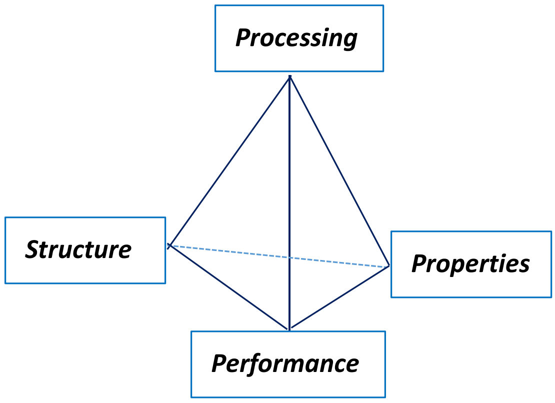
Chapter 1

1.Terms and concepts: Tetrahedron of Materials Science and Engineering



材料科学四面体

2.The development of materials: from the Stone Age to advanced materials, the timeline.

Stone Age(nature materials:stone,wood,clay,skins.etc) → Bronze Age →

Iron Age → Age of Advanced Materials(ceramic, semiconductors , polymers...)

3.What is Materials Science and Engineering? What are the four components of the tetrahedron of MSE?

MSE is the investigation of the relationships among processing, structure, properties, and performance of materials.

Four components: **Processing** → **Structure** → **Properties** → **Performance**

4.You need to be able to distinguish between natural materials and engineered materials.

Natural materials: From the nature,without processing.(stone,wood,clay,skins.etc)

Engineered materials :Synthetic material.(人工合成) (metal,plastics,glasses,fibers...)

5.Different scales: subatomic, atomic, microscopic, and macroscopic scales. Length scale unit conversion. Common sense of some length scale such as human hair, interatomic distance, etc.

Subatomic level :Electronic structure of individual atoms that defines interaction among atoms (interatomic bonding).

Atomic level :Arrangement of atoms in materials (for the same atoms can have different properties, e.g.two forms of carbon: graphite and diamond)

Microscopic structure :Arrangement of small grains of material that can be identified by microscopy.

Macroscopic structure :Structural elements that may be viewed with the naked eye.

Angstrom = 1Å = 1/10,000,000,000 meter = 10^{-10} m

Nanometer= 1 nm = 1/1,000,000,000 meter = 10^{-9} m

Micrometer = 1 mm = 1/1,000,000 meter = 10^{-6} m

Millimeter = 1 mm = 1/1,000 meter = 10^{-3} m

Interatomic distance ~ a few Å ;A human hair is ~ 50 mm ;Elongated bumps that make up the data track on CD are ~ 0.5 mm wide, minimum 0.83 mm long, and 125nm high

6.List at least six materials properties such as electrical property, optical property, etc, and what do they mean?

Mechanical properties（机械性能） – response to mechanical forces,strength, etc.

Electrical(电性能) and magnetic(磁性能) properties - response electrical and magnetic fields, conductivity, etc.

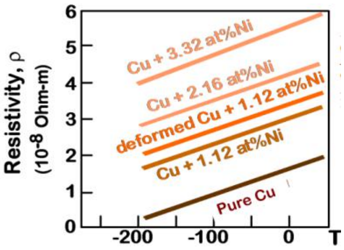
Thermal properties（热性能）-are related to transmission of heat and heat capacity.

Optical properties（光性能）-include to absorption, transmission and scattering of light.

Chemical stability（化学稳定性）-in contact with the environment -corrosion resistance.

7.For each materials property, I have included some figures in the lecture notes. You should be able to explain what can be inferred from reading those figures.

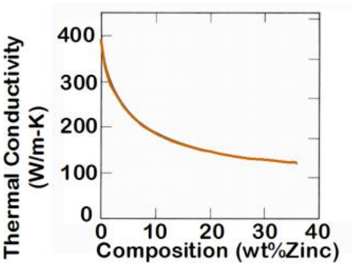
1.Electrical Resistivity of Copper:



Adding "impurity" atoms to Cu increases resistivity

Deforming Cu increases resistivity.

