An Introduction to Engineering Materials

MAAE 2700

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Introduction and Atomic Structure

Section 1

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Outlines

- Course outline (handout)
  - Textbook
  - WebCT
  - Instructor
  - TAs
  - Course content and textbook chapters
  - Marking schemes
  - Labs and PAs
- Course objectives
- Material classification and examples
- Evolution of materials
- Inadequate use of materials and processes
- Environmental and resource issues
- Questions

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WebCT

- Slides
  - Majority of the slides will be posted, however
    - Additional sample questions discussed in class will not be posted
    - Information presented on blackboard will be not posted
    - Images or slides with no copyright permissions will not be posted
  - Take notes and work on questions in class
- Group assignment (PA and Lab)
  - 9 groups (WebCT) – change request before Sept. 14.
  - Calendar (WebCT)
- Lab manuals and templates
- Assignments
- Announcement
- Grade posting (WebCT)

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Laboratories

- Study lab manual before each lab (this is particularly important since part of the lab report will be prepared during lab session)
- Attend lab on time (late arrival beyond 25 min. will not be admitted and will be considered as missed lab)
- Complete lab report using the template (print it in advance and add pages to it as needed)
- Submit lab report on time to drop box by MAE office (due within 2 days from the lab session, excluding weekends, holidays and university day)
- Lab report for Lab 5 due at the end of lab session
- 5%/day deduction for late submission
- More details provided in lab manual and course outline
- Missed lab due to medical or family reason
  - Contact TA within 24 hours after a missed lab and provide official medical certification or other document.
  - A makeup lab may be scheduled if the same lab is still running.

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PA and Quiz

- Assignment and PA
  - complete majority of the questions in each assignment before PA session
  - attend PA session and complete the remaining questions with help from TA
  - TA will provide solutions to assignment at PA
  - solutions will not be posted
  - 1 mark for each completed assignment toward final grade
- Quiz
  - 5 quizzes
  - At the start of the last hour in PA
  - Solutions to quizzes will be provided at the following PA session but not posted
  - No deferred quiz
  - 0% for missed quiz, except for
    - medical reason(s)
    - family emergency
    - compassionate grounds

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Instructors and TAs

- For assignment and quiz related questions, always see your TA first. Discuss with instructor for any unresolved question or concern.
- To make appointment, email: xhuang@mae.carleton.ca (allow two or more working days before the scheduled appointment)
- TA contacts posted on webCT

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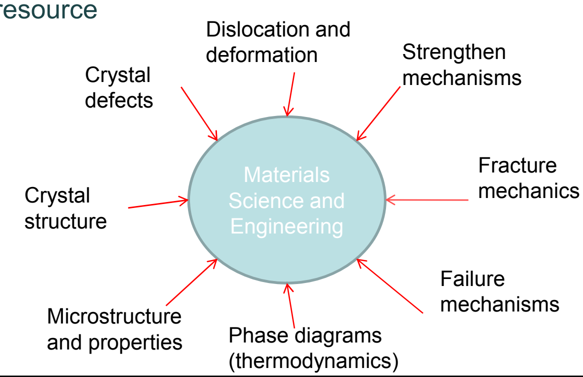
Course Objectives

- Understand the relationship between composition, process, structures and properties for common engineering materials
- Learn material's failure mechanisms and design against premature failure
- Select materials to make products with least life-cycle cost
- Recognize, new design opportunity, environment concerns and limited resource



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Classifications – Material Group

