

Study Unit 1: Introduction to Material Science and Bonding in Solid Materials

Introduction

This unit focuses on the historical perspectives of materials, meaning of materials science, types of materials, classification of materials. Atomic bonding and bonding types, Crystallography and x-ray diffraction, Defect structures, Amorphous structures in metals, ceramics, and polymers crystalline, crystal systems, crystallography, indices of planes and directions.

Learning outcomes

By the end of this course, you should be able to:

- i. Explain the terms Materials and Science
- ii. Identify different types of materials and their classifications
- iii. Explain structures in materials
- iv. Describe bonding in materials with relevant examples

Materials and Materials Science

Material is everything you can feel, see or touch, it exists in form of solid, liquid and gases. Generally, materials can be animate or inanimate. Inanimate solids are our major focus in the course. The inanimate solids that are used by scientists or engineers will be our major focus.

Historical Perspectives and Meaning of Material Science

Beginning of the Material Science - People began to make tools from stone – Start of the Stone Age about two million years ago. Natural materials: stone, wood, clay, skins, etc.

Three Age and Advent of Materials

The Stone Age ended about 5000 years ago with introduction of Bronze in the Far East. Bronze is an alloy (a metal made up of more than one element), copper + < 25% of tin + other elements.

Bronze: can be hammered or cast into a variety of shapes, can be made harder by alloying, corrode only slowly after a surface oxide film forms.

The Iron Age began about 3000 years ago and continues today. Use of iron and steel, a stronger and cheaper material changed drastically daily life of a common person.

Age of Advanced materials: throughout the Iron Age many new types of materials have been introduced (ceramic, semiconductors, polymers, composites...).

Classification of Materials

Metals

Materials in this group are composed of one or more metallic elements (e.g., iron, aluminium, copper, titanium, gold, and nickel), and often also non-metallic elements (e.g., carbon, nitrogen, and oxygen) in relatively small amounts. Atoms in metals and their alloys are arranged in a very orderly manner. Alloys are combination of one metal with one or more elements such that the combination behaves like metal. With regard to mechanical characteristics, these materials are relatively stiff and strong, yet are ductile (i.e., capable of large amounts of deformation without fracture), and are resistant to fracture, which accounts for their widespread use in structural applications. Metallic materials have large numbers of non-localized electrons; that is, these electrons are not bound to particular atoms. Many properties of metals are directly attributable to these electrons. For example, metals are extremely good conductors of electricity and heat, and are not transparent to visible light; a polished metal surface has a lustrous appearance. In addition, some of the metals (i.e., Fe, Co, and Ni) have desirable magnetic properties.

Ceramics

Ceramics are compounds between metallic and non-metallic elements; they are most frequently oxides, nitrides, and carbides. For example, common ceramic materials include aluminum oxide (or *alumina*, Al_2O_3), silicon dioxide (or *silica*, SiO_2), silicon carbide (SiC), silicon nitride (Si_3N_4), and, in addition, what some refer to as the *traditional ceramics*—those composed of clay minerals (i.e., porcelain), as well as cement and glass. With regard to mechanical behaviour, ceramic materials are relatively stiff and strong—stiffness and strengths are comparable to those of the metals. In addition, they are typically very hard. Historically, ceramics have exhibited extreme brittleness (lack of ductility) and are highly susceptible to fracture. However, newer ceramics are being engineered to have improved resistance to fracture; these materials are used for cookware, cutlery, and even automobile engine parts. Furthermore, ceramic materials are typically insulative to the passage of heat and electricity (i.e., have low electrical conductivities), and are more resistant to high temperatures and harsh environments than metals and polymers. With regard to optical characteristics, ceramics may be transparent, translucent, or opaque, and some of the oxide ceramics (e.g., Fe_3O_4) exhibit magnetic behavior.



Polymers

Polymers include the familiar plastic and rubber materials. Many of them are organic compounds that are chemically based on carbon, hydrogen, and other non-metallic elements (i.e., O, N, and Si). Furthermore, they have very large molecular structures, often chainlike in nature, that often have a backbone of carbon atoms. Some of the common and familiar polymers are polyethylene (PE), nylon, poly (vinyl chloride) (PVC), polycarbonate (PC), polystyrene (PS), and silicone rubber. These materials typically have low densities, whereas their mechanical characteristics are generally dissimilar to the metallic and ceramic materials—they are not as stiff nor as strong as these other material types. However, on the basis of their low densities, many times their stiffness and strengths on a per-mass basis are comparable to the metals and ceramics. In addition, many of the polymers are extremely ductile and pliable (i.e., plastic), which means they are easily formed into complex shapes.



Composite

A composite is composed of two (or more) individual materials, which come from the categories previously discussed—metals, ceramics, and polymers. The design goal of a composite is to achieve a combination of properties that is not displayed by any single material, and also to incorporate the best characteristics of each of the component materials. A large number of composite types are represented by different combinations of metals, ceramics, and polymers. Furthermore, some naturally occurring materials are composites—for example, wood and bone. However, most of those we consider in our discussions are synthetic (or human-made)

composites. One of the most common and familiar composites is fiberglass, in which small glass fibers are embedded within a polymeric material (normally an epoxy or polyester). The glass fibers are relatively strong and stiff (but also brittle), whereas the polymer is more flexible. Thus, fiberglass is relatively stiff, strong and flexible. In addition, it has a low density. Another technologically important material is the carbon fiber reinforced polymer (CFRP) composite—carbon fibres that are embedded within a polymer. These

materials are stiffer and stronger than glass fibre–reinforced materials but more expensive. CFRP composites are used in some aircraft and aerospace applications, as well as high-tech sporting equipment (e.g., bicycles, golf clubs, tennis rackets, and skis/snowboards) and recently in automobile bumpers.

Advanced Materials

Materials that are utilized in high-technology (or high-tech) applications are sometimes termed *advanced materials*. By *high technology* we mean a device or product that operates or functions using relatively intricate and sophisticated principles; examples include electronic equipment (camcorders, CD/DVD players, etc.), computers, fiber-optic systems, spacecraft, aircraft, and military rocketry. These advanced materials are typically traditional materials whose properties have been enhanced, and also newly developed, high-performance materials. They may be of all material types (e.g., metals, ceramics, polymers), and are normally expensive.

