

ME 254: Materials Engineering

Chapter 2: Atomic Structure and Interatomic Bonding

1st Semester 1435-1436 (Fall 2014)

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Outline

- ❑ Atomic structure and electron configurations
- ❑ Interatomic bonding: primary and secondary
 - ❑ Ionic
 - ❑ Covalent
 - ❑ Metallic
 - ❑ Secondary

WHY STUDY Atomic Structure and Interatomic Bonding?

From Chapter 1:



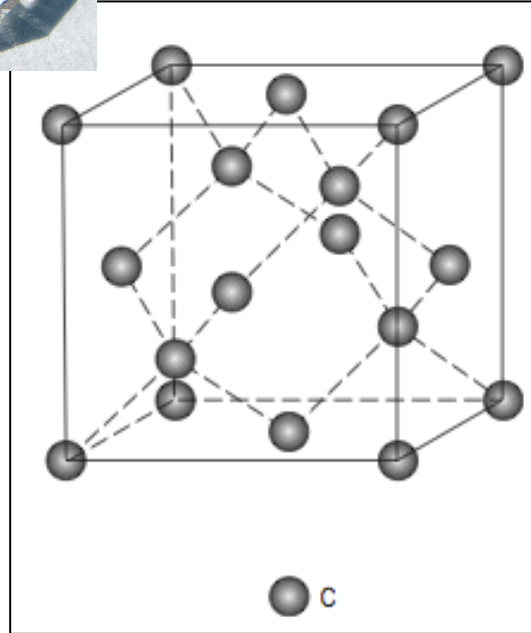
Some of the properties in solid materials strongly depend on the type of atomic structure and interatomic bonding

Carbon

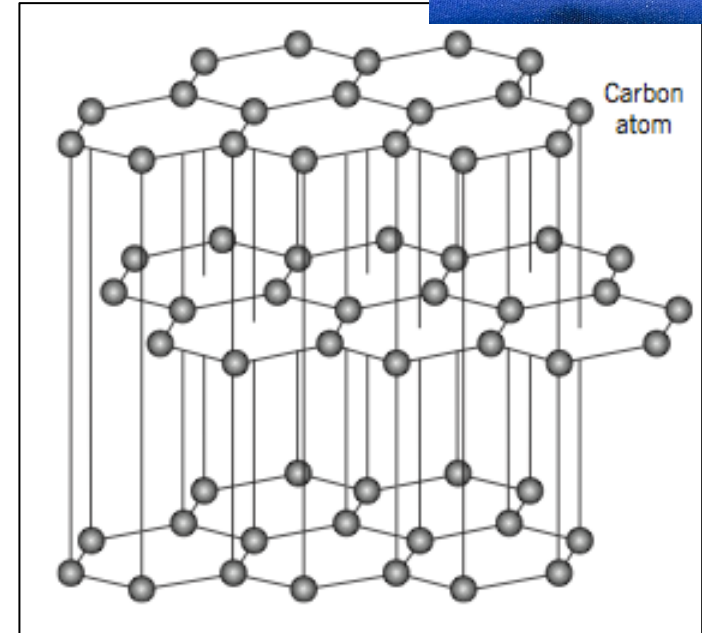


Diamond

vs. Graphite



Strong covalent



Strong covalent
+ weak van der Waals

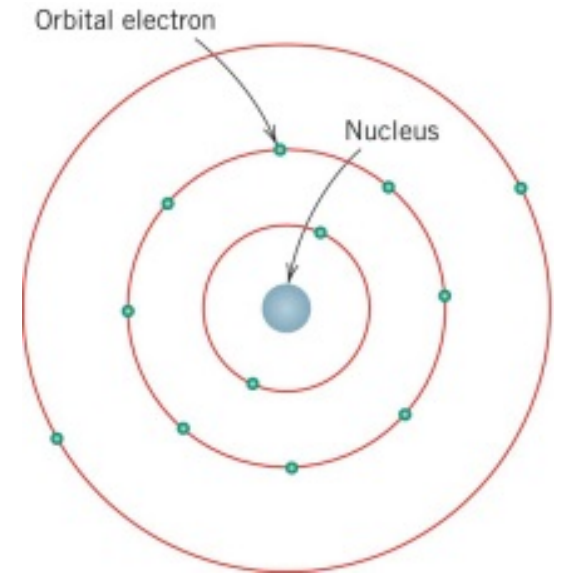
Interatomic
Bonding:

Properties:

Extremely hard, very
low electrical
conductivity

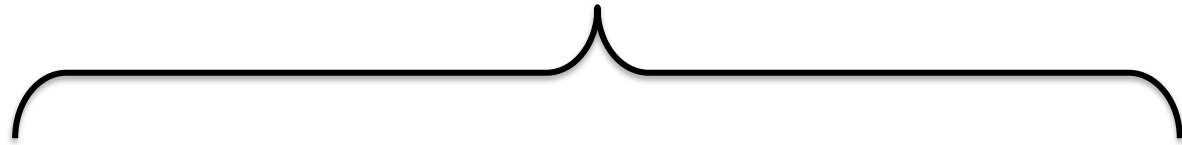
Soft, lubricant,
relatively high electrical
conductivity

Atomic Structure:



Fig_02_01

Atom



Nucleus

Proton (p^+) & neutron (n^0)

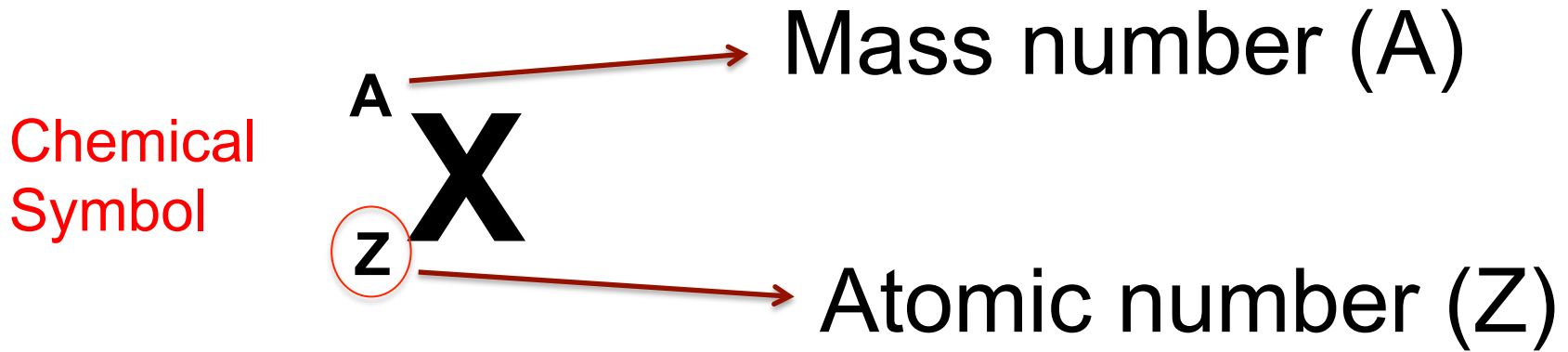
$1.6 \times 10^{-9} \text{ C}$
 $1.673 \times 10^{-27} \text{ kg}$

