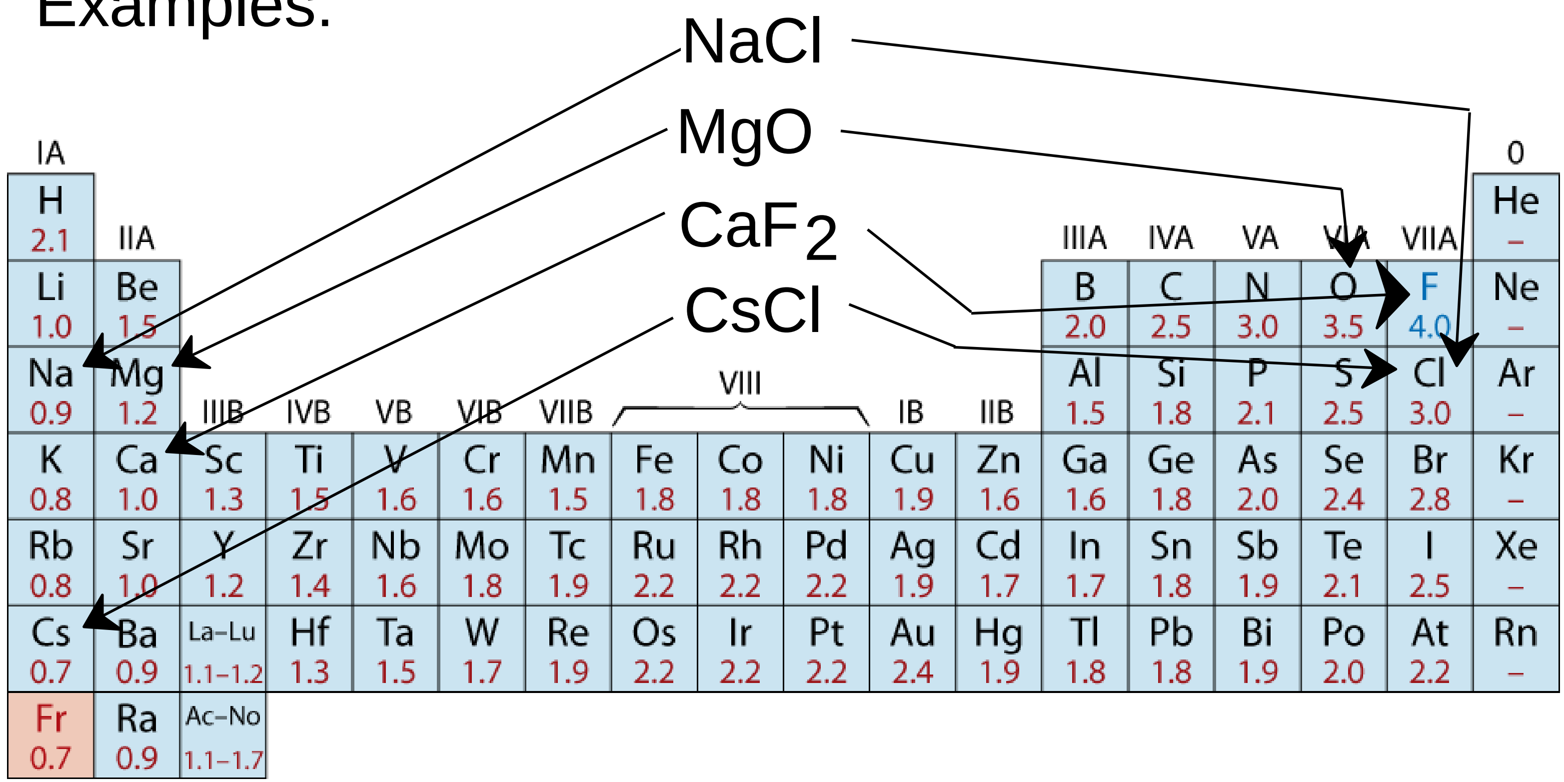
where ϵ_0 is the permittivity of a vacuum ($8.85 \times 10^{-12}\ F/m$), Z_1 and Z_2 are the valences of the two ion types, and e is the electronic charge ($1.602 \times 10^{-19}\ C$)

Mathematically, energy (E) and force (F) are related as $E = \int F\,\mathrm{d}r$

Ionic Bonding (cont.)