1. **Semiconductors:** Semiconductors have electrical properties that are intermediate between the electrical conductors (i.e., metals and metal alloys) and insulators (i.e., ceramics and polymers). Furthermore, the electrical characteristics of these materials are extremely sensitive to the presence of minute concentrations of impurity atoms, for which the concentrations may be controlled over very small spatial regions. Semiconductors have made possible the advent of integrated circuitry that has totally revolutionized the electronics and computer industries (not to mention our lives) over the past three decades.
2. **Biomaterials:** Biomaterials are employed in components implanted into the human body to replace diseased or damaged body parts. These materials must not produce toxic substances and must be compatible with body tissues (i.e., must not cause adverse biological reactions). All of the preceding materials—metals, ceramics, polymers, composites, and semiconductors—may be used as biomaterials. For example, some of the biomaterials that are utilized in artificial hip.
3. **Smart:** *Smart* (or *intelligent*) *materials* are a group of new and state-of-the-art materials now being developed that will have a significant influence on many of our technologies. The adjective *smart* implies that these materials are able to sense changes in their environment and then respond to these changes in predetermined manners—traits that are also found in living organisms. In addition, this “smart” concept is being extended to rather sophisticated systems that consist of both smart and traditional materials. Components of a smart material (or system) include some type of sensor (that detects an input signal), and an actuator (that performs a responsive and adaptive function). Actuators may be called upon to change shape, position, natural frequency, or mechanical characteristics in response to changes in temperature, electric fields, and/or magnetic fields.
4. **Nanomaterials:** One new material class that has fascinating properties and tremendous technological promise is the *nanomaterials*. Nanomaterials may be any one of the four basic types—metals, ceramics, polymers, and composites. However, unlike these other materials, they are not distinguished on the basis of their chemistry, but rather, size; the *Nano*-prefix denotes that the dimensions of these structural

entities are on the order of a Nano-meter (10^{-9} m)—as a rule, less than 100 nanometres (equivalent to approximately 500 atom diameters).

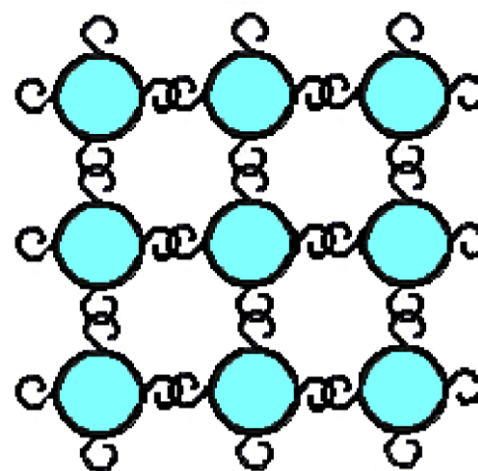
Molecules and molecular solids

Understanding of interatomic bonding is the first step towards understanding/explaining materials properties **Nature of Interatomic Bonding**. Why the individual atoms coalesce into larger structures and take on the characteristics and properties of many different materials? People were trying to answer this question for well over two millennia, since the time of the atomic hypothesis of Democritus, 440 B.C. Roman poet Lucretius (95-55 B.C.) wrote in *De Rerum Natura* (On the Nature of Things):

“What seems to us the hardened and condensed
Must be of atoms among themselves more hooked,
Be held compacted deep within, as it were
By branch-like atoms- of which sort the chief
Are diamond stones, despisers of all blows,
And stalwart flint and strength of solid iron...”

John Dalton (1766-1844) found the evidence of those "hooks" in his quantitative chemical measurements, making the foundation of modern atomic theory of matter.

The idea that everything is made of distinct atoms has been a subject of skeptical discussions as recently as the beginning of the twentieth century, before Einstein's observation of Brownian motion in 1905 and Max von Laue's observation of the diffraction of X-rays by crystals in 1912 provided strong support for the atomistic theory.



Structure of atoms

The bonding mechanisms between atoms are closely related to the structure of the atoms themselves.

Atoms = nucleus (proton and neutron) + electron

Charges: Electrons and protons have negative and positive charges of the same magnitude, 1.6×10^{-19} Coulombs. Neutrons are electrically neutral.

Masses: Protons and Neutrons have the same mass, 1.67×10^{-27} kg.

Mass of an electron is much smaller, 9.11×10^{-31} kg and can be neglected in calculation of atomic mass.

The atomic mass (A) = mass of protons + mass of neutrons

protons give chemical identification of the element, protons = atomic number (Z)
neutrons define isotope number

Atomic mass units. Atomic weight: The atomic mass unit (amu) is often used to express atomic weight. 1 amu is defined as 1/12 of the atomic mass of the most common isotope of carbon atom that has 6 protons (Z=6) and six neutrons (N=6).

$M_{\text{proton}} \approx M_{\text{neutron}} = 1.66 \times 10^{-24} \text{ g} = 1 \text{ amu}$.

The atomic mass of the ^{12}C atom is 12 amu.

The atomic weight of an element = weighted average of the atomic masses of the atoms naturally occurring isotopes. Atomic weight of carbon is 12.011 amu.

The atomic weight is often specified in mass per mole.

A mole is the amount of matter that has a mass in grams equal to the atomic mass in amu of the atoms (A mole of carbon has a mass of 12 grams).

The number of atoms in a mole is called the Avogadro number, $N_{\text{av}} = 6.023 \times 10^{23}$.