– Metals
– Ceramics and glasses
– Polymers
– Composites
– Semiconductor

– Examples

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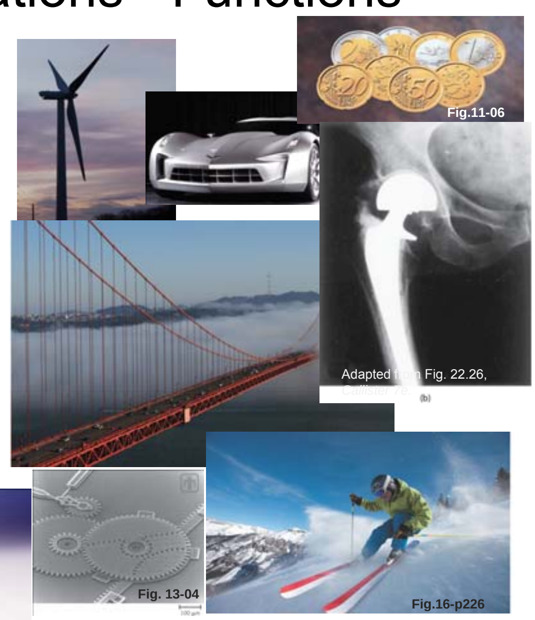
Classifications - Functions

- Functions
  - Aerospace
  - Automotive
  - Structural
  - Transportation
  - Bio-medical
  - Energy
  - Sports
  - Others



Material’s Selection

- Properties (do the job)
- Cost
- Availability
- Manufacturability
- Environmental concerns and recyclability

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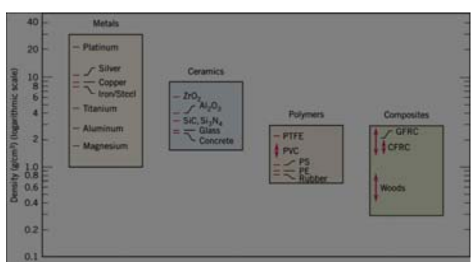
Properties

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

Canyon Bridge, Los Alamos, NM

Adapted from chapter-opening photograph, Chapter 17



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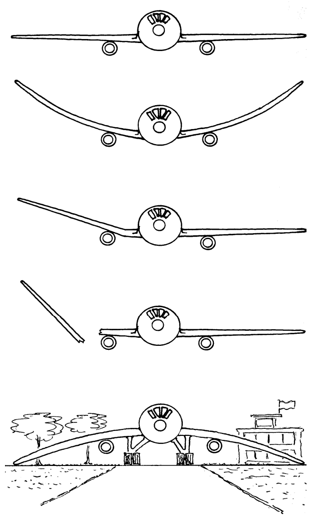
What will happen when a wrong material is chosen?



Stiff, strong, tough, light

Not stiff enough (need bigger stiffness E)

Not strong enough, plastic deformation (need bigger σ_y)

Not tough enough, fracture/failure (need bigger K_{ic})

Too heavy (need lower ρ)

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New Materials and Products

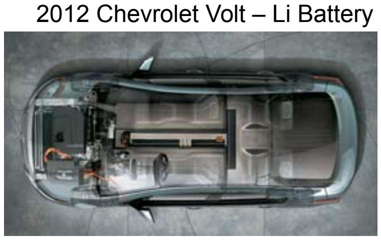
Michelin Tweel ™ Airless Tire

http://auto.howstuffworks.com/tweel-airless-tire.htm

Boeing 787 Dreamliner

http://boeing.mediaroom.com

2012 Chevrolet Volt – Li Battery



https://www.gm.ca/media/vehicles/current/chevrolet/volt/Volt_Brochure_EN.pdf

Composite Wind Turbine Blades

http://www.energy.siemens.com/hq/en/power-generation/renewables/wind-power/wind-turbines/?stc=wwecc120569

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Examples of Failures

Fast, brittle fracture

Rust

Fatigue Fracture – Cyclic loading from Waves

Challenger – O-ring failure (Tg)

Aloha Fuselage Failure

Atomic Structure and Bonding Types

Elements in Structure (4 levels)

- Atomic structure (s, p, d,…) - affecting bonding and certain properties
  - Examples: Elastic/Young's modulus (E), coefficient of thermal expansion (CTE) and melting temperature (Tm)
- Crystal structure (FCC, BCC, HCP, BCT) - affecting mechanical and physical properties
  - Examples: DBTT, elastic and plastic properties
- Microstructure (grain size, phases, defects) - affecting mechanical and physical properties
  - Examples: Hardness, strength, ductility, electrical/thermal conductivity
- Macrostructure (pores, cracks - what you see visually) - also affecting mechanical and physical properties
  - Examples: Fatigue strength, fracture toughness, strength, ductility