Predominant bonding in Ceramics

Examples:



Give up electrons

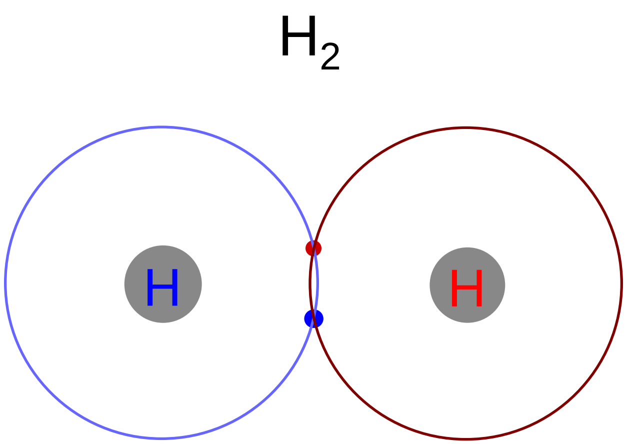
Acquire electrons

Covalent Bonding

- Similar electronegativities ∴ share electrons
- Bonds involve valence electrons – normally *s* and *p* orbitals are involved
- Example: H_2

Each H: has 1 valence e^-,
needs 1 more

Electronegativities
are the same.



• shared 1*s* electron from 1st hydrogen atom

• shared 1*s* electron from 2nd hydrogen atom

Fig. 2.12, *Calliser & Rethwisch 10e.*

Mixed Bonding

- Most common mixed bonding type is Covalent-Ionic mixed bonding

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\ \%)$$

where X_A & X_B are electronegativities of the two elements participating in the bond

Ex: MgO

$X_{Mg} = 1.2$
$X_O = 3.5$

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(3.5-1.2)^2}{4}}\right) \times (100\%) = 73.3\%$$

Metallic Bonding

- Electrons delocalized to form an "electron cloud"