1 amu/atom = 1 gram/mol

Example:

Atomic weight of iron = 55.85 amu/atom = 55.85 g/mol

Some simple calculations

The number of atoms per cm^3 , n, for material of density d (g/cm^3) and atomic mass M (g/mol):

$$n = N_{av} \times d / M$$

Graphite (carbon): $d = 2.3 \text{ g/cm}^3$,
 $M = 12 \text{ g/mol}$
 $n = 6 \times 10^{23} \text{ atoms/mol} \times 2.3 \text{ g/cm}^3 / 12 \text{ g/mol}$
 $= 11.5 \times 10^{22} \text{ atoms/cm}^3$

Diamond (carbon): $d = 3.5 \text{ g/cm}^3$,
 $M = 12 \text{ g/mol}$
 $n = 6 \times 10^{23} \text{ atoms/mol} \times 3.5 \text{ g/cm}^3 / 12 \text{ g/mol}$
 $= 17.5 \times 10^{22} \text{ atoms/cm}^3$

Water (H_2O) $d = 1 \text{ g/cm}^3$, $M = 18 \text{ g/mol}$
 $n = 6 \times 10^{23} \text{ molecules/mol} \times 1 \text{ g/cm}^3 / 18 \text{ g/mol}$
 $= 3.3 \times 10^{22} \text{ molecules/cm}^3$

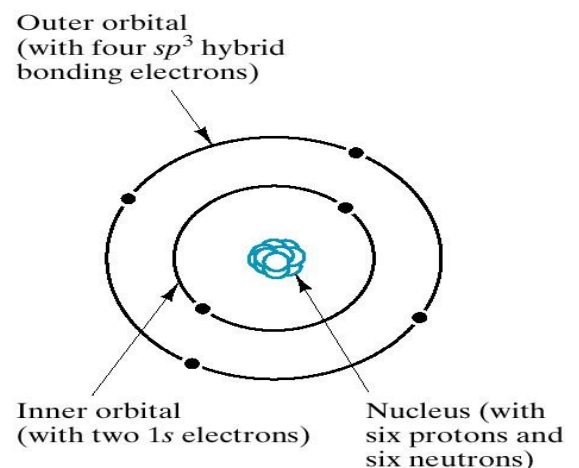
For material with $n = 6 \times 10^{22} \text{ atoms/cm}^3$ we can calculate mean distance between atoms $L = (1/n)^{1/3} = 0.25 \text{ nm}$. The scale of atomic structures in solids – a fraction of 1 nm or a few Å.

Electrons in Atoms

The electrons form a cloud around the nucleus, of radius of 0.05 – 2 nm. This picture looks like a mini planetary system. But quantum mechanics tells us that this analogy is not correct: Electrons move not in circular orbits, but in 'fuzzy' orbits. Actually, we cannot tell how it moves, but only can say what is the probability of finding it at some distance from the nucleus.

Only certain "orbits" or shells of electron probability densities are allowed. The shells are identified by a **principal quantum number n** , which can be related to the size of the shell, $n = 1$ is the smallest; $n = 2, 3 \dots$ are larger.

The second quantum number l , defines subshells within each shell. **Two more quantum numbers** characterize states within the subshells.



- The quantum numbers arise from solution of Schrodinger's equation
- Pauli Exclusion Principle: only one electron can have a given set of the four quantum numbers.

The number of available states in electron shells & subshells

Q. N., n	Subshells	of States	Per Subshell	Per Shell
1 (l=0)	<i>K-shell s s</i>	1	2	2
2 (l=0)	<i>L-shell p s</i>	1	2	8
2 (l=1) 3	<i>M-shell p d s</i>	3	6	
(l=0) 3	<i>N-shell p d f</i>	1	2	18
(l=1)		3	6	
3 (l=2)		5	10	
4 (l=0) 4		1	2	32
(l=1)		3	6	
4 (l=2)		5	10	
4 (l=3)		7	14	

Principal Number Number of Electrons

Each “orbit” or shell can accommodate only a maximum number of electrons, which is determined by quantum mechanics. In brief, the most inner *K-shell* can accommodate only two electrons, called *s-electrons*; the next *L-shell* two *s-electrons* and six *p-electrons*; the *M shell* can host two *s-electrons*, six *p-electrons*, and ten *d-electrons*; and so on.

Subshells by energy: 1s,2s,2p,3s,3p,4s,3d,4s,4p,5s,4d,5p,6s,4f,...

- Electrons that occupy the outermost filled shell – **the valence electrons** – they are responsible for bonding.
- Electrons fill quantum levels in order of increasing energy (only n, l make a significant difference).

Examples: Argon, Z = 18: $1s^2 2s^2 2p^6 3s^2 3p^6$
 Iron, Z = 26: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
 Krypton 36 = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

Electron configurations where all states within valence electron shell are filled are stable → unreactive inert or noble gas.

Periodic Table

The first accepted periodic table of elements was published in 1869 by Mendeleev. In the same year, a German chemist Lothar Meyer independently published a very similar table, but his contribution is generally ignored.

All elements in the periodic table have been classified according to the electron configuration.
Draft of the periodic table, Mendeleev, 1869

Periodic Table

Metal

Nonmetal

Intermediate

give up 1e⁻

give up 2e⁻

give up 3e⁻

accept 2e⁻

accept 1e⁻

inert gases

IA	IIA										IIIA	IVA	VA	VIA	VIIA	0			
1 H	2 He										5 B	6 C	7 N	8 O	9 F	10 Ne			
3 Li	4 Be										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar			
11 Na	12 Mg	IIIB	IVB	VB	VIB	VIIA	VIII			IB	IIB	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
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	Rare earth series	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	Acti-nide series	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds										

Electropositive elements:

Readily give up electrons

Electronegative elements:

Readily acquire electrons to become + ions. to become - ions.

Elements in the same column (Elemental Group) share similar properties. Group number indicates the number of electrons available for bonding.

0: Inert gases (He, Ne, Ar...) have filled subshells: chem. inactive

IA: Alkali metals (Li, Na, K...) have one electron in outermost occupied s subshell - eager to give up electron – chem. active

VIIA: Halogens (F, Br, Cl...) missing one electron in outermost occupied p shell - want to gain electron - chem. active

- Electronegativity - a measure of how willing atoms are to accept electrons
- Subshells with one electron → low electronegativity
- Subshells with one missing electron → high electronegativity
- Electronegativity increases from left to right

Metals are electropositive – they can give up their few valence electrons to become positively charged ions

Bonding Energies and Forces

In a typical potential well for two interacting atoms. The repulsion between atoms, when they are brought close to each other, is related to the Pauli principle: when the electronic clouds surrounding the atoms starts to overlap, the energy of the system increases abruptly. The origin of the attractive part, dominating at large distances, depends on the particular type of bonding.

$$F_1 = -F_2 = \frac{-dU(r_{12})}{d_{12}}$$

Forces can be calculated from the potential energy of interatomic interaction. For example, for a system of two atoms (e.g. a diatomic molecule), the potential depends only on the distance between the two atoms $U(r_{12})$

The electron volt (eV) – energy unit convenient for description of atomic bonding

Electron volt - the energy lost / gained by an electron when it is taken through a potential difference of one volt.

$$E = q \times V$$

for $q = 1.6 \times 10^{-19}$ Coulombs and $V = 1$ volt

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

Types of Bonding

The electronic structure of atoms defines the character of their interaction among each other. Filled outer shells result in a stable configuration as in noble inert gases. Atoms with incomplete outer shells strive to reach this noble gas configuration by sharing or transferring electrons among each other for maximal stability. Strong “primary” bonding results from the electron sharing or transfer.