Electron (e^-)

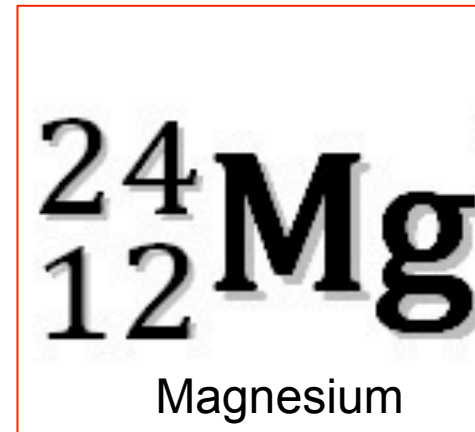
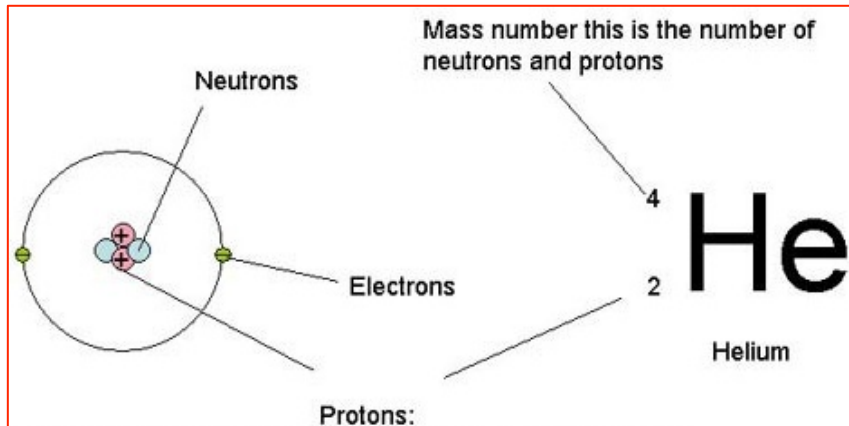
$-1.6 \times 10^{-9} \text{ C}$
 $9.11 \times 10^{-31} \text{ kg}$

Atomic number (Z) = number of protons (n_p) in nucleus
= number of electrons in neutral species **only**

Mass number (A) = number of protons + number of neutron



Example:



Isotopes

For all atoms of a given element, the number of protons is the same but the number of neutrons may be variable.

Isotopes: Atoms of the same element that have different number of neutrons.

Note the following:

- 1. Isotopes have the same proton numbers (Because they're from the same element)*
- 2. Isotopes have different atomic masses (Because they've different number of neutrons)*

Example:

Carbon-12, (A=12), Carbon-13, (A=13), Carbon-14, (A=14)

Atomic number (Z) for Carbon=6

→ No. of neutrons= 6, 7, & 8 for C-12, C-13, & C-14, respectively

- ❑ **Atomic mass:** mass of protons + mass of neutron
- ❑ **Atomic mass unit (amu):** it is a measure of atomic mass defined as $1/12$ of the atomic mass of the most common isotopes of carbon, ^{12}C .
- ❑ **Atomic weight (relative atomic mass):** The weighted average of the atomic masses of the atom's naturally occurring isotopes
- ❑ In one **mole** of a substance there are 6.023×10^{23} (Avogadro's number) atoms or molecules.
 $1 \text{ mole} \rightarrow 6.023 \times 10^{23} \text{ atoms}$
- ❑ $1 \text{ amu/atom} = 1 \text{ g/mole}$