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Atomic Structure - Review

- Atomic structure determines atomic bonding → ultimately determines material's properties
- Atomic number Z
- Electron configuration ($1S^2 2S^2$…)
- Atomic weight/mass and atomic mass unit (amu = 1/12 of ^{12}C)
- Cl: Valence (-1) and valence electrons (7)

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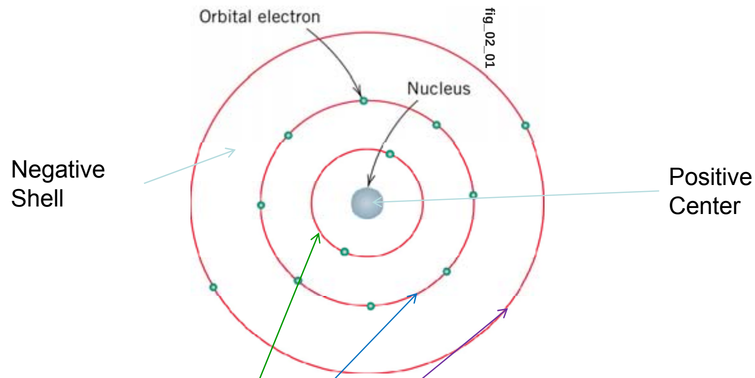
Bohr Atom - Review



Principal quantum number n and shell designation

n=1, K

n=2, L

n=3, M

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Definitions - Review

- Atomic number: number of protons in the nucleus (= number of electrons for neutral atom)
- Atomic mass unit: 1 amu = 1/12 of the atomic mass of ^{12}C (most common isotope)
  - 1 amu/atom = 1 g/mol (6.023×10^{23} atoms)
  - Fe: 55.85 amu/atom or 55.85 g/mol
- Atomic weight = atomic mass (by convention) (needed to convert at. % to wt. % and vice versa)
- Mole: in one mole of a substance there are 6.023×10^{23} atoms (Cu) or molecules (NaCl)

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Electrons and Electron Configuration - Review

- Every electrons in an atom is characterized by four quantum numbers:
  - Principal quantum number
    - n = 1,2,3,4,5 (K, L, M, N, O) - shell designation
    - Number of electrons per shell: 2, 8, 18, 32
  - Secondary quantum number
    - l = s, p, d, f - subshell
    - Number of electrons per subshell: 2, 6, 10, 14
  - 3^{rd} quantum number m_l (number of energy states when magnetic field is applied, 1, 3, 5 and 7)
  - 4^{th} quantum number m_s (spin moment, +1/2, -1/2)

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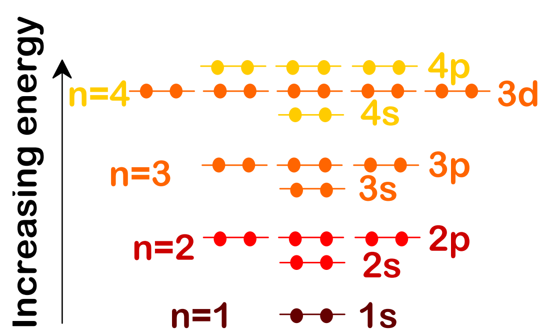
Electron Energy States - Review



4s before 3d

But

$3d^5 4s^1$

$3d^{10} 4s^1$

Write electron configurations:
Ar (Z=18)
Si (Z=14)
Cu (Z=29)
Zn (Z=30)
Fe (Z=26)
Cr (Z=24)

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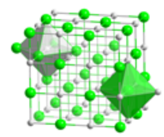
Valence and Valence Electrons - Review

- Valance electrons (N'): electrons occupy the outer most filled shell.
- Importance: participate in the bonding between atoms, affecting physical, thermal and chemical properties of solids.