Primary bonding: e^- are transferred or shared, Strong (100-1000 KJ/mol or 1-10 eV/atom)

- Ionic: Strong Coulomb interaction among negative atoms (have an extra electron each) and positive atoms (lost an electron). Example - Na^+Cl^-
- Covalent: electrons are shared between the molecules, to saturate the valency. Example - H_2
- Metallic: the atoms are ionized, loosing some electrons from the valence band. Those electrons form a electron sea, which binds the charged nuclei in place

**Secondary Bonding: no e^- transferred or shared Interaction of atomic/molecular dipoles
, Weak ($< 100 \text{ KJ/mol}$ or $< 1 \text{ eV/atom}$)**

- Fluctuating Induced Dipole (inert gases, H_2 , Cl_2 ...)
- Permanent dipole bonds (polar molecules - H_2O , HCl ...)
- Polar molecule-induced dipole bonds (a polar molecule induces a dipole in a nearby nonpolar atom/molecule)

Ionic Bonding (I) Ionic Bonding is typical for elements that are situated at the horizontal extremities of the periodic table. Atoms from the left (metals) are ready to give up their valence electrons to the (non-metallic) atoms from the right that are happy to get one or a few electrons to acquire stable or noble gas electron configuration. As a result of this transfer mutual ionization occurs: atom that gives up electron(s) becomes positively charged ion (cation), atom that accepts electron(s) becomes negatively charged ion (anion).

Formation of ionic bond:

- Mutual ionization occurs by electron transfer (remember electronegativity table)
- Ion = charged atom
- Anion = negatively charged atom
- Cation = positively charged atom

2. Ions are attracted by strong coulombic interaction

Oppositely charged atoms attract each other

An ionic bond is non-directional (ions may be attracted to one another in any direction)

Example: table salt (NaCl)

Na has 11 electrons, 1 more than needed for a full outer shell (Neon)

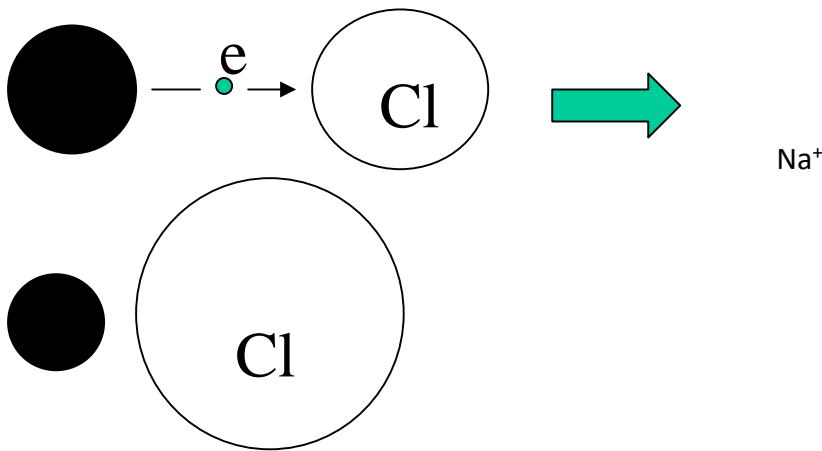
11 Protons Na $1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^1$

11 Protons Na⁺ $1\text{S}^2 2\text{S}^2 2\text{P}^6$ Donates e^- 10 e^- left

Chlorine has 17 electron, 1 more to complete the outer shell

17 Protons Cl $1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^2 3\text{P}^5$

17 Protons Cl⁻ $1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^2 3\text{P}^6$ Receives e^-

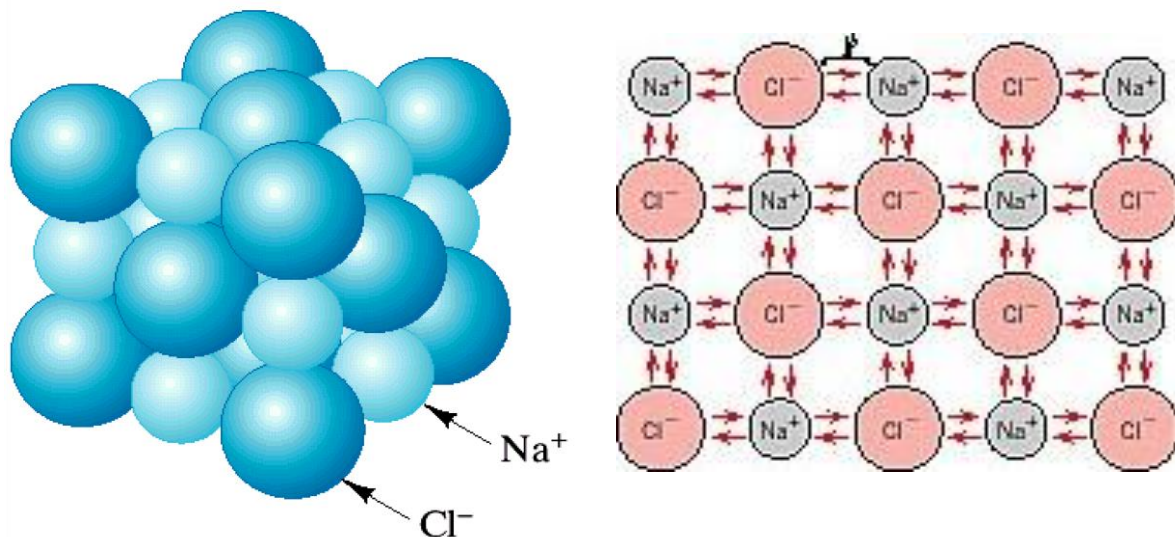


- Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable
- Note relative sizes of ions: Na shrinks and Cl expands

A strong electrostatic attraction between positively charged Na^+ ions and negatively charged Cl^- atoms along with $\text{Na}^+ - \text{Na}^+$ and $\text{Cl}^- - \text{Cl}^-$ repulsion result in the NaCl crystal structure which is arranged so that each sodium ion is surrounded by Cl^- ions and each Na^+ ion is surrounded by Cl^- ions, see the figure on the left.