PERIODIC TABLE

Atomic Properties of the Elements

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

18
VIII A

Group	Frequently used fundamental physical constants																Physical Measurement Laboratory				Standard Reference Data																																																																																															
	For the most accurate values of these and other constants, visit physics.nist.gov/constants 1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³ Cs																www.nist.gov/pml				www.nist.gov/srd																																																																																															
1 IA	2 IIA											13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIII A																																																																																																			
1 ¹ H Hydrogen 1.008 1s 13.5984	2 ⁴ He Helium 4.002602 1s ² 24.5874	<p>Speed of light in vacuum c 299 792 458 m s⁻¹ (exact)</p> <p>Planck constant h 6.626 07 × 10⁻³⁴ J s ($h = h/2\pi$)</p> <p>elementary charge e 1.602 177 × 10⁻¹⁹ C</p> <p>electron mass m_e 9.109 38 × 10⁻³¹ kg</p> <p>$m_e c^2$ 0.510 999 MeV</p> <p>proton mass m_p 1.672 622 × 10⁻²⁷ kg</p> <p>fine-structure constant α 1/137.035 999</p> <p>Rydberg constant R_∞ 10 973 731.569 m⁻¹</p> <p>$R_\infty c$ 3.289 841 960 × 10¹⁵ Hz</p> <p>$R_\infty hc$ 13.605 69 eV</p> <p>Boltzmann constant k 1.380 6 × 10⁻²³ J K⁻¹</p>																5 ¹⁰ B Boron 10.811 1s ² 2s ² 2p 8.2980	6 ¹² C Carbon 12.0111 1s ² 2s ² 2p ² 11.2603	7 ¹⁴ N Nitrogen 14.0071 1s ² 2s ² 2p ³ 14.5341	8 ¹⁶ O Oxygen 15.9994 1s ² 2s ² 2p ⁴ 13.6181	9 ¹⁹ F Fluorine 18.9984032 1s ² 2s ² 2p ⁵ 12.9678	10 ²⁰ Ne Neon 20.1797 1s ² 2s ² 2p ⁶ 21.5645	11 ²³ Na Sodium 22.98976928 [Ne]3s 5.1391	12 ²⁴ Mg Magnesium 24.3050 [Ne]3s ² 7.6462	13 ²⁷ Al Aluminum 26.9815386 [Ne]3s ² 3p 5.9858	14 ²⁸ Si Silicon 28.0855 [Ne]3s ² 3p ² 8.1517	15 ³¹ P Phosphorus 30.973762 [Ne]3s ² 3p ³ 10.4687	16 ³² S Sulfur 32.06 [Ne]3s ² 3p ⁴ 10.3600	17 ^{35.5} Cl Chlorine 35.45 [Ne]3s ² 3p ⁵ 12.9678	18 ⁴⁰ Ar Argon 39.948 [Ne]3s ² 3p ⁶ 15.7596	19 ³⁹ K Potassium 39.0983 [Ar]4s 4.3407	20 ⁴⁰ Ca Calcium 40.078 [Ar]4s ² 6.1132	21 ⁴⁵ Sc Scandium 44.955912 [Ar]3d ¹ 4s 6.5615	22 ⁴⁸ Ti Titanium 47.867 [Ar]3d ² 4s ² 6.8281	23 ⁵¹ V Vanadium 50.9415 [Ar]3d ³ 4s 6.7462	24 ⁵² Cr Chromium 51.9961 [Ar]3d ⁵ 4s 6.7695	25 ⁵⁵ Mn Manganese 54.938045 [Ar]3d ⁵ 4s ² 7.4340	26 ⁵⁶ Fe Iron 55.845 7.9025	27 ⁵⁹ Co Cobalt 58.933195 7.8810	28 ^{58.7} Ni Nickel 58.6934 7.6399	29 ^{63.5} Cu Copper 63.546 7.7284	30 ^{65.4} Zn Zinc 65.38 9.3942	31 ^{69.7} Ga Gallium 69.723 5.9993	32 ^{72.6} Ge Germanium 72.63 7.8994	33 ⁷⁵ As Arsenic 74.92160 9.7886	34 ^{78.96} Se Selenium 78.96 9.7524	35 ^{79.9} Br Bromine 79.904 11.8138	36 ^{83.8} Kr Krypton 83.798 13.9996	37 ^{85.5} Rb Rubidium 85.4678 4.1771	38 ^{87.62} Sr Strontium 87.62 5.6949	39 ^{88.91} Y Yttrium 88.90585 6.2173	40 ^{91.224} Zr Zirconium 91.224 6.6339	41 ^{92.906} Nb Niobium 92.90638 7.5889	42 ^{95.94} Mo Molybdenum 95.94 7.0924	43 ⁹⁸ Tc Technetium (98) [Kr]4d ⁵ 5s ² 7.1194	44 ^{101.07} Ru Ruthenium 101.07 7.3605	45 ^{102.91} Rh Rhodium 102.90550 7.4589	46 ^{106.42} Pd Palladium 106.42 8.3369	47 ^{107.8682} Ag Silver 107.8682 7.5782	48 ^{112.411} Cd Cadmium 112.411 8.9938	49 ^{114.818} In Indium 114.818 5.7864	50 ^{118.710} Sn Tin 118.710 7.3439	51 ^{121.760} Sb Antimony 121.760 8.6084	52 ^{127.60} Te Tellurium 127.60 9.0097	53 ^{126.90447} I Iodine 126.90447 10.4513	54 ^{131.293} Xe Xenon 131.293 12.1298	55 ^{132.9054519} Cs Cesium 132.9054519 3.8939	56 ^{137.327} Ba Barium 137.327 5.2117	57 ^{138.90473} La Lanthanum 138.90473 5.5769	58 ^{140.116} Ce Cerium 140.116 5.5386	59 ^{140.90765} Pr Praseodymium 140.90765 5.473	60 ^{144.242} Nd Neodymium 144.242 5.5250	61 ¹⁴⁵ Pm Promethium (145) [Xe]4f ⁵ 6s ² 5.582	62 ^{150.36} Sm Samarium 150.36 5.6437	63 ^{151.964} Eu Europium 151.964 5.6704	64 ^{157.25} Gd Gadolinium 157.25 6.1498	65 ^{158.92535} Tb Terbium 158.92535 6.1498	66 ^{162.50} Dy Dysprosium 162.50 5.9391	67 ^{164.93032} Ho Holmium 164.93032 6.0215	68 ^{167.259} Er Erbium 167.259 6.1077	69 ^{168.93421} Tm Thulium 168.93421 6.1843	70 ^{173.054} Yb Ytterbium 173.054 6.2542	71 ^{174.9668} Lu Lutetium 174.9668 5.4259	72 ^{175.053} Hf Hafnium 175.053 6.8251	73 ^{180.94788} Ta Tantalum 180.94788 7.5496	74 ^{183.84} W Tungsten 183.84 7.8640	75 ^{186.207} Re Rhenium 186.207 7.8335	76 ^{190.23} Os Osmium 190.23 8.4382	77 ^{192.217} Ir Iridium 192.217 8.9670	78 ^{195.084} Pt Platinum 195.084 8.9588	79 ^{196.966569} Au Gold 196.966569 9.2256	80 ^{200.59} Hg Mercury 200.59 10.4375	81 ^{204.38} Tl Thallium 204.38 [Hg]6p 6.1083	82 ^{207.2} Pb Lead 207.2 7.4167	83 ^{208.98040} Bi Bismuth 208.98040 7.2855	84 ⁽²⁰⁹⁾ Po Polonium (209) [Hg]6p 8.414	85 ⁽²¹⁰⁾ At Astatine (210) [Hg]6p 9.350	86 ⁽²²²⁾ Rn Radon (222) [Hg]6p 10.7485	87 ⁽²²³⁾ Fr Francium (223) [Rn]7s 4.0727	88 ⁽²²⁶⁾ Ra Radium (226) [Rn]7s 5.2784	89 ⁽²²⁷⁾ Ac Actinium (227) [Rn]6d ¹ 7s 5.8002	90 ^{232.0376} Th Thorium 232.0376 6.3067	91 ^{231.03688} Pa Protactinium 231.03688 5.89	92 ^{238.02891} U Uranium 238.02891 6.1941	93 ⁽²³⁷⁾ Np Neptunium (237) [Rn]5f ⁴ 6d ¹ 7s 6.2655	94 ⁽²⁴⁴⁾ Pu Plutonium (244) [Rn]5f ⁶ 7s 6.0258	95 ⁽²⁴³⁾ Am Americium (243) [Rn]5f ⁷ 7s 5.9738	96 ⁽²⁴⁷⁾ Cm Curium (247) [Rn]5f ⁸ 7s 5.9914	97 ⁽²⁴⁷⁾ Bk Berkelium (247) [Rn]5f ⁹ 7s 6.1978	98 ⁽²⁵¹⁾ Cf Californium (251) [Rn]5f ¹⁰ 7s 6.2617	99 ⁽²⁵²⁾ Es Einsteinium (252) [Rn]5f ¹¹ 7s 6.3676	100 ⁽²⁵⁷⁾ Fm Fermium (257) [Rn]5f ¹² 7s 6.50	101 ⁽²⁵⁸⁾ Md Mendelevium (258) [Rn]5f ¹³ 7s 6.58	102 ⁽²⁵⁹⁾ No Nobelium (259) [Rn]5f ¹⁴ 7s 6.65	103 ⁽²⁶²⁾ Lr Lawrencium (262) [Rn]5f ¹⁴ 7p 4.90

- Solids
- Liquids
- Gases
- Artificially Prepared

Atomic Number: 58

Ground-state Level: ¹G₄

Symbol: Ce

Name: Cerium

Standard Atomic Weight: [Xe]4f¹5d¹6s²

Ground-state Configuration: [Xe]4f¹5d¹6s²

Ionization Energy (eV): 5.5386

*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.

