



Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

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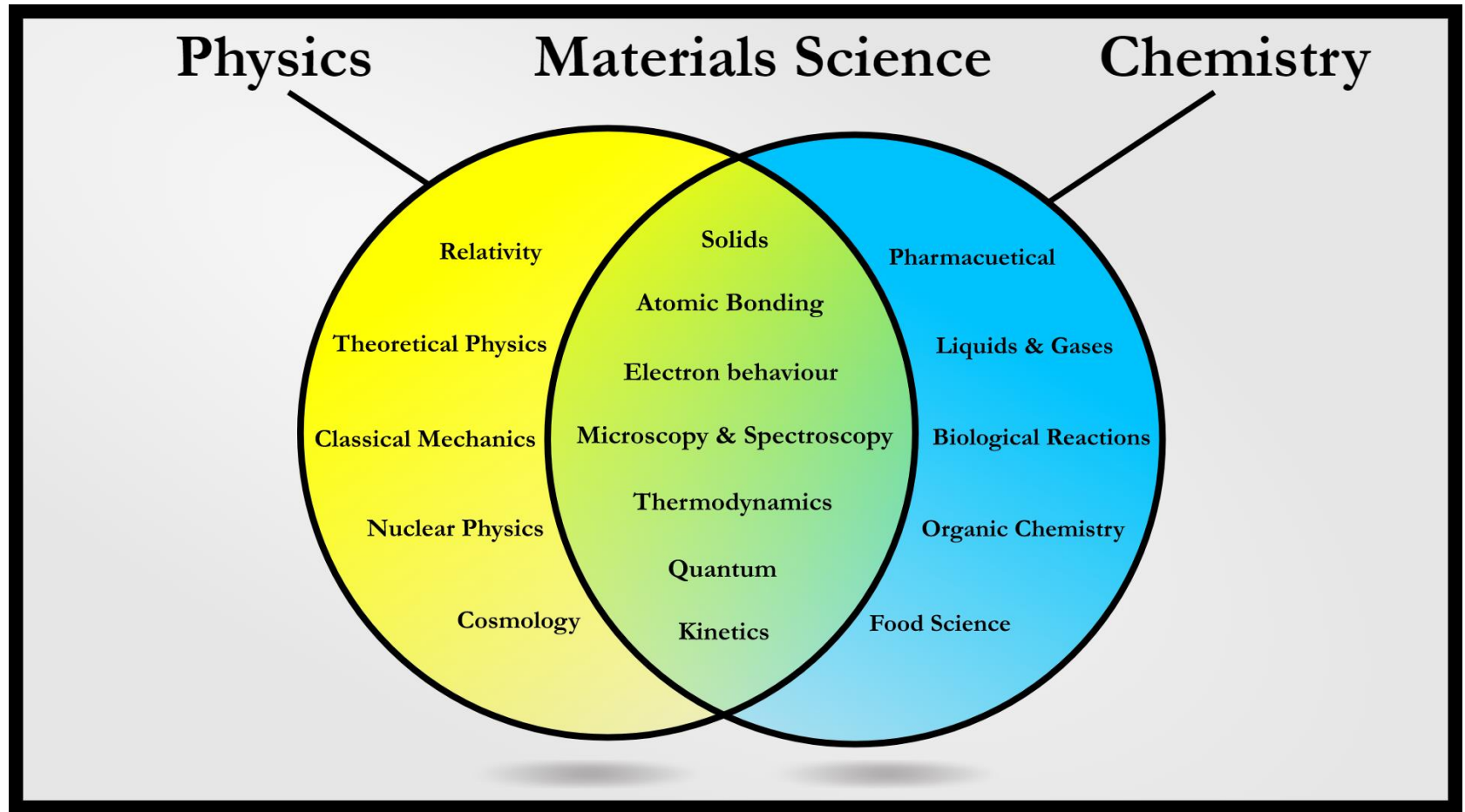
Chapter 1: Introduction to Materials Science & Engineering

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.

What is Materials Science & Engineering?

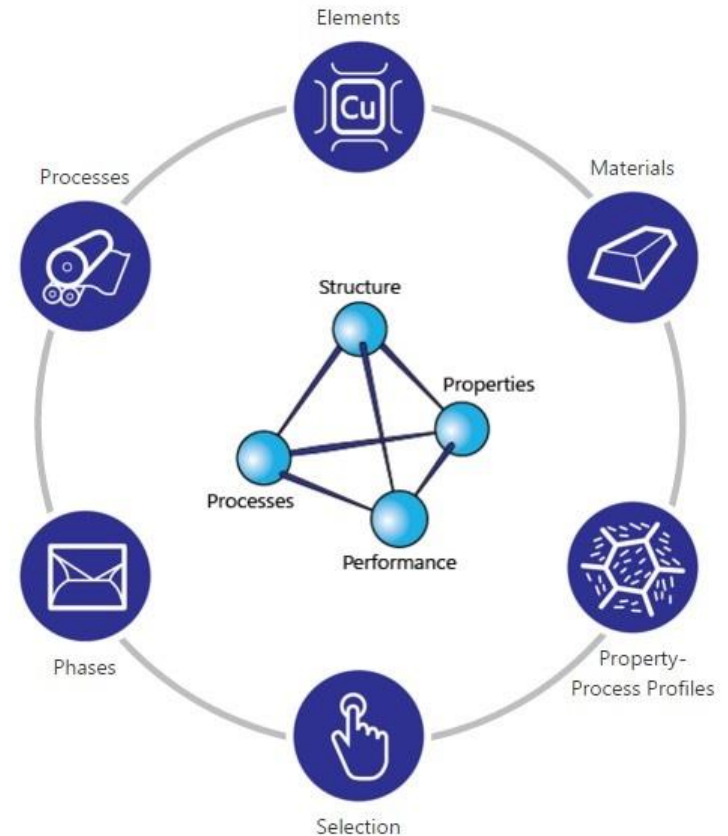
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<https://msestudent.com/13-reasons-why-you-should-study-materials-science-and-engineering/>