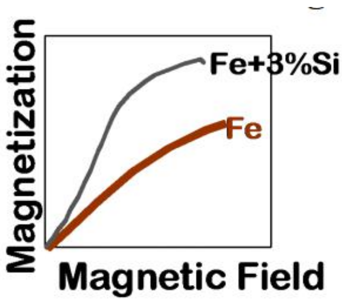
2.Thermal Conductivity of Copper:



It decreases when you add zinc!

(***Space Shuttle Tiles:***--Silica fiber insulation offers low heat conduction.)

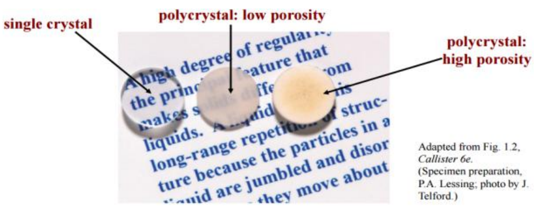
3.Magnetic Permeability vs. Composition:



Adding 3 atomic % Si makes Fe a better recording medium!

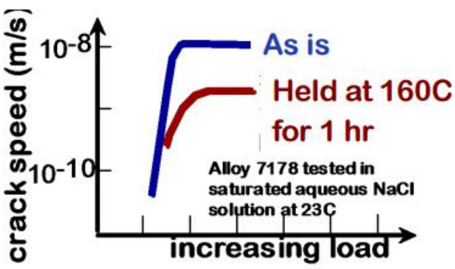
(***Magnetic Storage:***-Recording medium is magnetized by recording head)

4.Transmittance:



Aluminum oxide may be transparent, translucent, or opaque depending on the material structure.

5.Heat treatment:



slows crack speed in salt water!

8.List six different classifications of materials, i.e., types of materials and examples.

1.Metals :

- Iron and Steel
- Alloys and Superalloys (e.g. aerospace applications)
- Intermetallic Compounds (high-T structural materials)

2.Ceramics:

- Structural Ceramics (high-temperature load bearing)
- Refractories (corrosion-resistant, insulating)
- Whitewares (e.g. porcelains)
- Glass
- Electrical Ceramics (capacitors, insulators, transducers, etc.)
- Chemically Bonded Ceramics (e.g. cement and concrete)

3.*Polymers:*

- Plastics
- Liquid crystals
- Adhesives

4.Electronic Materials :

- Silicon and Germanium
- III-V Compounds (e.g. GaAs)
- Photonic materials (solid-state lasers, LEDs)

5.Composites:

- Particulate composites (small particles embedded in a different material)

• Laminate composites (golf club shafts, tennis rackets, Damaskus swords)

• Fiber reinforced composites (e.g. fiberglass)

6.Biomaterials:

• Man-made proteins (cytoskeletal protein rods or "artificial bacterium")

• Biosensors (Au-nanoparticles stabilized by encoded DNA for anthrax detection)

• Drug-delivery colloids (polymer based)

9.Cite the distinctive chemical or physical features of each class of materials.

1.Metals :Strong,ductile, conduct electricity and heat well, are shiny if polished.

2.Ceramics: Hard, brittle, insulators. (glass, porcelain)

3.Polymers: decompose at moderate temperatures(100~400oC), and are lightweight. (plastics, rubber)

4.Semiconductors : Their electrical properties depend strongly on minute proportions of contaminants。 (Si, Ge, GaAs)

5.Composites: Materials that are comprised of various parts; physical mixtures of two or more materials.Wood and Rock are natural composites,whereas concrete is a man-made (engineered) composite.

10.Standard materials selection process, i.e., what are the steps?

Pick application → properties → candidate materials → determine processing.

11.What are the future of Materials Science and Engineering? List several examples of future materials to be developed.

1.***Miniaturization :*** "Nanostructured" materials, with microstructure that has length scales between 1 and 100 nanometers with unusual properties. Electronic components,materials for quantum computing.

2.*Smart materials:* airplane wings that deice themselves,buildings that stabilize themselves in earthquakes…

3.*Environment-friendly materials:* biodegradable or photodegradable plastics, advances in nuclear waste processing, etc.