For a description of the data, visit physics.nist.gov/data
NIST SP 966 (March 2013)

Atomic weight:

2.2 Silicon has three naturally-occurring isotopes: 92.23% of ^{28}Si , with an atomic weight of 27.9769 amu, 4.68% of ^{29}Si , with an atomic weight of 28.9765 amu, and 3.09% of ^{30}Si , with an atomic weight of 29.9738 amu. On the basis of these data, confirm that the average atomic weight of Si is 28.0854 amu.

Example 1 (Problem 2.2)

2.2 Silicon has three naturally-occurring isotopes: 92.23% of ^{28}Si , with an atomic weight of 27.9769 amu, 4.68% of ^{29}Si , with an atomic weight of 28.9765 amu, and 3.09% of ^{30}Si , with an atomic weight of 29.9738 amu. On the basis of these data, confirm that the average atomic weight of Si is 28.0854 amu.

$$\begin{aligned}\text{Atomic_weight} &= 92.23/100 * 27.9769 \\ &+ 4.68/100 * 28.9765 \\ &+ 3.09/100 * 29.9738 \\ &= 28.0854 \text{ amu}\end{aligned}$$

Example 2:

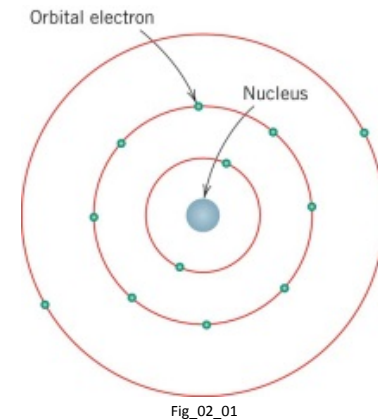
How many atoms of iron (Fe) in 1 g of Fe?

Atomic weight of Fe is 55.845 g/mol

Avogadro number = 6.023×10^{23}

See Homework 2

Electronic Structure



- Electrons are assumed to revolve around the atomic nucleus in discrete orbitals
- Energies of electrons are quantized; that is, electrons are permitted to have only specific values of energy
- Each orbital at discrete energy level is determined by quantum numbers.

-

Quantum

n = principal (energy level-shell)
 l = subsidiary (orbitals, subshell)
 m_l = magnetic
 m_s = spin

Designation

K, L, M, N, O (1, 2, 3, etc.)
 s, p, d, f (0, 1, 2, 3, ..., $n-1$)
1, 3, 5, 7 ($-l$ to $+l$)
 $1/2, -1/2$

- ❑ **Valence electrons:** The electrons in the outermost occupied electron shell, which participate in inter-atomic bonding.
- ❑ Many of the physical and chemical properties of solids are based on the valence electrons.
- ❑ Stable electron configurations = valence electrons shells are completely filled (e.g. inert gasses)

Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
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SURVEY OF ELEMENTS

- Most elements: **Electron configuration 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)

PERIODIC TABLE Atomic Properties of the Elements

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

11 $2s_{1/2}$
Na
Sodium
22.98976928
[Ne]3s
5.1391

Frequently used fundamental physical constants
For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.626 07 $\times 10^{-34}$ J s	($h = h/2\pi$)
elementary charge	e	1.602 177 $\times 10^{-19}$ C	
electron mass	m_e	9.109 38 $\times 10^{-31}$ kg	
$m_e c^2$		0.510 999 MeV	
proton mass	m_p	1.672 622 $\times 10^{-27}$ kg	
fine-structure constant	α	1/137.035 999	
Rydberg constant	R_∞	10 973 731.569 m^{-1}	
$R_\infty c$		3.289 841 960 $\times 10^{15}$ Hz	
$R_\infty hc$		13.605 69 eV	
Boltzmann constant	k	1.380 6 $\times 10^{-23}$ J K^{-1}	

- Solids
- Liquids
- Gases
- Artificially Prepared

Physical Measurement Laboratory www.nist.gov/pml		Standard Reference Data www.nist.gov/srd			
13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
5 B Boron 10.811 $1s^2 2s^2 2p^1$ 8.2990	6 C Carbon 12.0111 $1s^2 2s^2 2p^2$ 14.5341	7 N Nitrogen 14.007 $1s^2 2s^2 2p^3$ 10.4867	8 O Oxygen 15.999 $1s^2 2s^2 2p^4$ 13.6181	9 F Fluorine 18.9984032 $1s^2 2s^2 2p^5$ 17.4228	10 Ne Neon 20.1797 $1s^2 2s^2 2p^6$ 21.5645
13 Al Aluminum 26.9815386 $[\text{Ne}]3s^2 3p^1$ 5.9858	14 Si Silicon 28.0855 $[\text{Ne}]3s^2 3p^2$ 8.1517	15 P Phosphorus 30.973762 $[\text{Ne}]3s^2 3p^3$ 10.4867	16 S Sulfur 32.06 $[\text{Ne}]3s^2 3p^4$ 10.3600	17 Cl Chlorine 35.45 $[\text{Ne}]3s^2 3p^5$ 12.9676	18 Ar Argon 39.948 $[\text{Ne}]3s^2 3p^6$ 15.7596
31 Ga Gallium 69.723 $[\text{Ar}]3d^{10} 4s^1 4p^2$ 5.9993	32 Ge Germanium 72.63 $[\text{Ar}]3d^{10} 4s^2 4p^2$ 7.8994	33 As Arsenic 74.9216 $[\text{Ar}]3d^{10} 4s^2 4p^3$ 9.7886	34 Se Selenium 78.96 $[\text{Ar}]3d^{10} 4s^2 4p^4$ 9.7524	35 Br Bromine 79.904 $[\text{Ar}]3d^{10} 4s^2 4p^5$ 11.8138	36 Kr Krypton 83.798 $[\text{Ar}]3d^{10} 4s^2 4p^6$ 14.5131
49 In Indium 114.818 $[\text{Kr}]4d^{10} 5s^2 5p^2$ 5.7864	50 Sn Tin 118.710 $[\text{Kr}]4d^{10} 5s^2 5p^2$ 7.3439	51 Sb Antimony 121.760 $[\text{Kr}]4d^{10} 5s^2 5p^3$ 8.6084	52 Te Tellurium 127.60 $[\text{Kr}]4d^{10} 5s^2 5p^4$ 9.0097	53 I Iodine 126.90447 $[\text{Kr}]4d^{10} 5s^2 5p^5$ 10.4513	54 Xe Xenon 131.29 $[\text{Kr}]4d^{10} 5s^2 5p^6$ 13.4464
81 Tl Thallium 204.38 $[\text{Hg}]6s^2 6p^1$ 6.1083	82 Pb Lead 207.2 $[\text{Hg}]6s^2 6p^2$ 7.4187	83 Bi Bismuth 208.98040 $[\text{Hg}]6s^2 6p^3$ 7.2855	84 Po Polonium (209) $[\text{Hg}]6s^2 6p^4$ 8.414	85 At Astatine (210) $[\text{Hg}]6s^2 6p^5$ 9.350	86 Rn Radon (222) $[\text{Xe}]6s^2 6p^6$ 10.972
113 Uut Ununtrium (284)	114 Fl Flerovium (289)	115 Uup Ununpentium (288)	116 Lv Livermorium (293)	117 Uus Ununseptium (294)	118 Uuo Ununoctium (294)