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

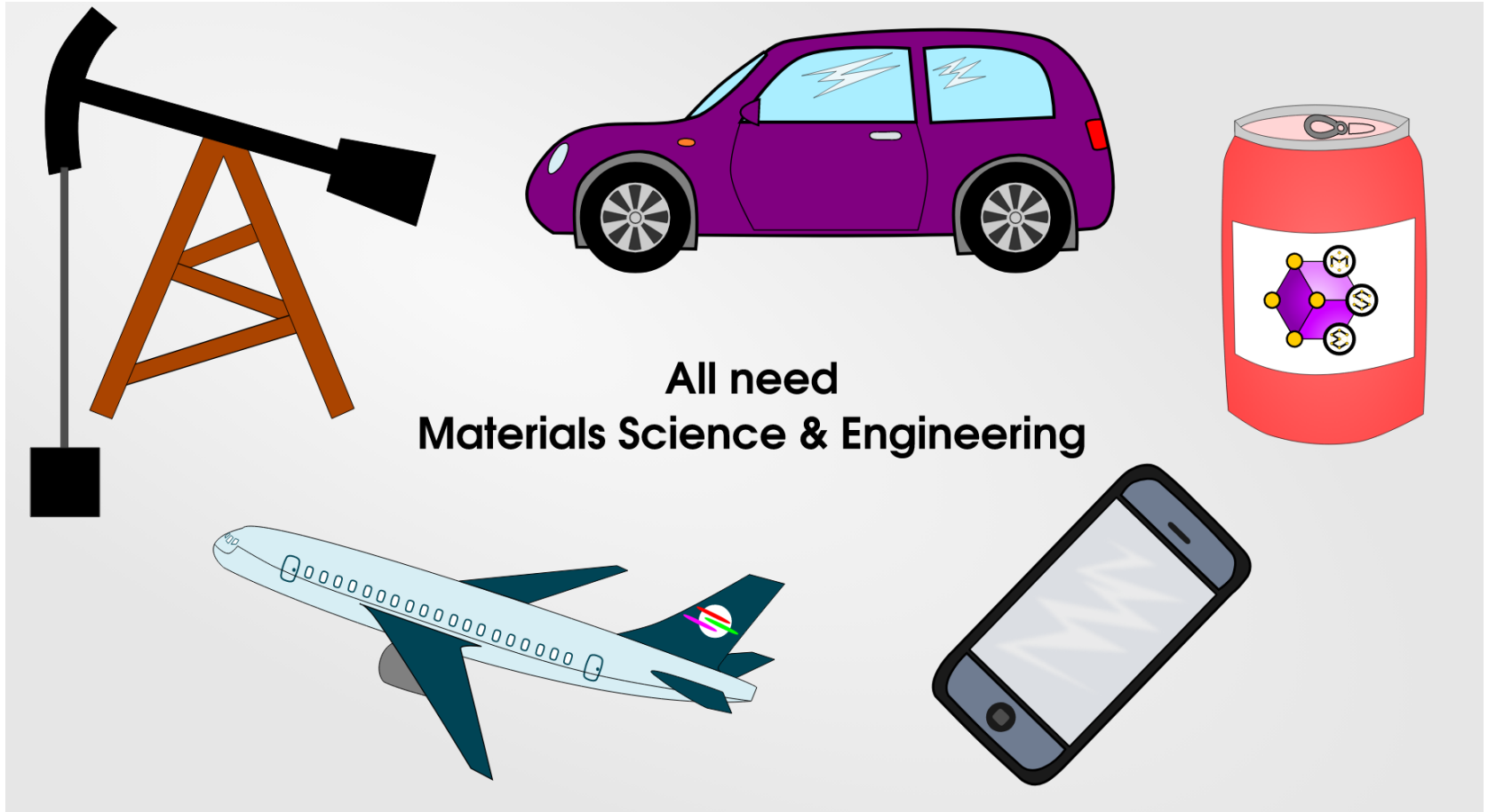


<http://www.stemclopedia.com/Matsci.html>

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?



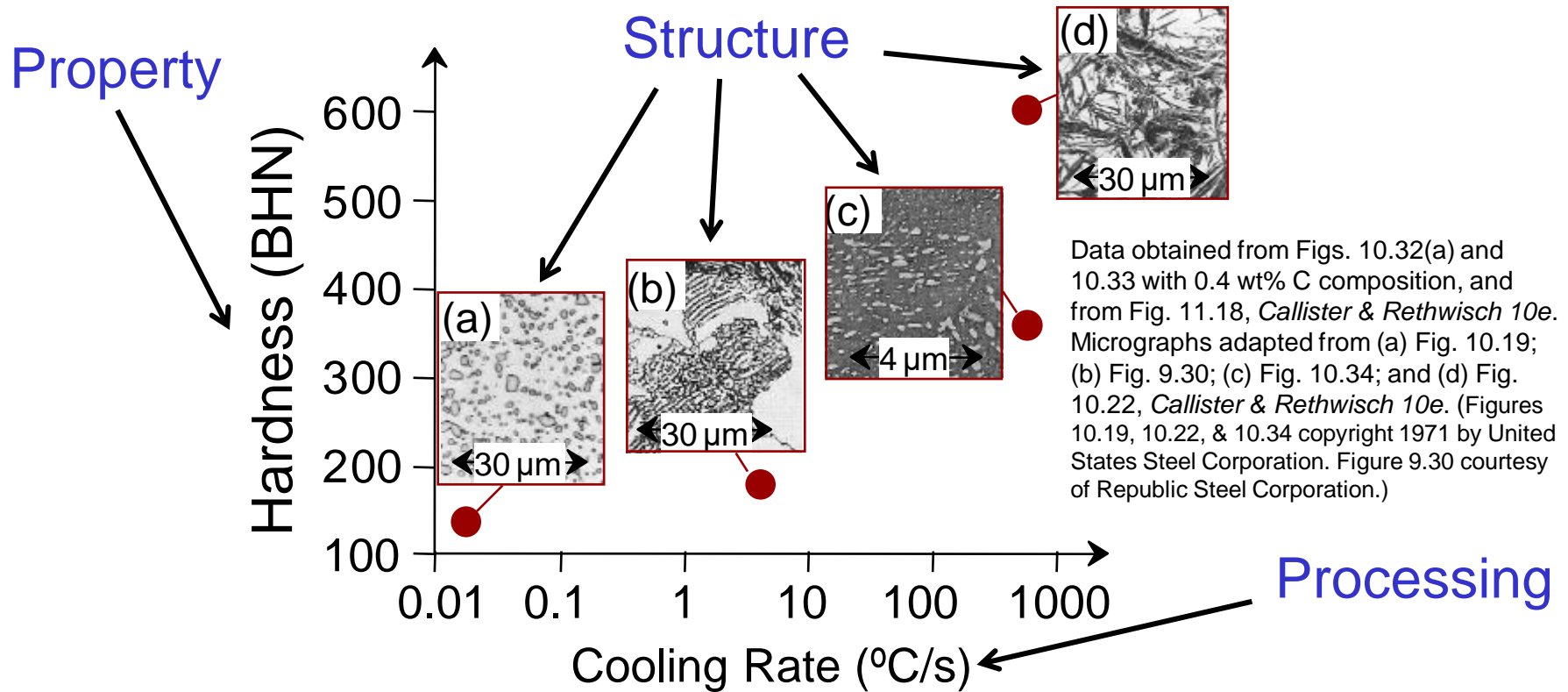
<https://msestudent.com/13-reasons-why-you-should-study-materials-science-and-engineering/>

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**



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:

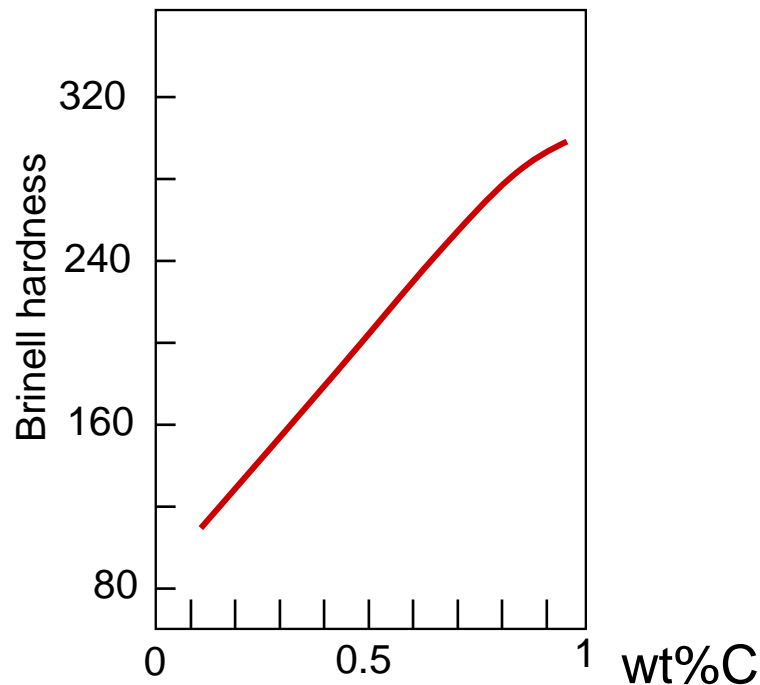


Fig. 10.31, *Callister & Rethwisch 10e*.
[Data taken from *Metals Handbook: Heat Treating*, Vol. 4, 9th edition, V. Masseria (Managing Editor), 1981. Reproduced by permission of ASM International, Materials Park, OH.]

- Increasing carbon content increases hardness of steel.

Electrical Properties

Factors that affect **electrical resistivity** – for copper:

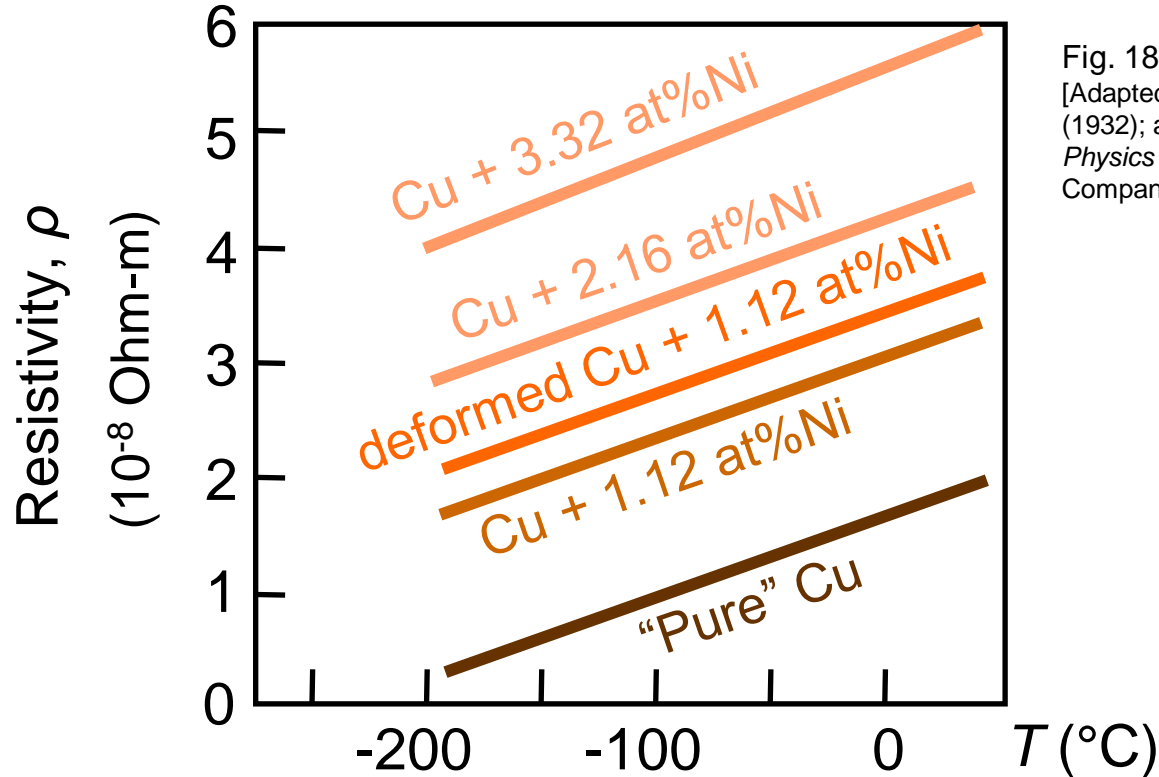


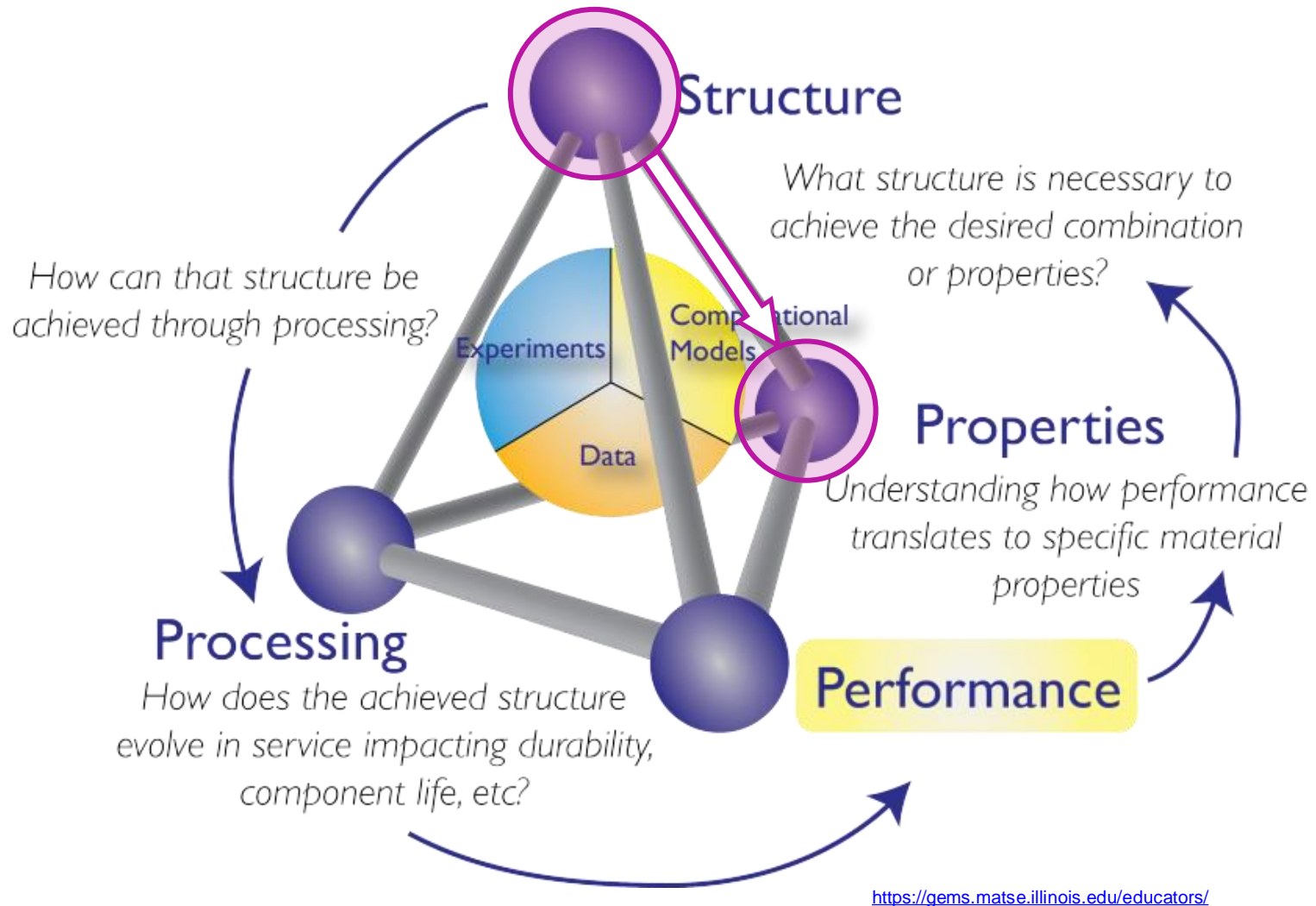
Fig. 18.8, *Callister & Rethwisch 9e*.
[Adapted from: J.O. Linde, *Ann Physik* **5**, 219 (1932); and C.A. Wert and R.M. Thomson, *Physics of Solids*, 2nd edition, McGraw-Hill Company, New York, 1970.]

- 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



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

$$1 \text{ amu/atom} = 1 \text{ g/mol}$$

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

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 #

n = principal (shell)

ℓ = azimuthal (subshell)

m_ℓ = magnetic (no. of orbitals)

m_s = spin

- Designation/Values

K, L, M, N, O (1, 2, 3, 4, etc.)

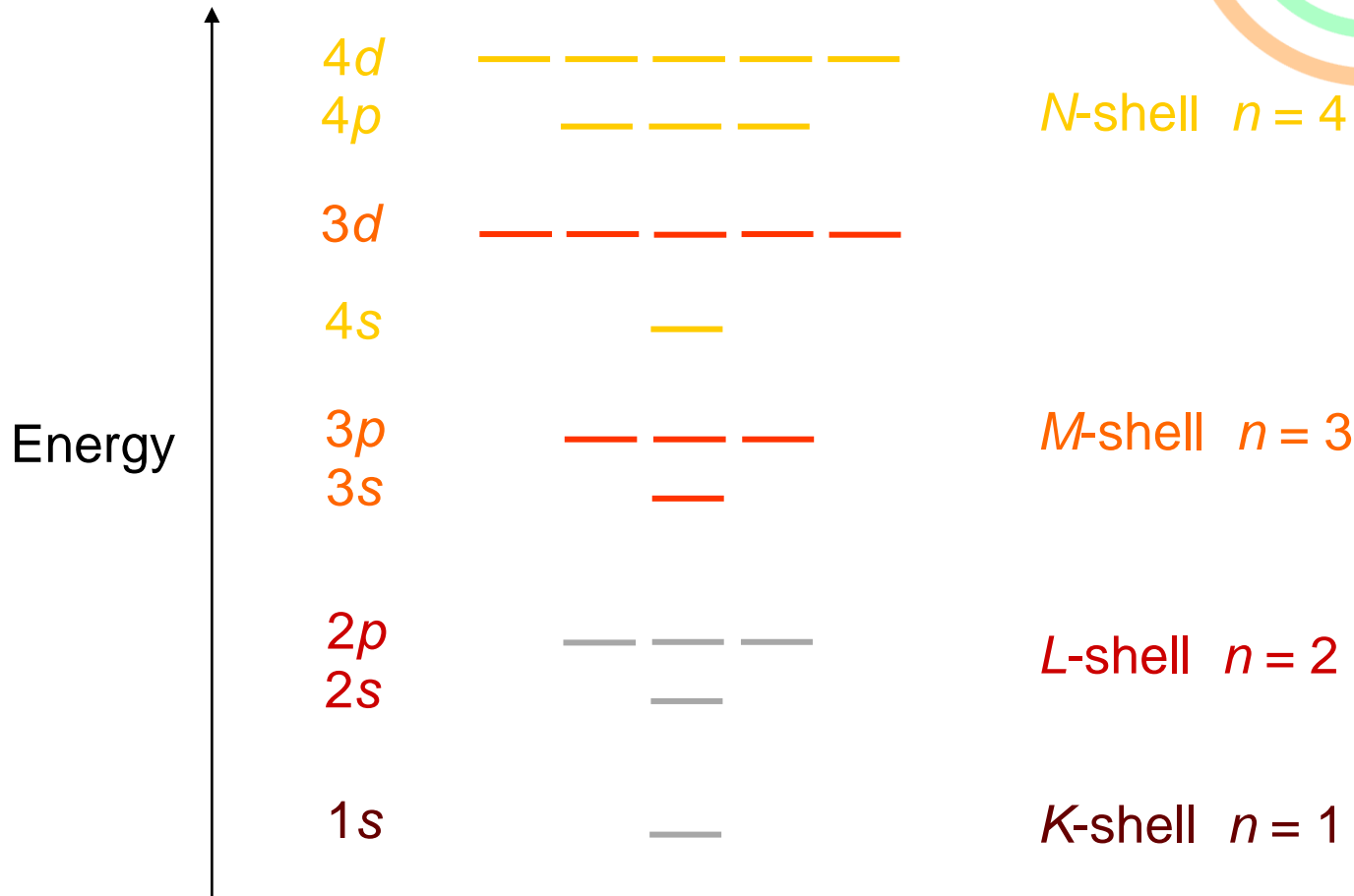
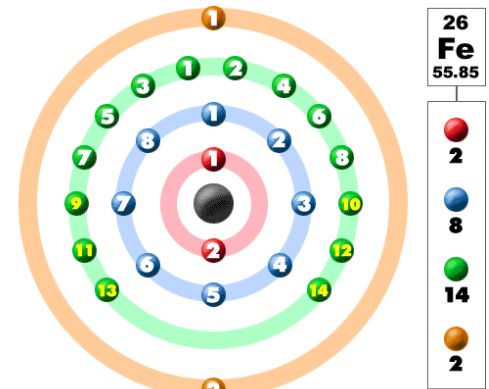
s, p, d, f (0, 1, 2, 3, ..., $n-1$)