Any mechanical force that tries to disturb the electrical balance in an ionic crystal meets strong resistance: ionic materials are strong and brittle. In some special cases, however, significant plastic deformation can be observed,

e.g. NaCl



Attractive coulomb interaction between charges of opposite sign:

$$U_A = \frac{1}{4\pi\epsilon_0} \times \frac{q_1 q_2}{r} = \frac{-A}{r}$$

Repulsion due to the overlap of electron clouds at close distances (Pauli principle of Quantum Mechanics)

$$U_B = \frac{B}{r^n}$$

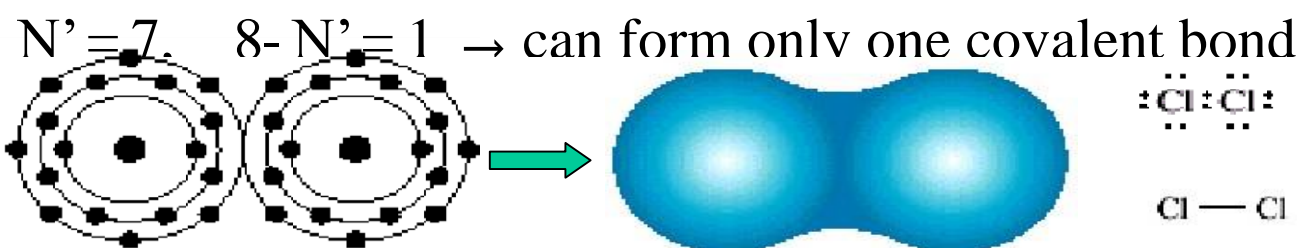
$$U = U_A + U_R = \frac{-A}{r} + \frac{B}{r^n}$$

In covalent bonding, electrons are shared between the molecules, to saturate the valency. In this case the electrons are not transferred as in the ionic bonding, but they are localized between the neighboring ions and form directional bond between them. The ions repel each other, but are attracted to the electrons that spend most of the time in between the ions.

Formation of covalent bonds:

- Cooperative sharing of valence electrons • Can be described by orbital overlap
- Covalent bonds are HIGHLY directional
- Bonds - in the direction of the greatest orbital overlap
- Covalent bond model: an atom can covalently bond with at most $8 - N'$, N' = number of valence electrons

Example: Cl_2 molecule. $Z_{\text{Cl}}=17$ ($1s^2 2s^2 2p^6 3s^2 3p^5$)

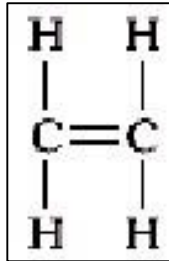


Covalent Bonding (II)

Example: Carbon materials. $Z_c = 6$ ($1S^2 2S^2 2P^2$) $N' = 4$, $8 - N' = 4 \rightarrow$ can form up to four covalent bonds

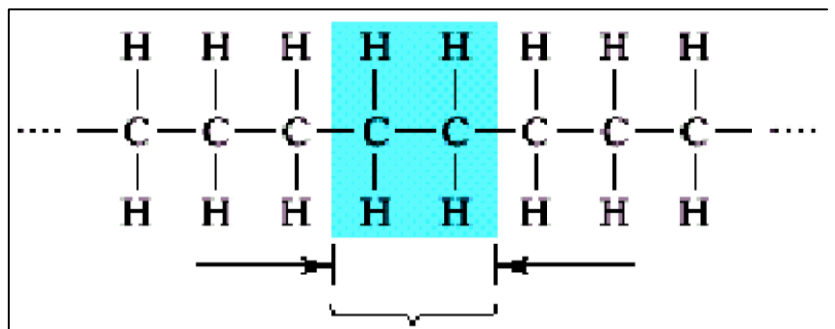
ethylene

molecule:



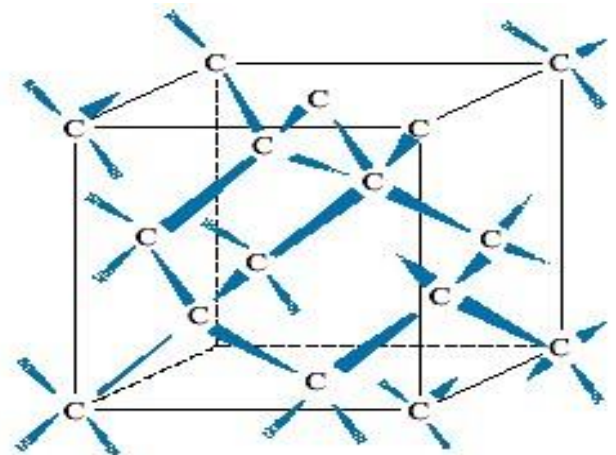
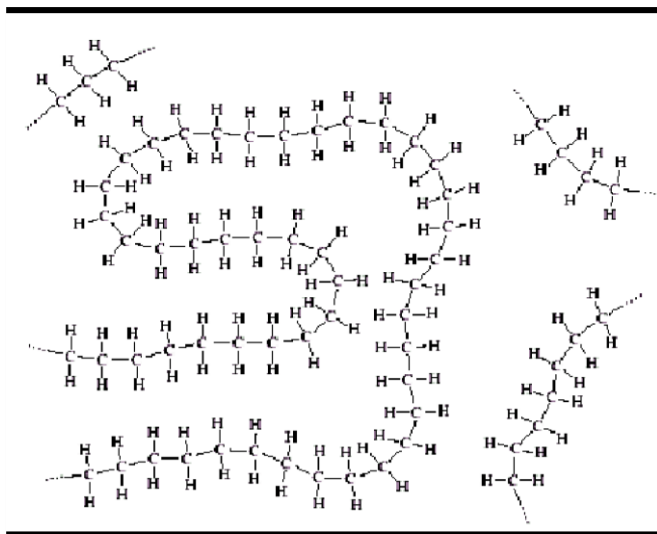
polyethylene

molecule:



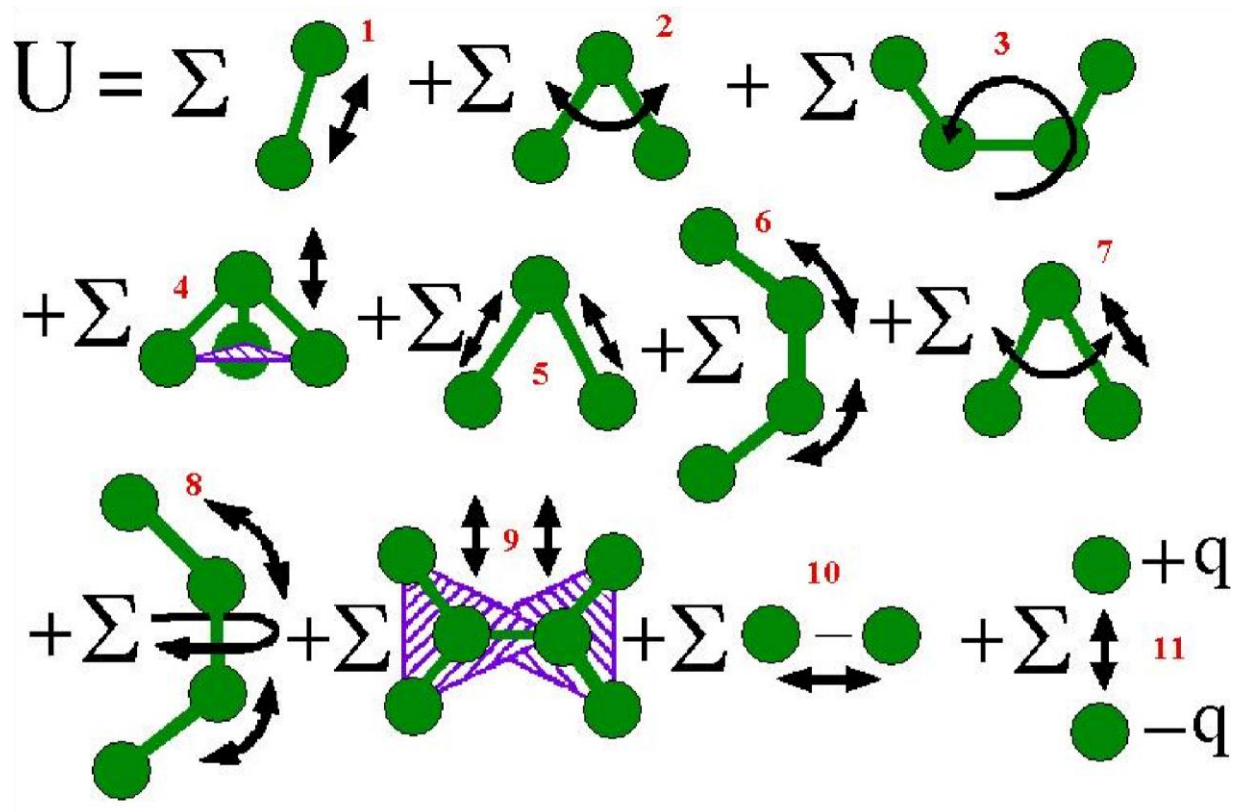
diamond:

(each C atom has four covalent bonds with four other carbon atoms)



2-D schematic of the "spaghetti-like" structure of solid polyethylene. The potential energy of a system of

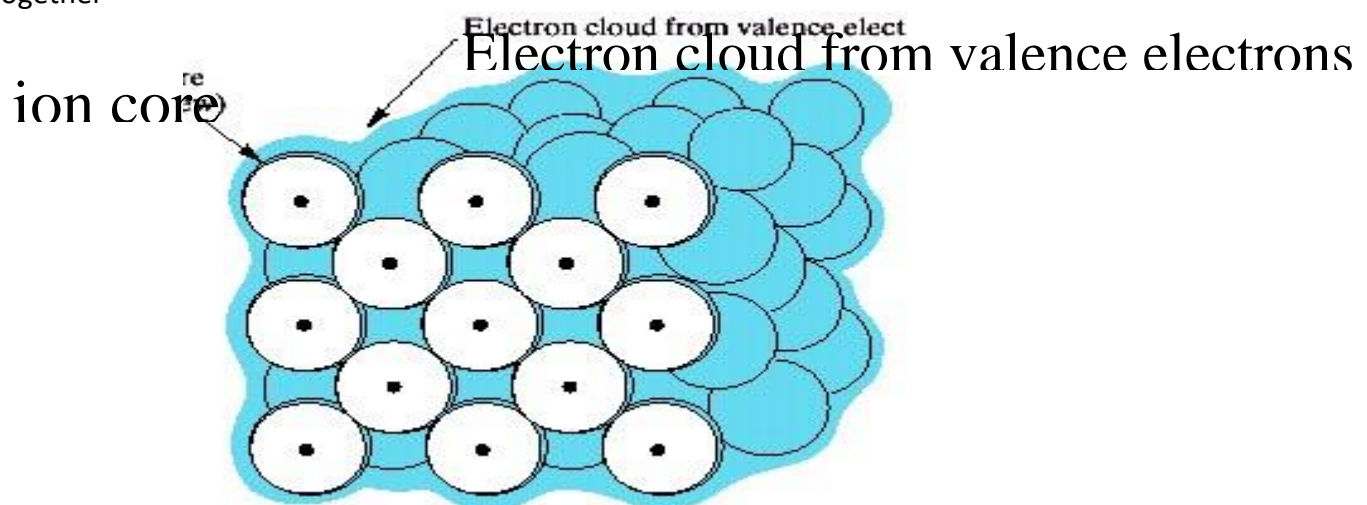
covalently interacting atoms depend not only on the distances between atoms, but also on angles between bonds...



Metallic Bonding

Valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the positive ions together.

- A metallic bond is non-directional (bonds form in any direction) → atoms pack closely together

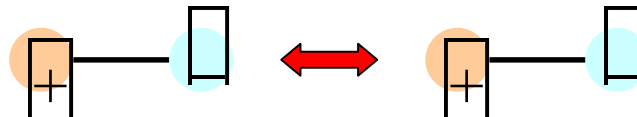


The “bonds” do not “break” when atoms are rearranged – metals can experience a significant degree of plastic deformation.