Period

Group
1
IA

2
IIA

3
IIIB

4
IVB

5
VB

6
VIB

7
VIIB

8
VIII

9
VIII

10
VIII

11
IB

12
IIB

Atomic Number: 58
Ground-state Level: G_4^0
Symbol: Ce
Name: Cerium
Standard Atomic Weight: 140.116
Ground-state Configuration: [Xe]4f5d6s^2
Ionization Energy (eV): 5.5386

Lanthanides		Actinides												
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
138.90547 $[\text{Xe}]5d^1 6s^2$ 5.5789	140.116 $[\text{Xe}]4f5d6s^2$ 5.5386	140.90765 $[\text{Xe}]4f^3 6s^2$ 5.473	144.242 $[\text{Xe}]4f^4 6s^2$ 5.5250	144.9128 $[\text{Xe}]4f^5 6s^2$ 5.582	150.36 $[\text{Xe}]4f^6 6s^2$ 5.6437	151.964 $[\text{Xe}]4f^7 6s^2$ 5.6704	157.25 $[\text{Xe}]4f^7 6s^2$ 5.9391	158.92535 $[\text{Xe}]4f^9 6s^2$ 5.8638	162.500 $[\text{Xe}]4f^10 6s^2$ 6.0215	164.93032 $[\text{Xe}]4f^11 6s^2$ 6.0215	167.259 $[\text{Xe}]4f^12 6s^2$ 6.1077	168.93421 $[\text{Xe}]4f^13 6s^2$ 6.1843	173.054 $[\text{Xe}]4f^14 6s^2$ 6.2542	174.9668 $[\text{Xe}]4f^14 6s^2$ 5.4259
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
(227) $[\text{Rn}]5f^7 6s^2$ 5.3802	232.03806 $[\text{Rn}]5f^4 6s^2$ 6.3067	231.03688 $[\text{Rn}]5f^6 6s^2$ 5.89	238.02891 $[\text{Rn}]5f^4 6s^2$ 6.1941	237 $[\text{Rn}]5f^6 6s^2$ 6.2655	244 $[\text{Rn}]5f^8 6s^2$ 6.0258	243 $[\text{Rn}]5f^7 6s^2$ 5.9738	247 $[\text{Rn}]5f^9 6s^2$ 5.9914	247 $[\text{Rn}]5f^10 6s^2$ 6.1978	251 $[\text{Rn}]5f^11 6s^2$ 6.2617	252 $[\text{Rn}]5f^12 6s^2$ 6.3676	257 $[\text{Rn}]5f^13 6s^2$ 6.50	258 $[\text{Rn}]5f^14 6s^2$ 6.58	259 $[\text{Rn}]5f^14 6s^2$ 6.65	262 $[\text{Rn}]5f^14 6s^2$ 4.90

[†]Based upon ^{12}C . () indicates the mass number of the longest-lived isotope.

^{*}IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.

For a description of the data, visit physics.nist.gov/data
NIST SP 966 (March 2013)

The Periodic Table

- Columns: Similar **Valence** Structure

Annotations for valence electrons:

- give up 1e⁻ (Group 1)
- give up 2e⁻ (Group 2)
- give up 3e⁻ (Group 3)
- accept 2e⁻ (Group 16)
- accept 1e⁻ (Group 17)
- inert gases (Group 18)

1 H	2 He											10 Ne	11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar														
3 Li	4 Be											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					
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 Tm	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
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	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og			

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

Electronegative elements:
Readily acquire electrons
to become - ions.



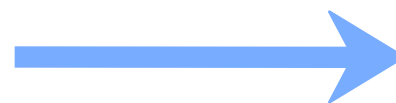
Electronegativity

- Ranges from 0.9 to 4.1,
- 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	3.1	3.5	4.1	-
Na	Mg																Ar
1.0	1.3	IIIB	IVB	VB	VIB	VIIIB	VIII			IB	IIB	Al	Si	P	S	Cl	-
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.9	1.1	1.2	1.3	1.5	1.6	1.6	1.7	1.7	1.8	1.8	1.7	1.8	2.0	2.2	2.5	2.8	-
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.9	1.0	1.1	1.2	1.3	1.3	1.4	1.4	1.5	1.4	1.4	1.5	1.5	1.7	1.8	2.0	2.2	-
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.9	0.9	1.1	1.2	1.4	1.4	1.5	1.5	1.6	1.5	1.4	1.5	1.5	1.6	1.7	1.8	2.0	-
Fr	Ra	Ac	Lanthanides: 1.0-1.2														
0.9	0.9	1.0	Actinides: 1.0-1.2														



Smaller electronegativity



Larger electronegativity

INTERATOMIC BONDING

Atomic Bonds

Primary interatomic bonds

- depends on the electron structures of the atoms
- Seeks stable electron structures (by filling the outermost electron shell)