1, 3, 5, 7 ($-\ell$ to $+\ell$)

$\frac{1}{2}, -\frac{1}{2}$

Electron Energy States

- have discrete **energy values**
- tend to occupy lowest available energy state



Survey of Elements

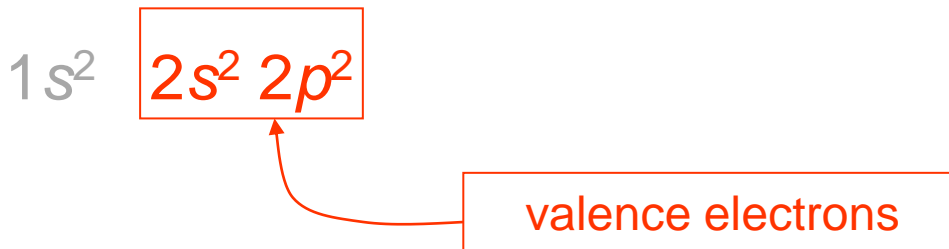
- Most elements: Electron configurations **not stable**.

<u>Element</u>	<u>Atomic #</u>	<u>Electron configuration</u>
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)



The Periodic Table

- Elements in each column: Similar **valence** electron structure

give up 1e⁻

give up 2e⁻

give up 3e⁻

accept 2e⁻

accept 1e⁻

inert gases

0 2

He

Ne

Ar

Kr

Xe

Rn

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

IA IIA IIIA IVA VA VIA VIIA VIII IB IIB

1 H 2 He

3 Li 4 Be 5 B 6 C 7 N 8 O 9 F 10 Ne

11 Na 12 Mg 13 Al 14 Si 15 P 16 S 17 Cl 18 Ar

19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr

37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe

55 Cs 56 Ba 57 La 58 Ce 59 Pr 60 Nd 61 Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy 67 Ho 68 Er 69 Tm 70 Yb 71 Lu 72 Hf 73 Ta 74 W 75 Re 76 Os 77 Ir 78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn

87 Fr 88 Ra 89 Ac 90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es 100 Fm 101 Md 102 No 103 Lr 104 Rf 105 Db 106 Sg 107 Bh 108 Hs 109 Mt 110 Ds

Rare earth series

Actinide series

Metal

Nonmetal

Intermediate

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																	0
H																	He
2.1																	–
IIA												IIIA	IVA	VA	VIA	VIIA	
Li	Be											B	C	N	O	F	Ne
1.0	1.5											2.0	2.5	3.0	3.5	4.0	–
Na	Mg											Al	Si	P	S	Cl	Ar
0.9	1.2											1.5	1.8	2.1	2.5	3.0	–
		IIIB	IVB	VB	VIB	VIIIB	VIII			IB	IIB						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8	–
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5	–
Cs	Ba	La–Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.7	0.9	1.1–1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	–
Fr	Ra	Ac–No															
0.7	0.9	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] $3s^2$

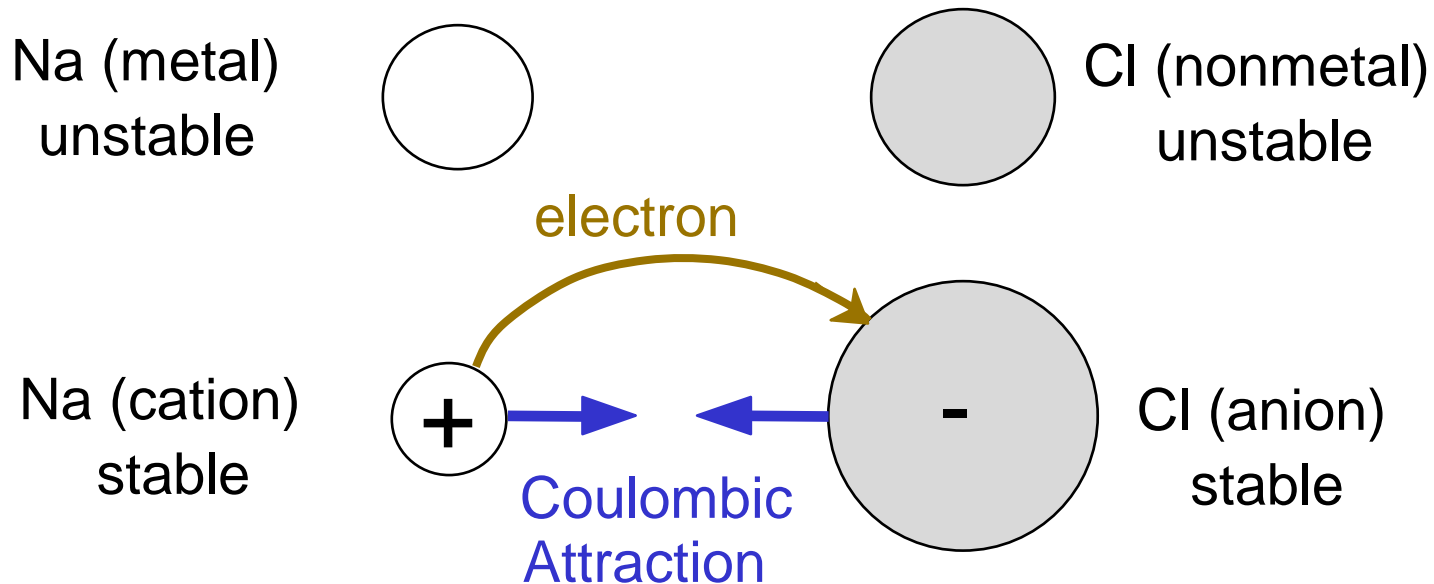
O $1s^2 2s^2 2p^4$

Mg²⁺ $1s^2 2s^2 2p^6$
[Ne]

O²⁻ $1s^2 2s^2 2p^6$
[Ne]