Valence/valence number = number of electrons to be added (+) or removed (-) to form an inert gas electron configuration

Ar (Z=18) $1S^2 2S^2 2p^6 3S^2 3P^6$ – Valence electron 8
Si (Z=14) $1S^2 2S^2 2p^6 3S^2 3P^2$ – Valence electron=4, valence = 4
Cu (Z=29) $1S^2 2S^2 2p^6 3S^2 3P^6 3d^{10} 4S^1$
Zn (Z=30) $1S^2 2S^2 2p^6 3S^2 3P^6 3d^{10} 4S^2$
Fe (Z=26) $1S^2 2S^2 2p^6 3S^2 3P^6 3d^6 4S^2$
Cr (Z=24) $1S^2 2S^2 2p^6 3S^2 3P^6 3d^5 4S^1$

Wustite (FeO)
Hematite (Fe_2O_3)
Magnetite (Fe_3O_4)



Determine valences:
Si (Z=14)
Zn (Z=30)
Fe (Z=26)
Cr (Z= 24)

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Periodic Table - Review

- Row, column, atomic mass/weight, atomic number, symbols for common elements.
- Electronegativity
  - Describes the tendency of an atom to gain electrons
  - Related the position of an atom in the periodic table
  - Helps to determine the % of ionic bonding in molecules with mixed bonding type (ionic + covalent)

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Periodic Table - Review

Transition metals: partially filled **d** electron states and one or two electron in the next higher energy shell

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 2.1																	2 He –
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne –
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar –
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr –
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe –
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn –
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

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

Electronegative elements: Readily acquire electrons to become - ions.

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Primary Bonds

- All atoms have the tendency to form stable or inert gas electron configurations.
- This can be achieved by: gaining, losing, or sharing electrons.
- Primary bonding type:
  - Ionic bonding
  - Covalent bonding
  - Metallic bonding

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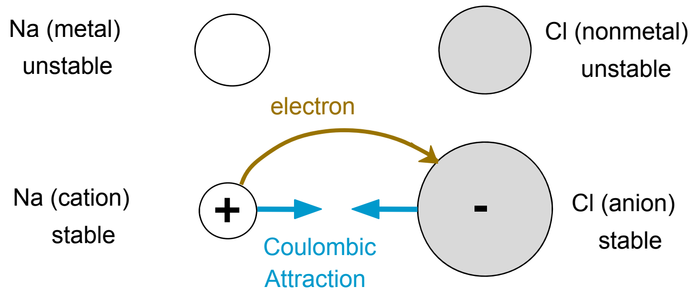
Ionic Bonding
(between metal and nonmetal)



Requires electron transfer

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Ionic Bonding

Ionic bond – metal + nonmetal

metal → donates electrons

nonmetal → accepts electrons

Dissimilar electronegativities

ex: MgO   Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$ O $1s^2\ 2s^2\ 2p^4$

[Ne] $3s^2$

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

[Ne]   [Ne]

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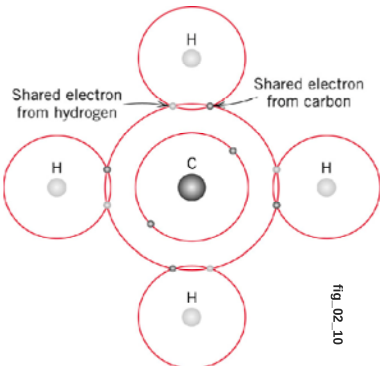
Covalent Bonding

(Molecules with nonmetals or metal+nonmetal or metal)

Methane (70% natural gas)



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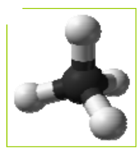
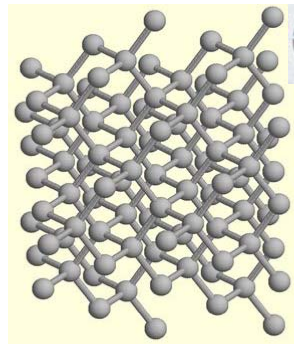
4 covalent bonds for C

1 covalent bond for H





Covalent bonding in diamond

C-C

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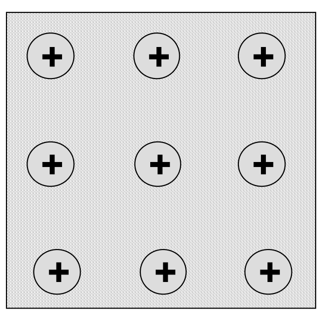
Metallic Bonding