Secondary, van der Waals, or physical bonds

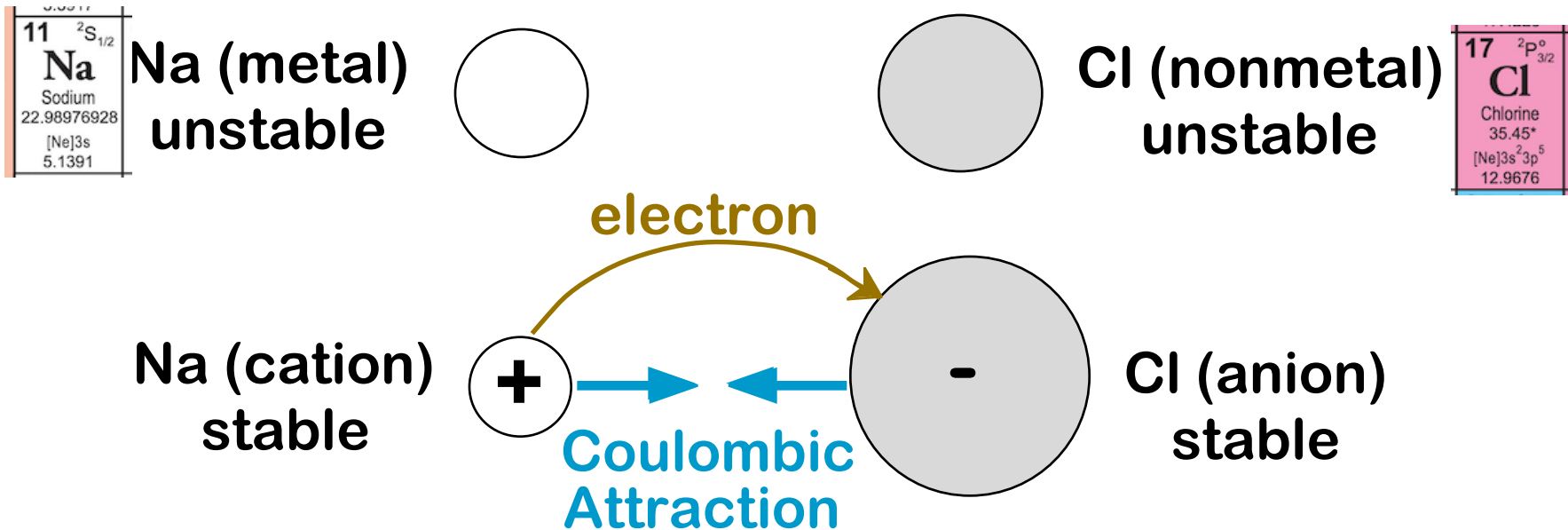
Ionic bonding

Covalent bonding

Metallic bonding

1. IONIC BONDING

- Occurs between + and - ions.
- Requires **electron transfer**.
- Example: NaCl



EXAMPLES: IONIC BONDING

- Predominant bonding in **Ceramics**

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	IIIB	IVB	VB	VB	VIB	VIII			IB	IIB						Cl	Ar
0.9	1.2											Al	Si	P	S		3.0	-
												1.5	1.8	2.1	2.5			
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	1.8	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	57-71 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	89-100 Ac-No																
0.7	0.9	1.1-1.7																


Give up electrons


Acquire electrons

Ionic materials (materials with predominate ionic bonding):

- ❑ Most **ceramic** materials have ionic bonding
- ❑ Bonding energy is relatively large → High melting temperature
- ❑ Ionic materials are hard and brittle
- ❑ Electrically and thermally insulative
- ❑ Covalent bonding is nondirectional

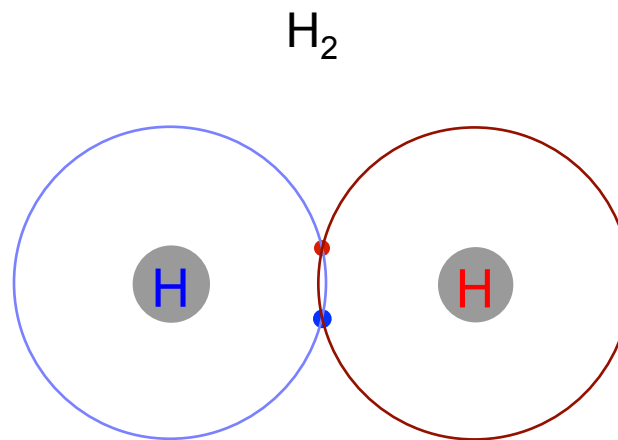
2. Covalent Bonding

- Requires **shared electrons**
- similar **electronegativity** \therefore share electrons

Example: H₂

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

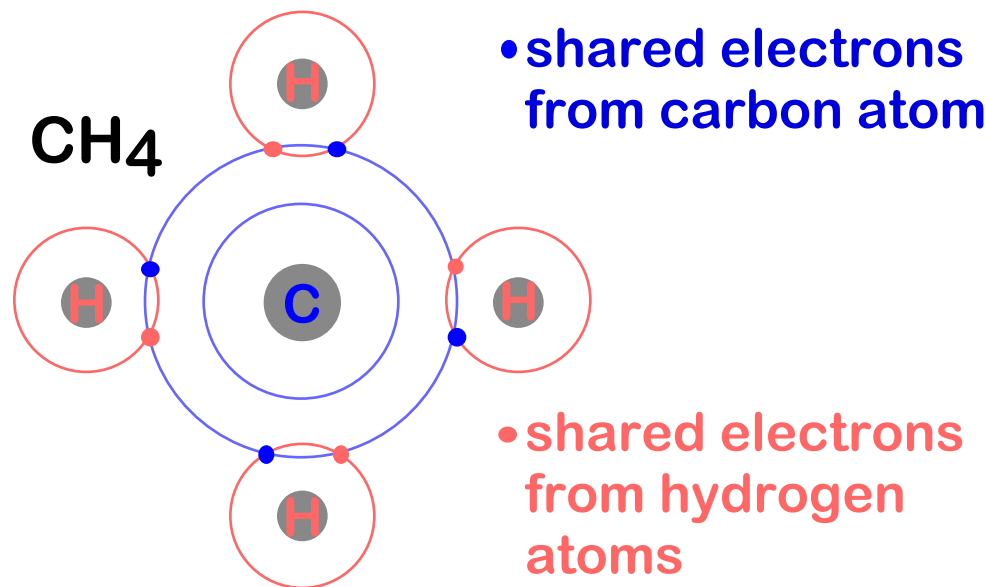
2. COVALENT BONDING

- Requires **shared electrons**
- Example: CH₄

C: has 4 valence e,
needs 4 more

H: has 1 valence e,
needs 1 more

**Electronegativities
are comparable.**



2. COVALENT BONDING

- ❑ Available in
 - Most nonmetallic elemental molecules (H_2 , Cl_2 , F_2 , etc)
 - CH_4 , H_2O , HF , etc
 - Elemental solids such as diamond, silicon, germanium
 - Polymers

- ❑ Bonding may be weak or strong

- ❑ Ionic bonding is directional

It should be noted that partially ionic and partially covalent bonding are possible

3. METALLIC BONDING

- ✓ Primary bond for **metals** and their **alloys**
- ✓ Arises from a sea of **donated valence electrons**