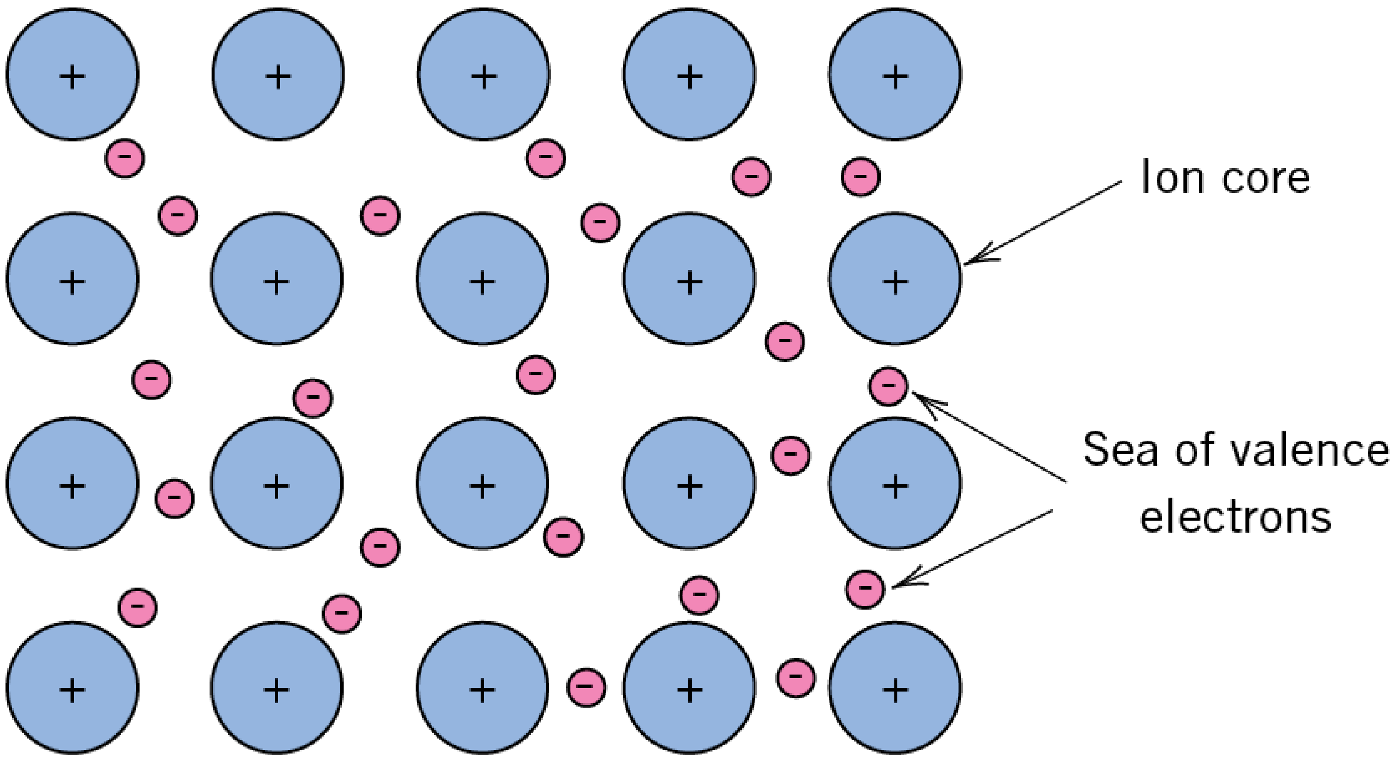
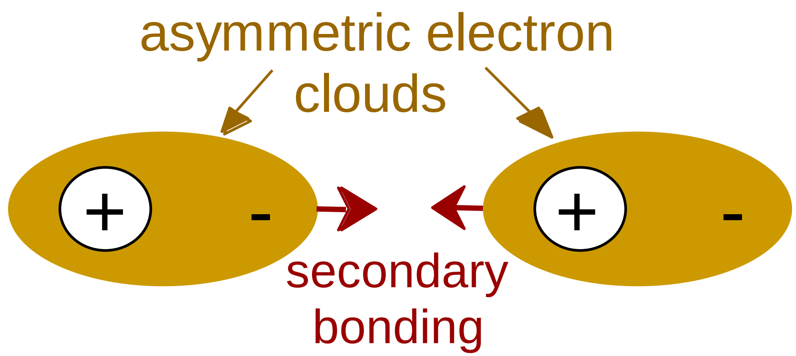


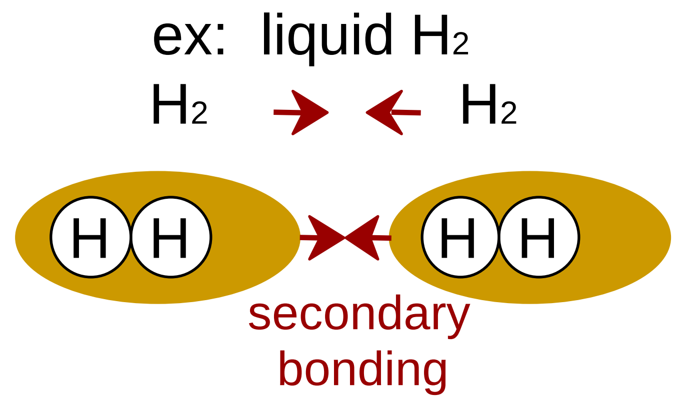
Fig. 2.19*b*, *Callister & Rethwisch 10e.*