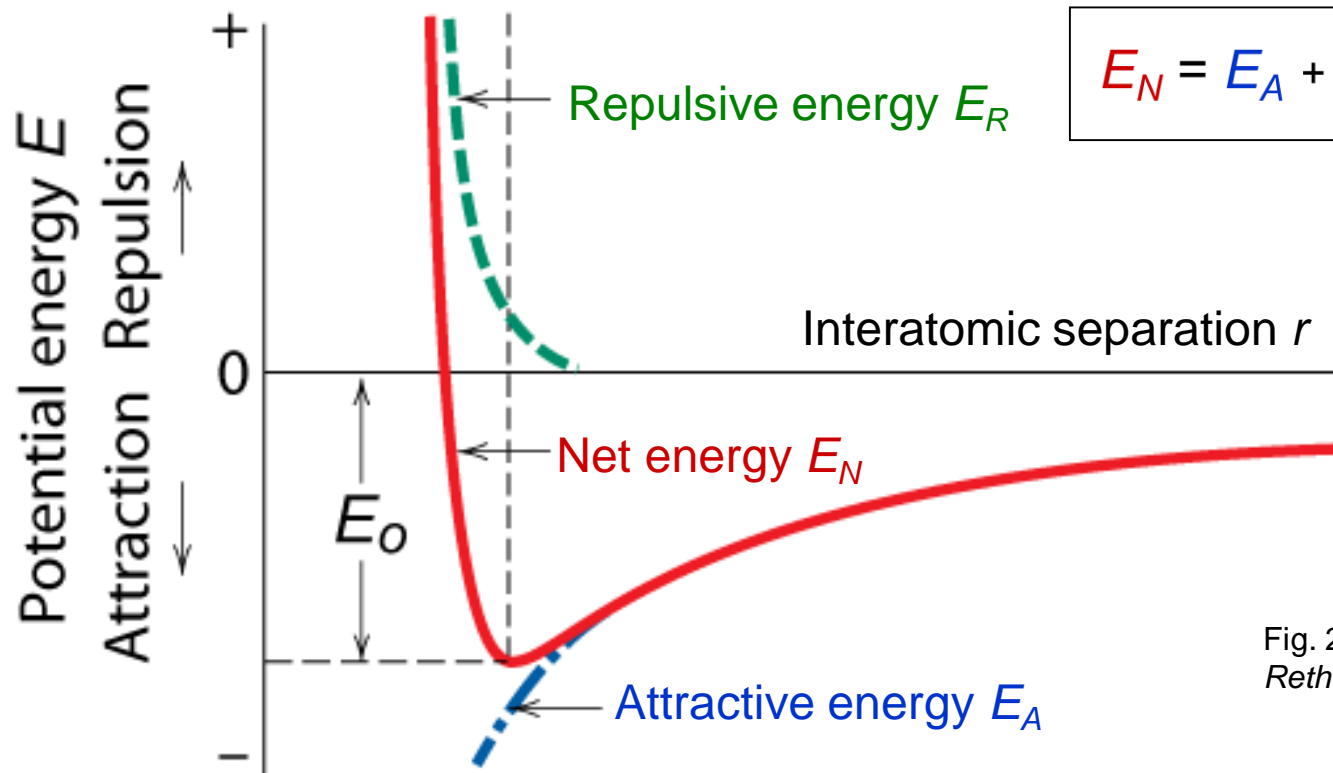
Ionic Bonding

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

Mathematically, energy (E) and force (F) are related as $E = \int F \, dr$

Ionic Bonding (cont.)

Predominant bonding in **Ceramics**

Examples:

NaCl

MgO

CaF₂

CsCl

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

← Give up electrons

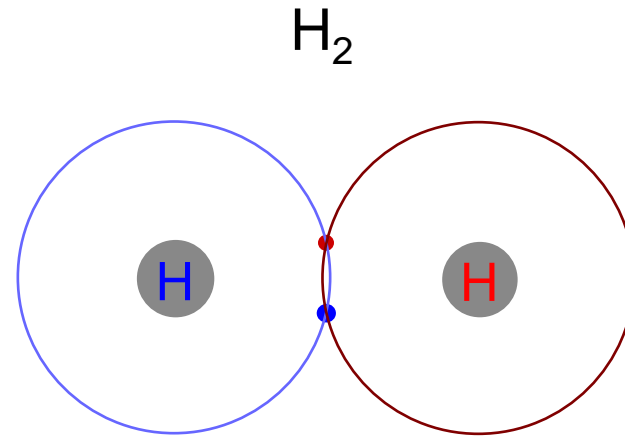
→ Acquire electrons

Covalent Bonding

- Similar electronegativities \therefore 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 1s electron
from 1st hydrogen
atom

• shared 1s 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

$$\begin{aligned} X_{\text{Mg}} &= 1.2 \\ X_{\text{O}} &= 3.5 \end{aligned}$$

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

Metallic Bonding

- Electrons delocalized to form an “electron cloud”

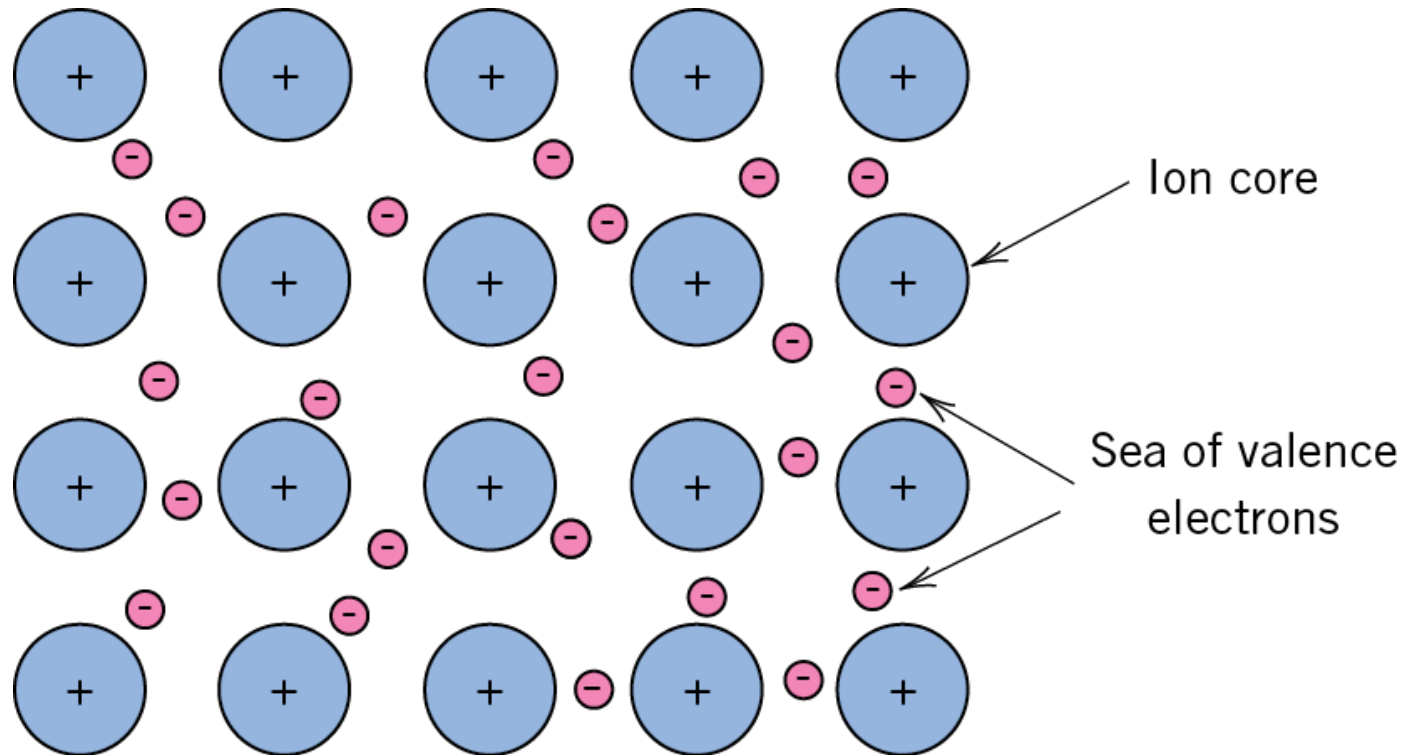
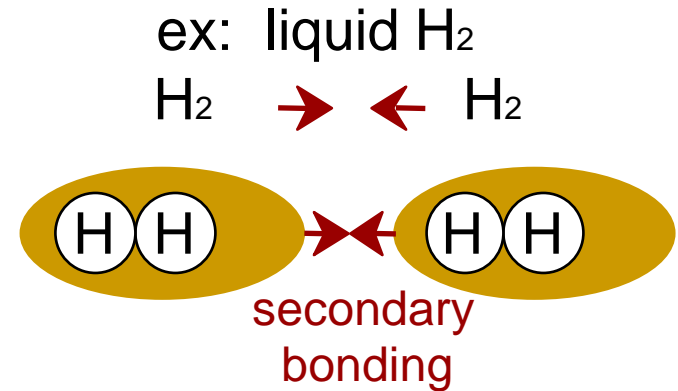
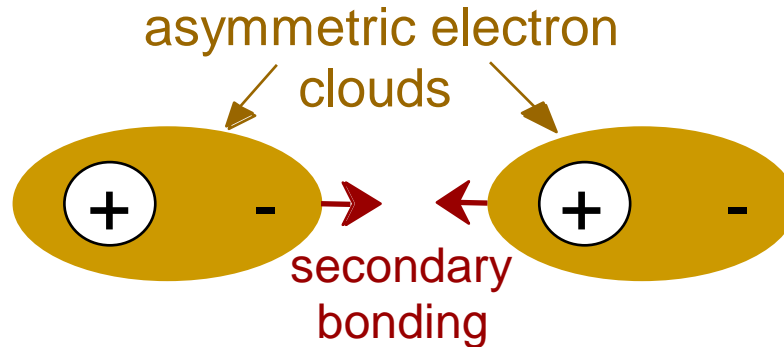