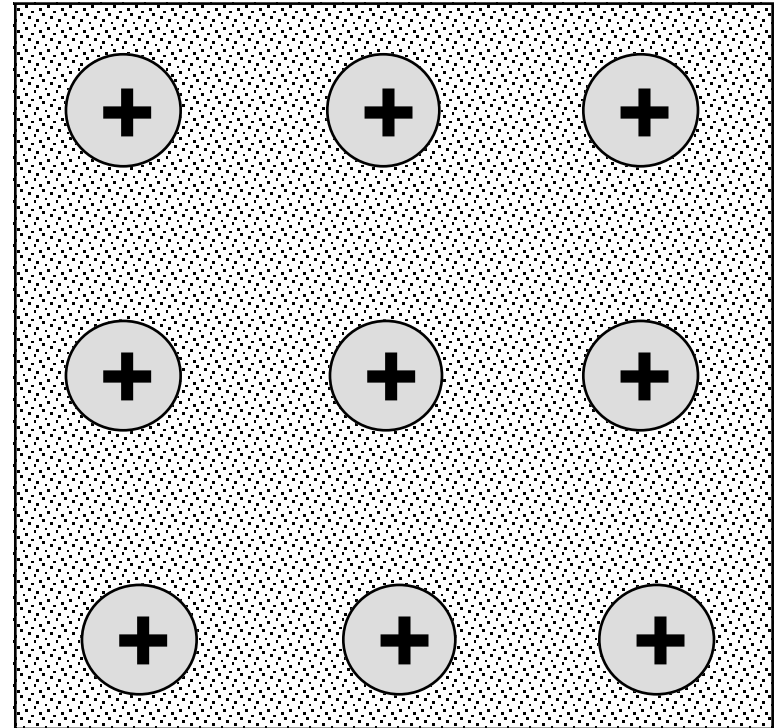
① Metallic elements have 1, 2, or 3 valence electrons
→ Electron clouds
(negative charge)

+

② Non valence electrons and atomic nuclei → ions cores (positive charge)

=

forms Metallic bonding

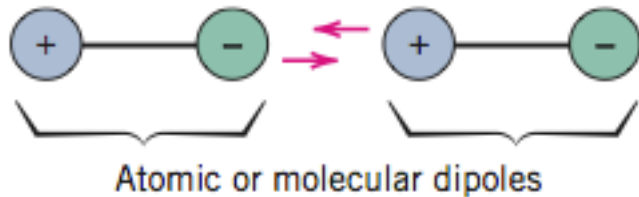


3. METALLIC BONDING

- ❑ Primary bond for metals
- ❑ Good electric and thermal conductivities (because of the free electrons)
- ❑ Bonding may be weak or strong
- ❑ Metallic bonding is nondirectional

Secondary Bonding or van der Waals Bonding

- Secondary bonding arise from interaction between atomic or molecular **dipoles**



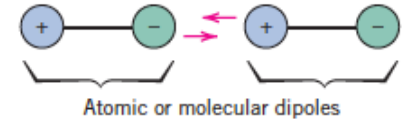
Dipole is a pair of equal yet opposite electrical charges that are separated by a small distance.

- Weak bonding (10 kJ/mol)
- Can exist between all atoms or molecules
- *Fluctuating induced dipole bond, polar molecule- induced dipole bond, permanent dipole bond, and hydrogen bond (see **section 2.7**)*

Atomic Bonds

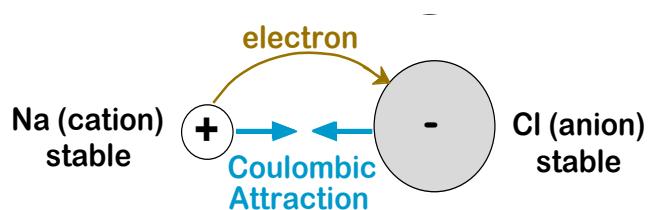
Primary interatomic bonds

Secondary, van der Waals, or physical bonds



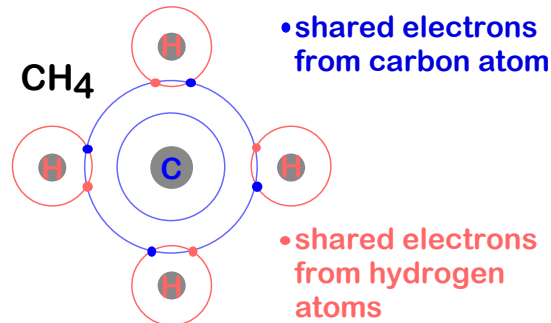
Ionic bonding

Atoms give up their valence electrons to other atoms



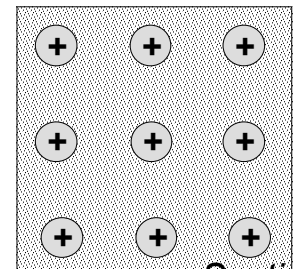
Covalent bonding

share electrons between adjacent atoms



Metallic bonding

Arises from a sea of donated valence electrons



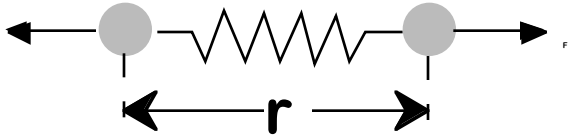
SUMMARY: BONDING

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional semiconductors, ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

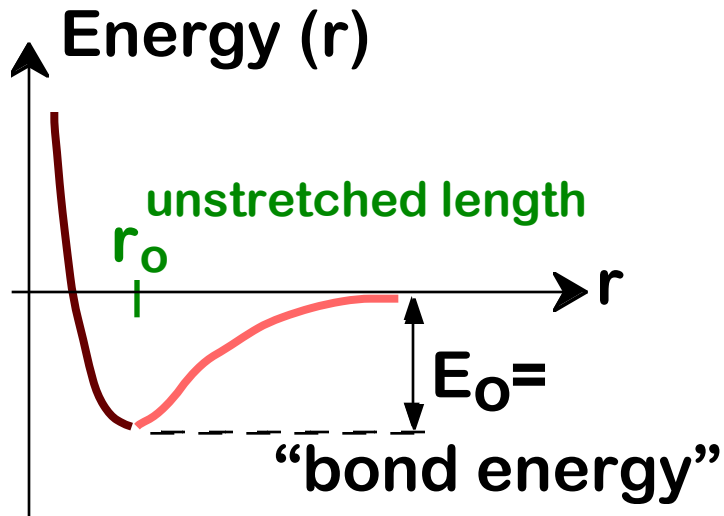
Relationships between bonding and some physical properties