(primary bond for metals and their alloys)

(For elements with valence electron number N'=1, 2, 3)



- Arises from a sea of donated valence electrons (1, 2, or 3 from each atom).
- The electrons are shared among all – non specific or non-directional

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Mixed Bonding

- Ionic-covalent mixed bonding

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

where X_A & X_B are electronegativities of elements A and B
(For two elements with different electronegativities, there will be some % of ionic bond between them)

Ex: MgO

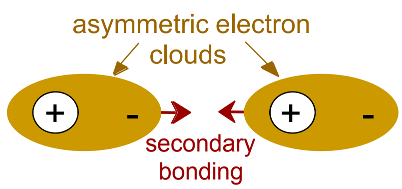
$X_{Mg} = 1.2$
$X_O = 3.5$

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(3.5-1.2)^2}{4}}\right) \text{x } (100\%) = 73.4\% \text{ ionic}$$

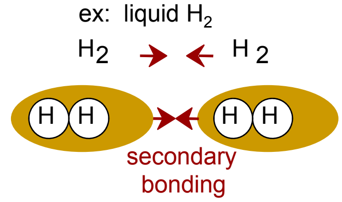
Secondary Bonding

Arises from interaction between dipoles (also called van der Waals Bonding)

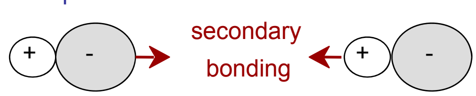
- Fluctuating dipoles



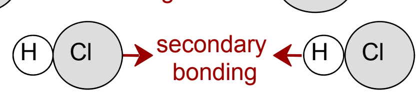
ex: liquid H_2



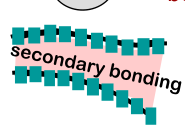
- Permanent dipoles - molecule induced



e.g. Liquid HCl or H_2O



Polymer

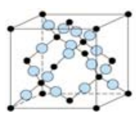


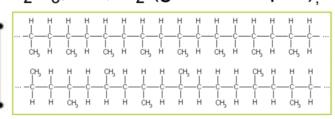
Summary of Bonding Types

Type	Bond Energy	Comments
Ionic	Large	Ceramics
Covalent	Variable Large – diamond Small – Bismuth (Tm=270°C)	Semiconductors Ceramics Within polymer chains
Metallic	Variable Large-Tungsten Small-Mercury	Metals
Secondary	Smallest	inter-chain (polymer) inter-molecular

Identify the bonding type(s): Fe, SiC, SiO_2, Al_2O_3, Ice, N_2 (gas and liquid), polypropylene (ketchup bottle)

$$\left(1-e^{-\frac{(X_A-X_B)^2}{4}}\right)x100$$





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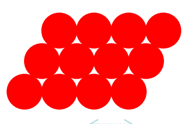
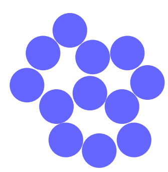
Crystal Structure and Bonding Energy

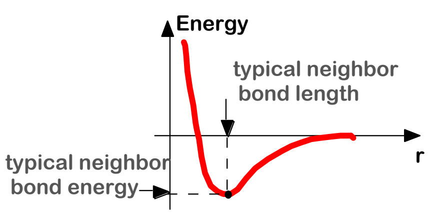


Crystalline Material

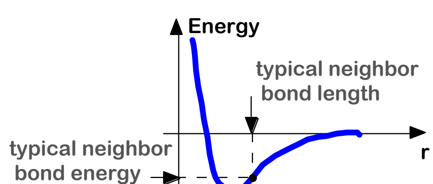


Non- crystalline Material

(e.g. glass, liquid metal, metal glass)



Dense, regular-packed structures in a lower energy state.