Chapter 2

1.Terms and Concepts: see summary of the chapter.

2.Understand the basic concepts: charges, masses, atomic weight, atomic mass,atomic mass unit, atomic number, mole, Avogadro's number, the number of atoms per cm3, their conversion and some simple calculations.

Atoms = nucleus + electrons

Nucleus = protons (+) + neutrons(-)

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

masses: Protons and Neutrons have the same mass, 1.67×10^{-27} kg.*(M_P=M_N)*

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

The atomic mass (A) = mass of protons (atomic number *(Z)*)+ mass of neutrons*(N)*

protons gives chemical identification of the element;

neutrons defines isotope number.

The atomic mass unit (amu): amu is often used to express **atomic weight**.

Mp ≈ Mn = 1.66 x 10-24 g = 1 amu=1/12 The atomic mass of the ^{12}C atom

*The atomic weight of an element :*The atomic weight of an element =weighted average of the atomic masses of the atoms naturally occurring isotopes.

$$\overline{A}_M = \sum_i f_{iM} A_{iM} \qquad \overline{A}_{(Si)} = f^{28}{}_{Si} A^{28}{}_{Si} + f^{29}{}_{Si} A^{29}{}_{Si} + f^{30}{}_{Si} A^{30}{}_{Si}$$ **(HW4-4)**

Atomic weight of carbon is 12.011 amu.

Mole:1amu=1g/mol

A mole of carbon has a mass of 12 grams.

The Avogadro's number: The number of atoms in a mole .

Nav = 6.023×10^{23}. Nav = 1 gram/1 amu.

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

The number of atoms per cm3, n, for material of density d (g/ cm3) and atomic mass M (g/mol): n= Nav×d / M L = $(1/n)^{1/3}$(distance between atoms)（**HW3-1，4**）

3.Name the two atomic models, and note the difference between them. What are the key assumptions in each model?

①BOHR ATOMIC MODEL:

Bohr made several postulates:

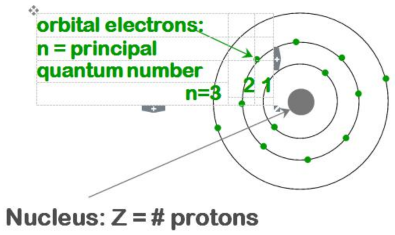
1.Electrons exist in certain stable, circular orbits about the nucleus.

(电子存在于围绕核的某些稳定的圆形轨道中。)

2.The electrons may shift to an orbits of higher or lower energy, thereby gaining or losing energy equal to the difference in energy levels. **hν= E2-E1**

(电子可以转移到更高或更低能量的轨道，从而获得等于能级差异的能量)

3.The angular momentum pθ of the electron in an orbit is always an integral multiple of h/2π.（轨道中电子的角动量 pθ总是 h/2π的整数倍）.（1 h/2π=1 ħ）



Nucleus: Z = # protons

= 1 for hydrogen to 94 for plutonium N = # neutrons

Energy of electrons are quantized（量化）：

Make quantum jump to change energy.

Higher energy (absorption of energy) ; Lower energy (emission of energy)（高吸低放）

Problems : 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.

（电子运动轨道不确定——是电子云形态）

Probability and Uncertainty Principle： probability density function

②Wave-Mechanical Model：

several postulates:

1.Electron is considered to exhibit both wavelike and particle-like characteristics.

（电子具有波状和颗粒状特性）

2.An electron is not treated as a particle moving in a discrete orbital, but rather, position is considered to be the probability of an electron's being at various locations around the nucleus.

（电子不被视为在离散轨道中移动的粒子，而是位置被认为是电子在核周围的各种位置的概率。）

3.Position is described by a probability distribution or electron cloud.

（位置由概率分布或电子云描述）

4.Know the important concepts associated with the two atomic models, such as quantum mechanics, quantum jump, energy level, energy state, finite energy, fuzzy orbits, probability density, probability distribution, electron cloud, etc.

5.Know how Schrodinger equation（薛定谔方程） is expressed and its physical meaning.