PROPERTIES FROM BONDING: T_M

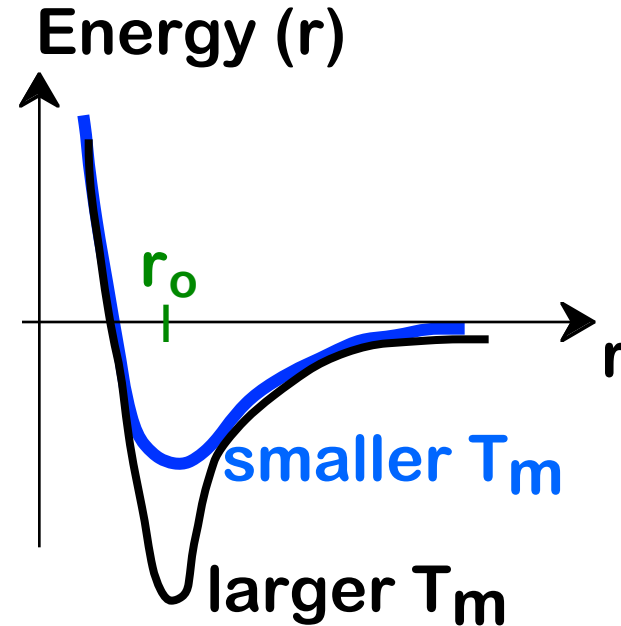
- **Bond length, r**



- **Bond energy, E_0**



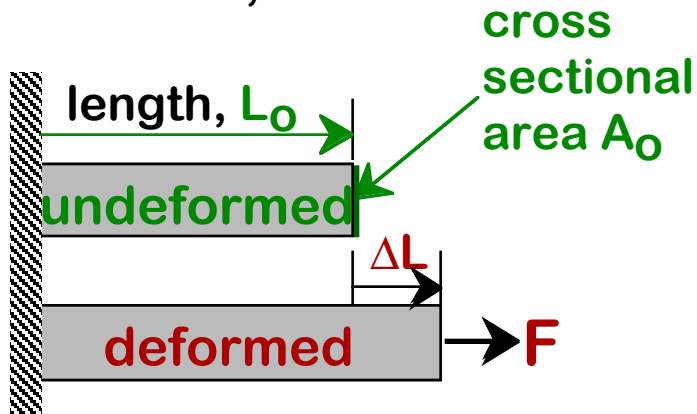
- **Melting Temperature, T_m**



T_m is larger if E_0 is larger.

PROPERTIES FROM BONDING: E

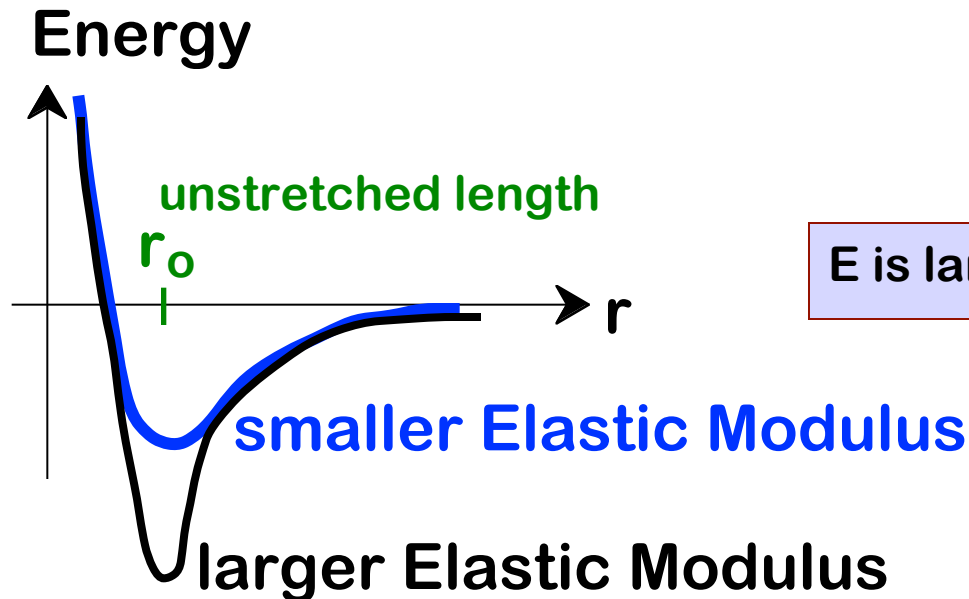
- Elastic modulus, E



Elastic modulus

$$\frac{F}{A_0} = E \frac{\Delta L}{L_0}$$

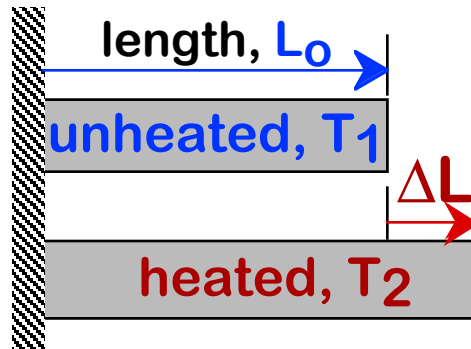
- $E \sim$ curvature at r_0



E is larger if E_0 is larger.

PROPERTIES FROM BONDING: α

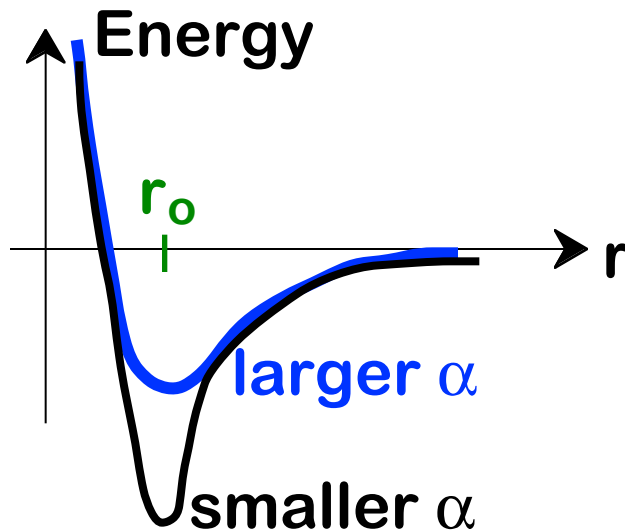
- Coefficient of thermal expansion, α



coeff. thermal expansion

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

- $\alpha \sim$ symmetry at r_0



α is larger if E_0 is smaller.

SUMMARY: PRIMARY BONDS

Ceramics

(Ionic & covalent bonding):

Large bond energy

large T_m

large E

small α

Metals

(Metallic bonding):

Variable bond energy

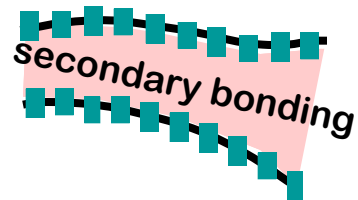
moderate T_m

moderate E

moderate α

Polymers

(Covalent & Secondary):



Directional Properties

Secondary bonding dominates

small T

small E

large α

Chapter 2: Summary

1) Atomic structure and electron configurations

2) Interatomic bonding

(primary & secondary, van der Waals, bonding)