Fig. 2.19b, Callister & Rethwisch 10e.

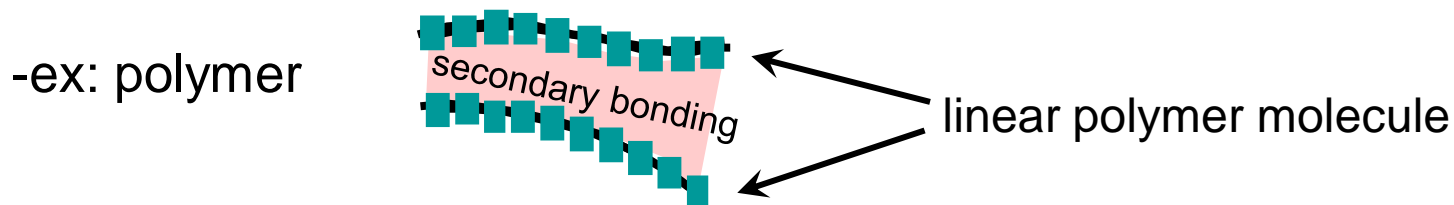
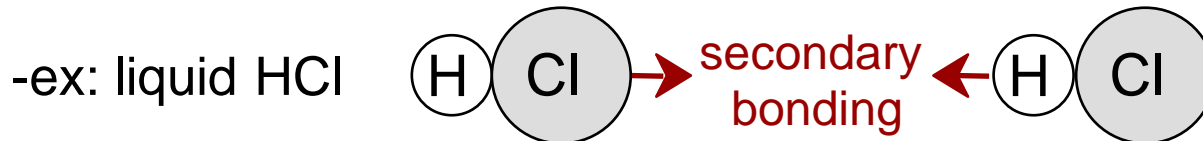
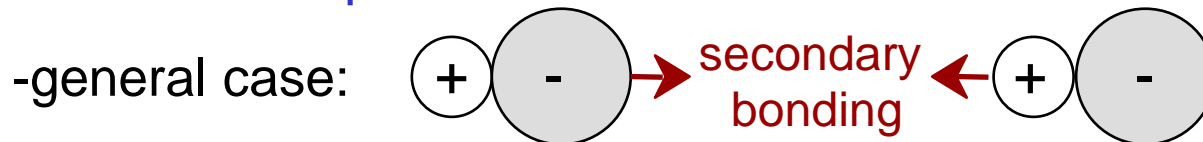
Secondary Bonding

Arises from attractive forces between **dipoles**

- Fluctuating **dipoles**



- Permanent **dipoles**



Secondary Bonding

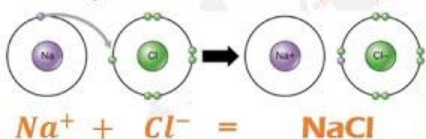
Types of Bonding

Primary bonds

Electrostatic forces which keep the atoms of a solid together are known as primary bonds. These are also called interatomic bonds

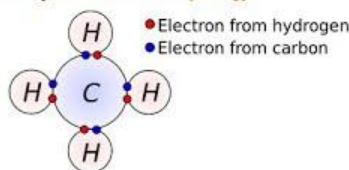
Ionic bonds

- Atoms of different elements transfer electrons from one to the other so that both have stable outer shells and at the same time become **ions**.
one positively charged and the other negatively charged.
- The binding force is strictly electrostatic.
- No. of +Ve charges = No. of negative charges.
- The attractive bonding forces are coulombic; that is, positive and negative ions, by virtue of their net electrical charge, attract one another.
- Example : Sodium Chloride (NaCl)



Covalent bonds

- Bond resulting from sharing of pairs of valence electrons by two or more atoms is known as a covalent bond.
- Elements forming molecules with covalent bonding must have four or more valence electrons that is the Carbon, Phosphorus, Sulphur, and Chlorine etc.
- Hydrogen is an exceptional case. It also enters into covalent bond with the above mentioned elements.
- In covalent bonding, stable electron configurations are assumed by the sharing of electrons between adjacent atoms.
- Example : Methane (CH_4)

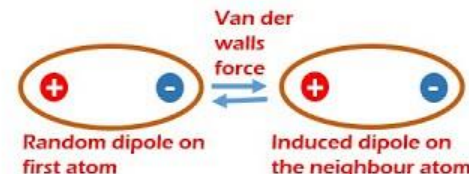


Metallic bonds

- Atoms of the same or different elements give up their valence electrons to form an 'electron gas' / 'electron cloud' / a 'sea of electron' throughout the space occupied by the atoms.
-
- These ions are held together by forces that are similar to those of ionic bond, but here between the ions and the electrons, the bonds formed is metallic bonds.
 - This type of bond is seen in the elements having low number of valence electron say one, two or at most three.