Schrodinger equation（薛定谔方程）： $\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}[E-V(x)]\psi(x)=0$

6.What do the four quantum numbers mean, i.e., n, l, ml, ms? Where did the four quantum numbers come from?

Principal quantum number n（主量子数）: n=1,2,3,4……（K,L,M,N……）

The angular quantum number l （角量子数）： l=0,1,2,3……n-1（s,p,d,f……）

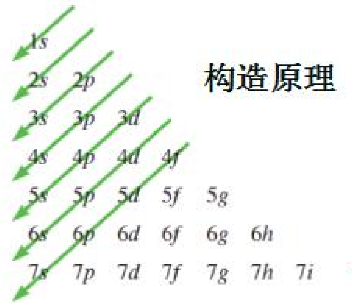
Magnetic quantum number ml（磁量子数）： ml=0,∓1，∓2，……∓l

Spin quantum number ms (自旋量子数）： ms=∓1/2

7.What is the Pauli Exclusion Principle?

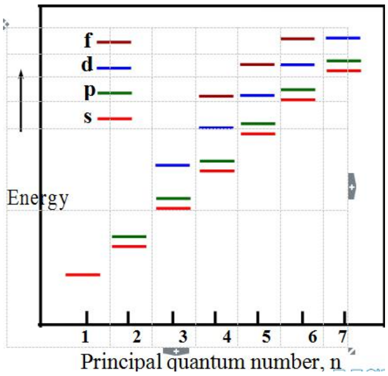
Pauli Exclusion Principle: only one electron can have a given set of the four quantum numbers.(同一原子中不能存在运动状态完全相同的电子，或者说同一原子中不能存在四个量子数完全相同的电子.)

8.What is the order of the subshell energy state? 1s, 2s, 2p, 3s, …



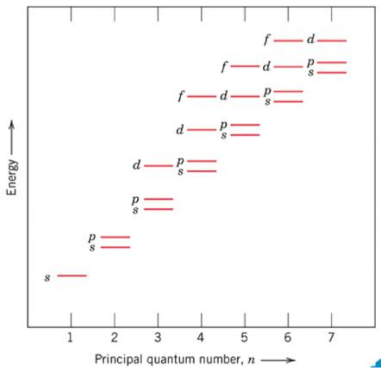
Principal Q. N., n	Subshells	Number of States	Number of Electrons Per Subshell	Per Shell
1 (l=0)	s	1	2	2
2 (l=0)	s	1	2	8
2 (l=1)	p	3	6	
3 (l=0)	s	1	2	18
3 (l=1)	p	3	6	
3 (l=2)	d	5	10	
4 (l=0)	s	1	2	32
4 (l=1)	p	3	6	
4 (l=2)	d	5	10	
4 (l=3)	f	7	14	

$2n^2$



•1s,2s, 2p,3s,3p,4s, 3d,4s,4p,5s,

4d,5p,6s,4f,…



•1s,2s, 2p,3s,3p,4s, 3d,4s,4p,5s,

4d,5p,6s,4f,…

9.What is the definition of valence electrons?

the valence electrons: Electrons that occupy the outermost filled shell.they are responsible for bonding.

10.You should be able to write down electron configuration of given elements.

(见附件）HW4-5 HW6-4

11.Features of the Periodic Table of Elements.

Materials of engineering interest are:

Polymers (based on carbon in Group 4B)

Ceramics (combinations of elements from Groups 1-5B and oxygen, carbon, or nitrogen)

Metallic materials (Groups 1 and 2, and transition metal elements)

12.Understand the concept of electronegativity and know how electronegativity varies with different columns of elements in the periodic table.