Secondary Bonding

Arises from attractive forces between dipoles

- Fluctuating dipoles



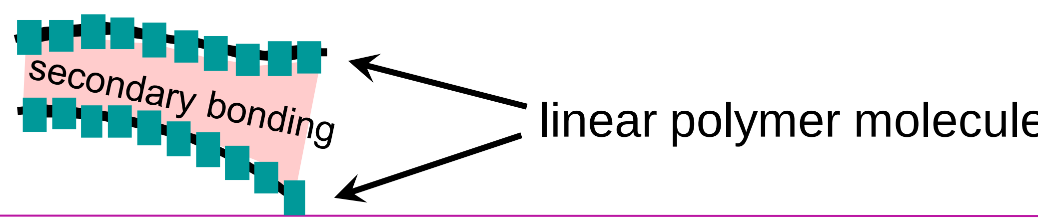


- Permanent dipoles

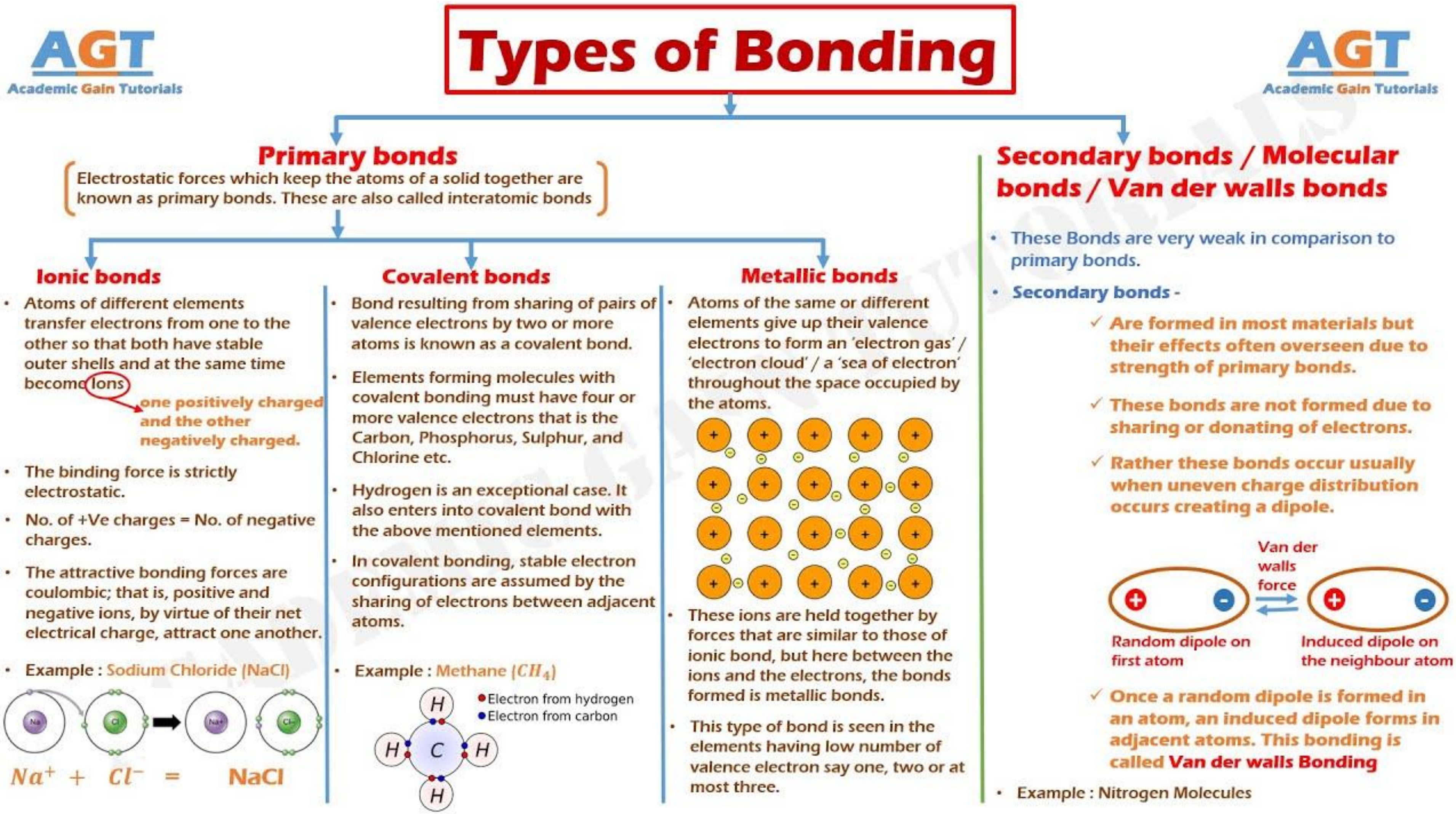
-general case:

-ex: liquid HCl

-ex: polymer



Secondary Bonding



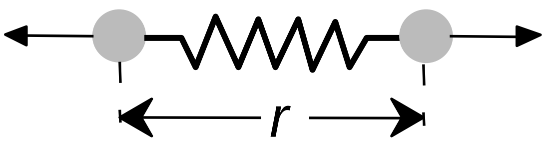
https://www.youtube.com/watch?v=eVdL-ipUa1Y

Atomic Structure (cont.)

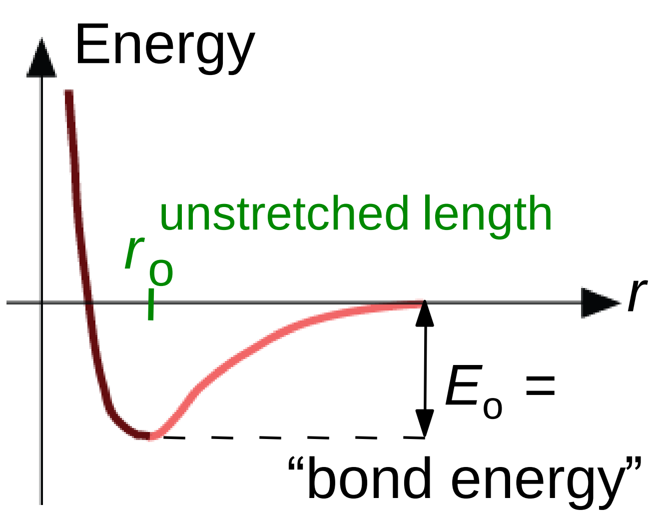
- Some of the following properties are determined by an atom's electronic structure:
  1) Chemical
  2) Electrical
  3) Thermal
  4) Optical

Properties Related to Bonding I: Melting Temperature (T_m)