Deviated from the lowest energy state

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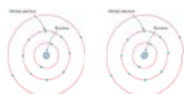
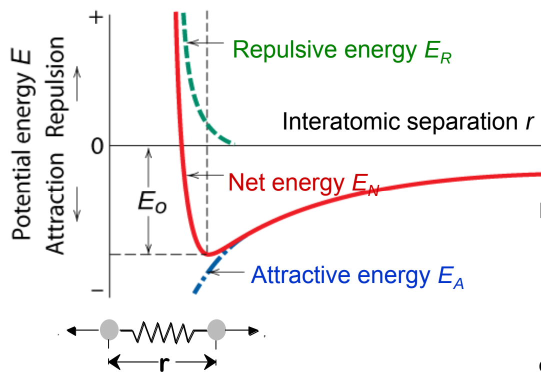
Bonding Energy (at equilibrium spacing)

Energy balance of attractive and repulsive terms



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



Equilibrium spacing r_0 (=R_1+R_2)

How to determine the bonding energy experimentally?

Importance:

- Stiffness
- Melting point
- Coefficient of thermal expansion of pure substances

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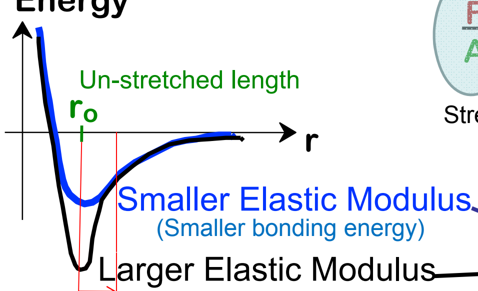
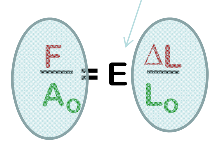
Bonding Energy and Elastic Modulus E



Elastic Modulus



Stress and Strain

Larger bonding energy = lower energy state = stronger bond = higher melting temperature = higher elastic modulus = lower CTE

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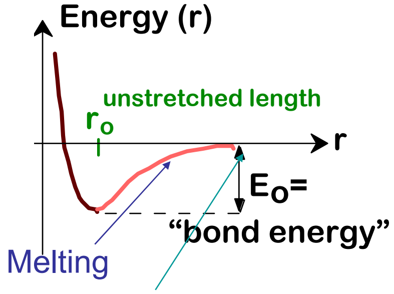
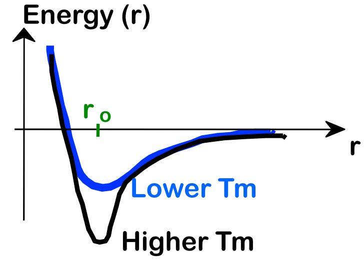
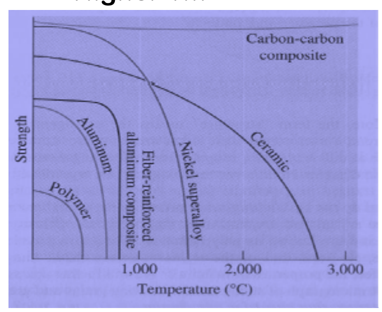
Bonding Energy and Melting Temperature T_m







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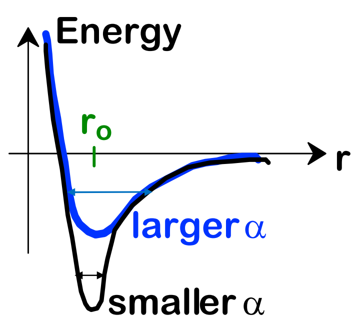
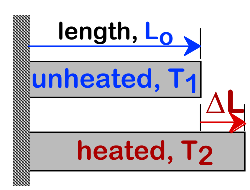
Bonding Energy and CTE (α)



A larger bonding energy means deeper and narrower trough/well – lower α

Coefficient of thermal expansion

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



Engineering Implications

- Mismatch for dissimilar materials (thermal stress)
- Temperature sensor
- Design of low CTE: Kovar, Invar

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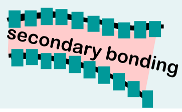
Summary

Material Class	Bonding Type	Properties
Ceramics	(Ionic & covalent bonding)	Large bond energy large T_m large E small α
Metals	Metallic Bonding	Variable bond energy moderate T_m moderate E moderate α
Polymers 	Covalent & Secondary	Directional properties Secondary bonding dominates small T_m small E large α

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