Electronegative ：→增强(得电子能力)(Electronegativity increases from left to right)

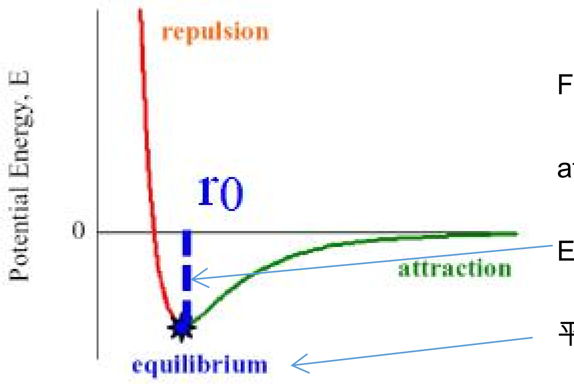
a measure of how willing atoms are to accept electrons

Subshells with one electron - low electronegativity

Subshells with one missing electron -high electronegativity

Metals are electropositive – they can give up their few valence electrons to become positively charged ions（金属正电性）

13.Schematically plot attractive, repulsive, and net energies versus interatomic separation for two atoms; note on this plot the equilibrium separation and the bonding energy.

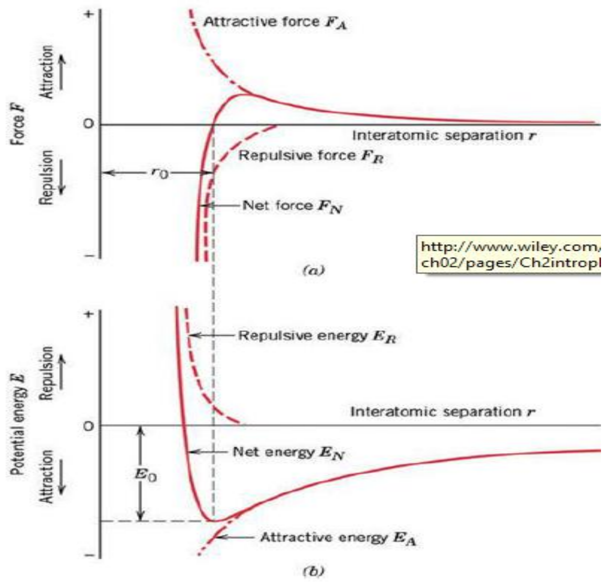


FN=FA+FR

at balance   FA+FR=0

E0 bonding energy

平衡态



$$E = \int F dr$$

$$E_N = \int_{\infty}^{r} F_N dr = \int_{\infty}^{r} F_A dr + \int_{\infty}^{r} F_R dr = E_A + E_R$$

14.What is electron volt? How is it converted to Joules?

Electron volt **:** volt 1 eV = 1.6 x 10-19 J

15.What are primary bonding types and what are secondary bonding types?

There are 4 important mechanisms by which atoms are bonded in engineering materials:

Metallic bonds   Covalent bonds   Ionic bonds   Van der Waals bonds

The first 3 types are strong and called ***primary bonds***. Van der Waals bonds are ***secondary bonds*** and weaker.

16.How is bonding energy associated with each type of bond?

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). eg.- Na^+ and Cl^- ***(transferred)***

Covalent: electrons are shared between the molecules, to saturate the valency. eg. - H_2 ***(shared)***

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 KJ/mol or < 1 eV/atom)

Fluctuating Induced Dipole bonds (inert gases, H_2, Cl_2…)振动诱导偶极键

Permanent dipole bonds (polar molecules - H_2O, HCl...)永久偶极键

Polar molecule-induced dipole bonds (a polar molecule like induce a dipole in a nearby nonpolar atom/molecule)极性分子诱导偶极键

17.Briefly describe ionic, covalent, metallic, hydrogen, and van der Waals bonds. This includes many pages from the lecture notes, so please read carefully and see if you understand the content.

Ionic Bonding　: transfer e-

Ion（离子） Anion（阴离子） Cation（阳离子）

1.Features of Ionic Bonding

Occurs between + and - ions.(正负离子间发生）

Requires electron transfer.（电子转移）

Large difference in electronegativity required.（大电负性差异）

Example: NaCl

2..$E=E_A+E_R= -K_A/r +K_B/r^n$

eg. NaCl:relative sizes of ions: Na shrinks and Cl expands(Na 缩 Cl 胀）

system of atoms, that is, electron transfer is energetically favorable

3.Ionic Bonding ↑→melting point（熔点）↑→Elastic Modulus（弹性模量 E）↑

→CTE（热膨胀系数）↓

4.constitute：金+非金

Covalent Bonding ：share e-

1.Features of Covalent Bonding

Cooperative sharing of valence electrons（价电子共享）

Can be described by orbital overlap（轨道重叠）

Covalent bonds are HIGHLY directional（高度定向）

Bonds - in the direction of the greatest orbital overlap（最大轨道重叠向）

Covalent bond model: an atom can covalently bond with at most 8-N’, N’ = number of valence electrons