Secondary bonds / Molecular bonds / Van der Waals bonds

- These Bonds are very weak in comparison to primary bonds.
- Secondary bonds -
 - Are formed in most materials but their effects often overseen due to strength of primary bonds.
 - These bonds are not formed due to sharing or donating of electrons.
 - Rather these bonds occur usually when uneven charge distribution occurs creating a dipole.



- Once a random dipole is formed in an atom, an induced dipole forms in adjacent atoms. This bonding is called **Van der Waals Bonding**

- Example : Nitrogen Molecules

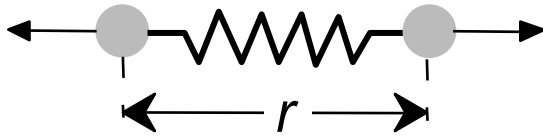
<https://www.youtube.com/watch?v=eVdL-ipUa1Y>

Atomic Structure (cont.)

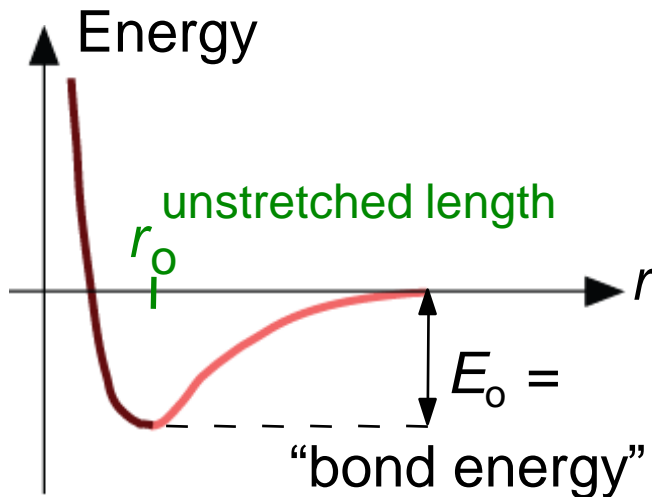
- ❑ Some of the following properties are determined by an atom's electronic structure:
 - 1) Chemical
 - 2) Electrical
 - 3) Thermal
 - 4) Optical

Properties Related to Bonding I: Melting Temperature (T_m)

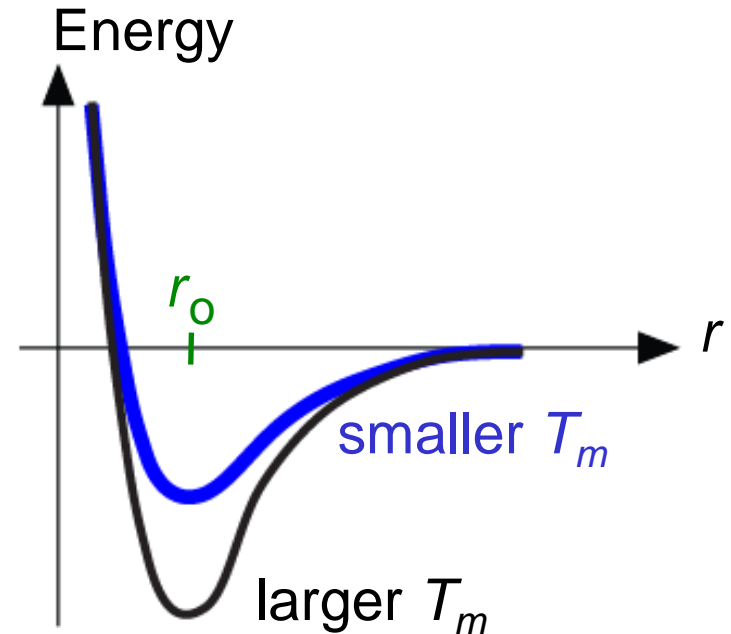
- Bond length, r



- Bond energy, E_0



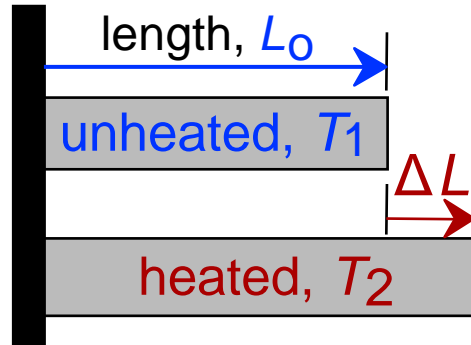
- Melting Temperature, T_m



The larger E_0 , the higher T_m

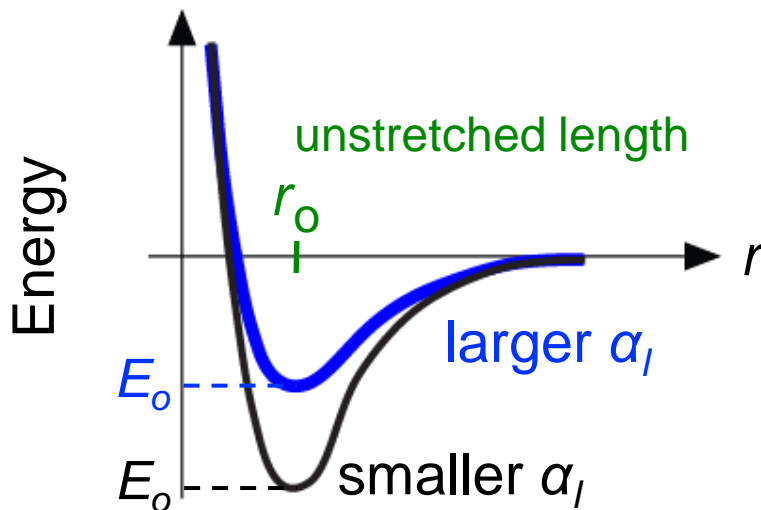
Properties Related to Bonding II: Coefficient of Thermal Expansion (α_l)

- Coefficient of thermal expansion, α_l



$$\frac{\Delta L}{L_0} = \alpha_l (T_2 - T_1)$$

The smaller E_0 , 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_f

Metals

(Metallic bonding):

Variable bond energy

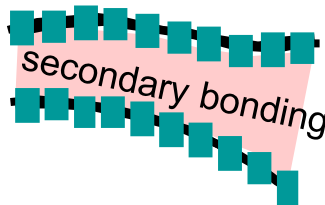
moderate T_m

moderate E

moderate α_f

Polymers

(Covalent & Secondary):



Weak bond energy (between chains)

Secondary bonding responsible for most physical properties

low T_m

small E

large α_f

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?