Examples of typical metallic bonding: Cu, Al, Au, Ag, etc. Transition metals (Fe, Ni, etc.) form mixed bonds that are comprising of metallic bonds and covalent bonds involving their 3d-electrons. As a result the transition metals are more brittle (less ductile) than Au or Cu.

Secondary Bonding

Secondary = van der Waals = physical (as opposite to chemical bonding that involves e^- transfer) bonding results from interaction of atomic or molecular dipoles and is weak, ~ 0.1 eV/atom or ~ 10 kJ/mol.

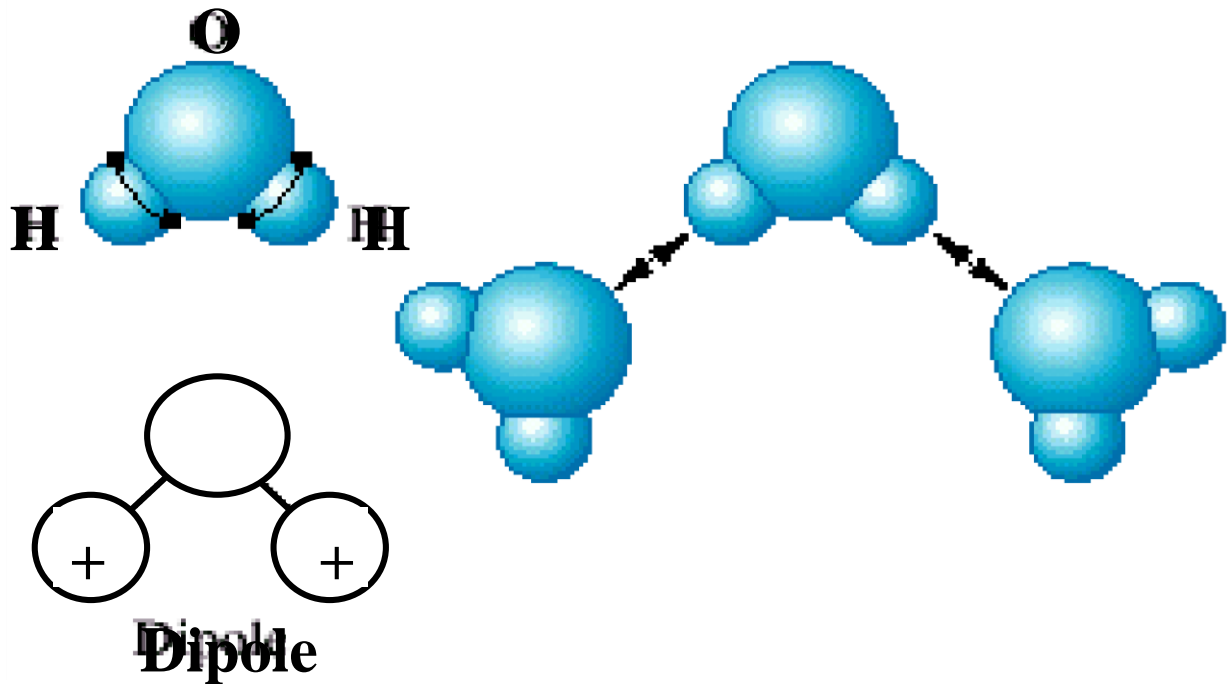


Permanent dipole moments exist in some molecules (called **polar molecules**) due to the asymmetrical arrangement of positively and negatively charged regions (HCl, H₂O). Bonds between adjacent polar molecules – **permanent dipole bonds** – are the strongest among secondary bonds.

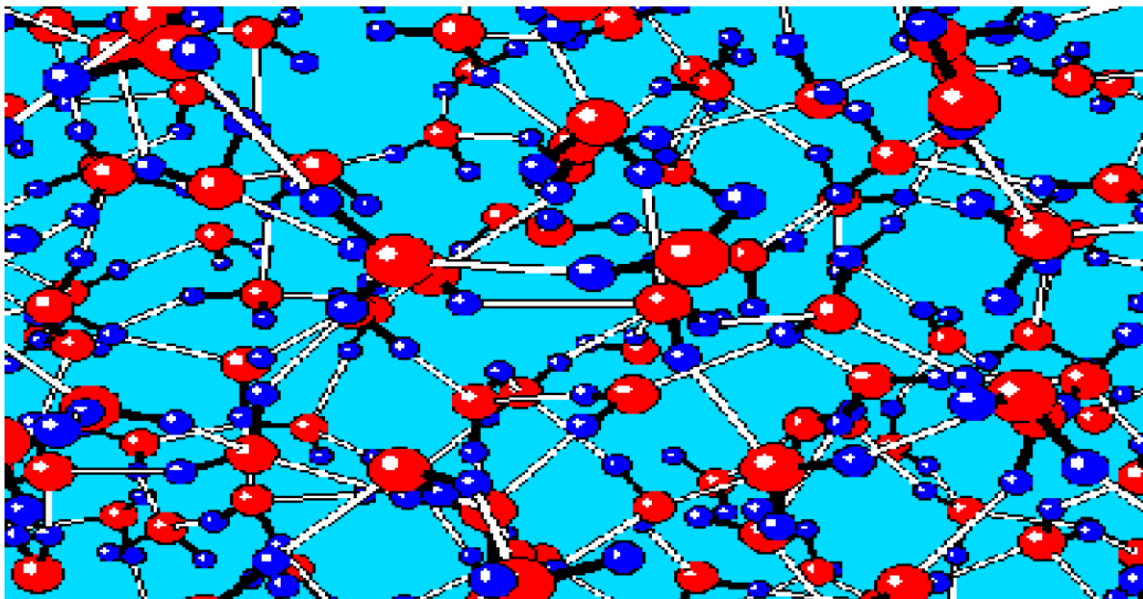
Polar molecules can induce dipoles in adjacent non-polar molecules and a bond is formed due to the attraction between the permanent and induced dipoles.