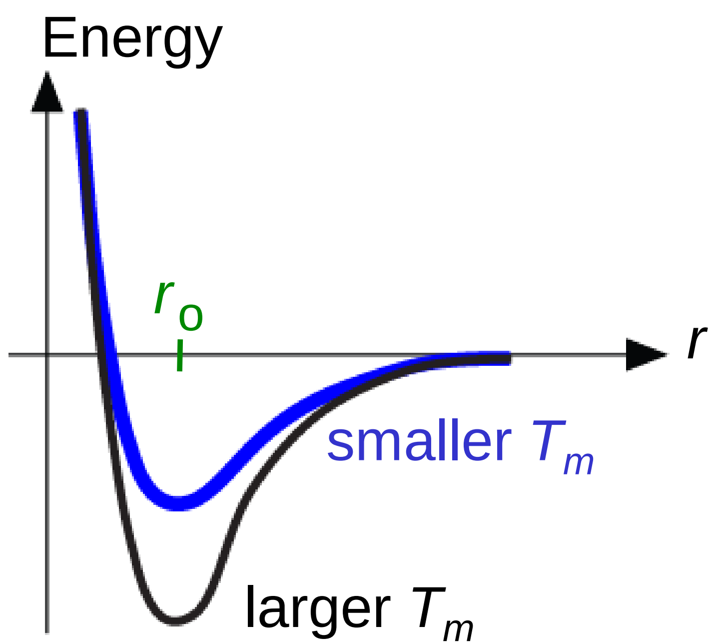
- Bond length, r



- Bond energy, E_o



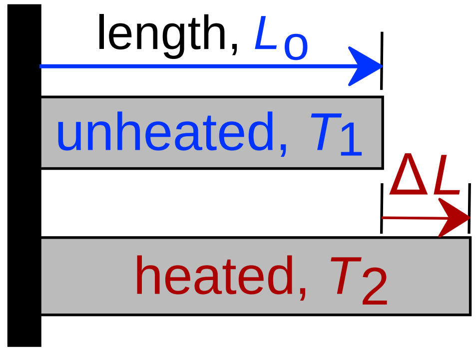
- Melting Temperature, T_m



The larger E_o, the higher T_m

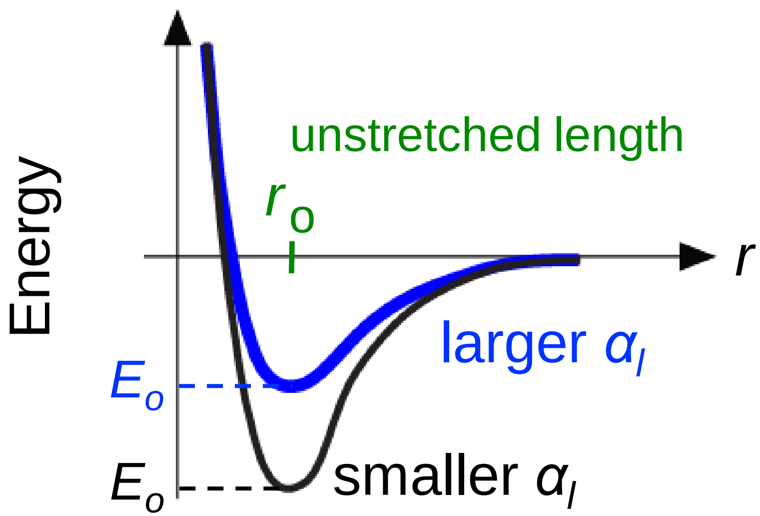
Properties Related to Bonding II: Coefficient of Thermal Expansion (α_l)

- Coefficient of thermal expansion, α_l



$$\frac{\Delta L}{L_o} = \alpha_l (T_2 - T_1)$$

The smaller E_o, the larger α_l.



- Increase in bond length is due to asymmetry of the E vs. r curve. This results in an increase in α_l.
- As E_0 increases this asymmetry decreases.

Summary: Properties Related to Bonding Type and Bonding Energy

Ceramics

(Ionic & covalent bonding):

Large bond energy

- high T_m
- large E
- small α_l

Metals

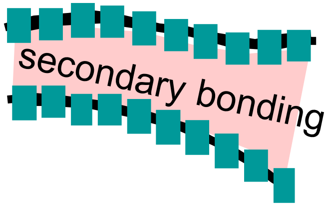
(Metallic bonding):

Variable bond energy

- moderate T_m
- moderate E
- moderate α_l

Polymers

(Covalent & Secondary):



Weak bond energy (between chains)

Secondary bonding responsible for most physical properties

- low T_m
- small E
- large α_l

Summary

- **Valence electrons** occupy the outermost unfilled electron shell.
- **Primary bonding types** include covalent, ionic, and metallic bonding.
- The percent ionic character of a covalent-ionic mixed bond between two elements depends on their **electronegativities**.
- Secondary or **van der Waals bonds** are weaker than the primary bonding types.
- A material's chemical, electrical, thermal, and optical properties are determined by **electronic configuration**.

Announcements

Reading: Textbook Ch. 1-2

Assignment: Open today; DL: 18:00 Sunday

Problem for next Lecture:

How to best stack oranges?

https://plus.maths.org/content/sites/plus.maths.org/files/abstractpics/%5Buid%5D/%5Bsite-date%5D/oranges_icon.jpg

Questions?