2.eg.CH4(methane molecule) C2H4(ethylene molecule) Cl2 polyethylene molecule(聚乙烯） diamond（金刚石）

3.Constitute：

A.相同非金属元素分子（H2 Cl2 F2）

B.不同非金元素分子（CH4 H2O HNO3 HF）

C.元素固体（金刚石 硅 锗及周期表右手边元素组合的固化：GaAs InSb SiC）

Metallic Bonding :

1.Features of Metallic Bonding

Arises from a sea of donated valence electrons

Primary bond for metals and their alloys (金属及合金主键）

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

non-directional (bonds form in any direction) → atoms pack closely（非定向 密集）

2.Constitute：金属 or 合金

Secondary Bonding

1.Features of 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（范德华力 弱结合）

An electrical dipole exists whenever there is some separation of positive and negative portions of an atom or molecule.（正负分离，存在电偶极子）

The bonding results from coulombic attraction（结合力——库仑力吸引）

2.Classification

Fluctuating Induced Dipole bonds (inert gases, H_2, Cl_2…)振动诱导偶极键

Permanent dipole bonds (polar molecules - H_2O, HCl...)永久偶极键

Polar molecule-induced dipole bonds (a polar molecule like induce a dipole in a nearby nonpolar atom/molecule)极性分子诱导偶极键

3.Bonds between adjacent polar molecules strongest among secondary bonds.(相邻极性

分子键最强）

4.Hydrogen bond :HF H2O NH3

"Hydrogen bond" – secondary bond formed between two permanent dipoles in adjacent water molecules.在相邻水分子中的两个永久偶极子之间形成的第二键

Molecules: Primary bonds inside, secondary bonds among each other

18.What materials and materials class exhibit each of the bonding types? Remember only the typical ones.

19.What bonds are directional and what are non-directional?

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

20.What is a polar molecule?

polar molecules. : Permanent dipole moments exist in some molecules by virtue of an asymmetrical arrangement of positively and negatively charged regions; such molecules are termed polar molecules.（通过带正电荷和带负电荷的区域的不对称排列，在一些分子中存在永久偶极矩；这样的分子被称为极性分子。）HCl H2O

21.What does secondary bond include? What are the features of such secondary bonds?

22.What is hydrogen bond? Give an example.

(18.21.22 题见 17 题答案）

23.Table 2.3 should be important in terms of typical substances for each different bonding type.

Table 2.3 Bonding Energies and Melting Temperatures for Various Substances

Bonding Type	Substance	Bonding Energy kJ/mol (kcal/mol)	Bonding Energy eV/Atom, Ion, Molecule	Melting Temperature (°C)
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_2O	51 (12.2)	0.52	0

24.Relationship between bonding energy and melting temperature, elastic modulus, and coefficient of thermal expansion, and why?

Bonding energy↑→melting point（熔点）↑→Elastic Modulus（弹性模量 E）↑

→CTE（热膨胀系数）↓

Table 2.2 A Listing of the Expected Electron Configurations for Some of the Common Elements[a]

Element	*Symbol*	*Atomic Number*	*Electron Configuration*
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 2s^2 2p^6$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
Potassium	K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium	Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium	Sc	21	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
Titanium	Ti	22	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Vanadium	V	23	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
Chromium	Cr	24	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Manganese	Mn	25	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$
Iron	Fe	26	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
Cobalt	Co	27	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
Nickel	Ni	28	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
Copper	Cu	29	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
Zinc	Zn	30	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
Arsenic	As	33	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$
Selenium	Se	34	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$
Bromine	Br	35	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$
Krypton	Kr	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

[a] When some elements covalently bond, they form *sp* hybrid bonds. This is especially true for C, Si, and Ge.