Even in electrically symmetric molecules/atoms an electric dipole can be created by fluctuations of electron density distribution. Fluctuating electric field in one atom A is felt by the electrons of an adjacent atom, and induces a dipole moment in this atom. This bond due to fluctuating induced dipoles is the weakest (inert gases, H₂, Cl₂).

Example: hydrogen bond in water. The H end of the molecule is positively charged and can bond to the negative side of another H₂O molecule (the O side of the H₂O dipole)

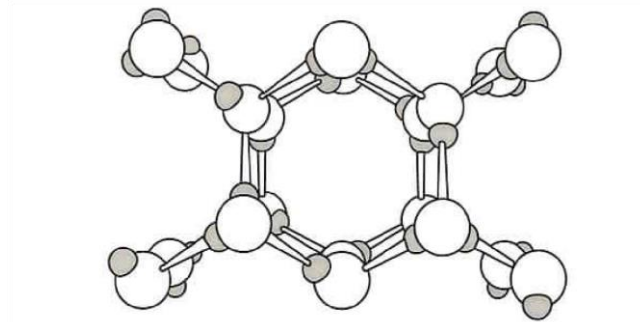


“Hydrogen bond” – secondary bond formed between two **permanent dipoles** in adjacent water molecules. Hydrogen bonding in liquid water from a molecular-level simulation

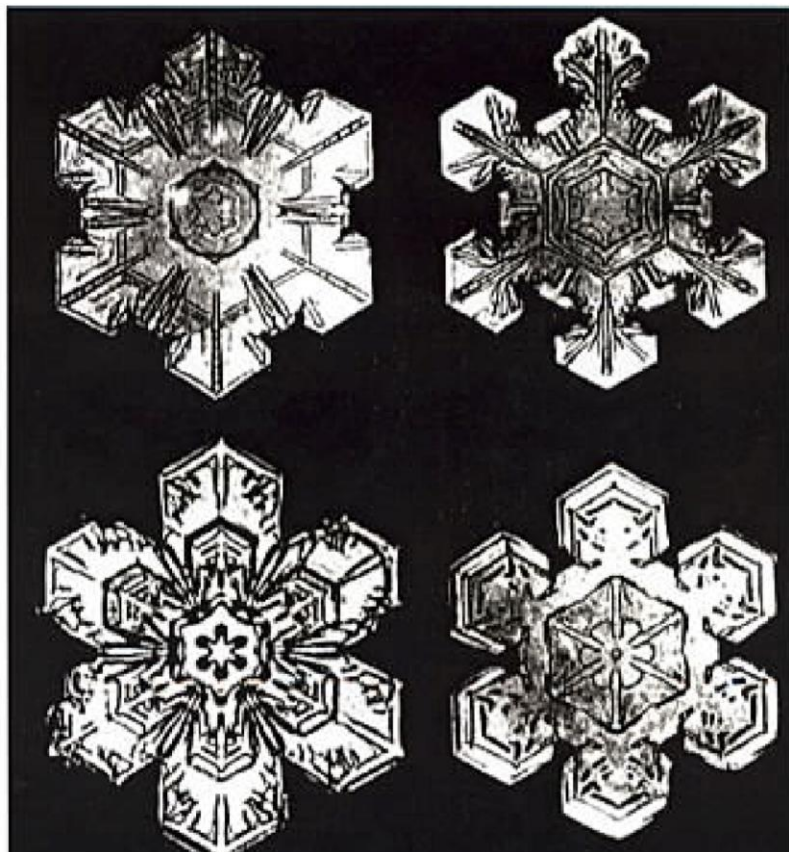


Molecules: Primary bonds inside, secondary bonds among each other

The Crystal Structures of Ice



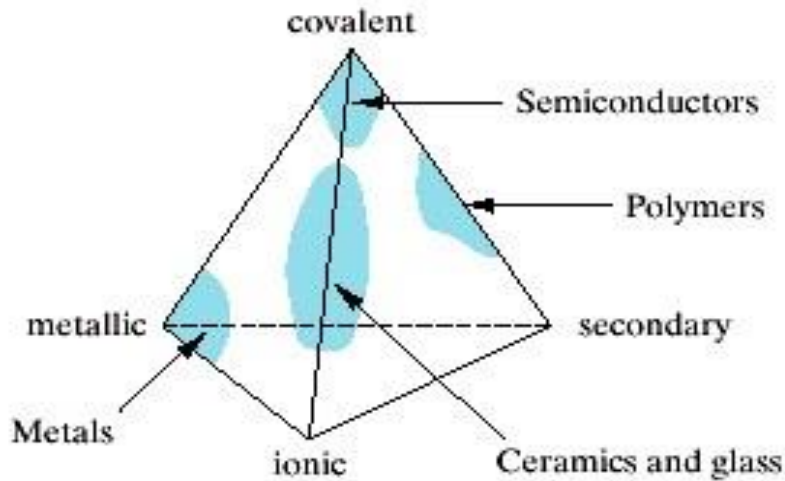
Hexagonal Symmetry of Ice Snowflakes



Figures by Paul R. Howell

Bonding in real materials

In many materials more than one type of bonding is involved (ionic and covalent in ceramics, covalent and secondary in polymers, covalent and ionic in semiconductors).



Examples of bonding in Materials:

Metals: Metallic

Ceramics: Ionic / Covalent

Polymers: Covalent and Secondary

Semiconductors: Covalent or Covalent / Ionic

Correlation between bonding energy and melting temperature

Table 2.3 Bonding Energies and Melting Temperatures for Various Substances

Bonding Type	Substance	Bonding Energy		Melting Temperature (°C)
		<i>kJ/mol (kcal/mol)</i>	<i>eV/Atom, Ion, Molecule</i>	
Ionic	NaCl	640 (153)	3.3	801
	MgO	1000 (239)	5.2	2800
Covalent	Si	450 (108)	4.7	1410
	C (diamond)	713 (170)	7.4	>3550
Metallic	Hg	68 (16)	0.7	-39
	Al	324 (77)	3.4	660
	Fe	406 (97)	4.2	1538
	W	849 (203)	8.8	3410
van der Waals	Ar	7.7 (1.8)	0.08	-189
	Cl ₂	31 (7.4)	0.32	-101
Hydrogen	NH ₃	35 (8.4)	0.36	-78
	H ₂ O	51 (12.2)	0.52	0