

Introduction to Materials Science and Engineering

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Materials Science and Engineering

합금설계 + 공정조절 ➡ Microstructure Control of Materials



Better Material Properties



Atomic structure



Crystal structure

14 Bravais Lattice



- Only 14 different types of unit cells are required to describe all lattices using symmetry
- simple (1), body-centered (2), base-centered (2) face-centered (4 atoms/unit cell)

What is microstructure?

Microstructure originally meant the structure inside a material that could be observed with the aid of a microscope.

In contrast to the crystals that make up materials, which can be approximated as collections of atoms in specific packing arrangements (crystal structure), microstructure is the collection of defects in the materials.

What defects are we interested in?
 Interfaces (both grain boundaries and interphase boundaries), which are planar defects,
 Dislocations (and other line defects), and
 Point defects (such as interstititals and vacancies as well as solute atoms in solution)



Important!!!

Understanding and Controlling Phase Transformation of Materials

Phase Transformation

- Solidification: Liquid **Solid**
- Phase transformation in Solids
 - 1) Diffusion-controlled phase transformation ;

Generally long-distance atomic migration

- Precipitation transformation
- Eutectoid transformation ($S \implies S_1 + S_2$)

- etc.

2) Diffusionless transformation ;

Short-distance atomic migration

- Martensitic transformation

미세구조 조절: 2) Secondary phase control during solidification Phase Diagram of Iron-Carbon Alloy



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미세구조 조절: 2) Secondary phase control during solidification Equilibrium Phases of Iron-Carbon Alloy





Isothermal Transformation Diagram of a Eutectoid Iron-Carbon Alloy



➡ Phase Transformation 제어을 통한 microstructure의 조절 가능

Control of Phases by Heat Treatment



Control of Mechanical Properties by Proper Heat Treatment in Iron-Carbon Alloy



Martensite

Brittle

Tip of needle shape grain







Proper heat treatment (tempering)



Tempered martensite



Very small & spherical shape grain

Good strength, ductility, toughness





High performance materials

- High/low temperature
- High specific strength (strength/weight)
- High electrical performance
 - High/low dielectric, Ferroelectric, Superconductor
- Nano materials
- Bio-materials
- High performance coatings
- Structural materials
- Optical materials (LED, OLED, Fluorescent)
- Magnetic/Superconducting materials
- Materials are involved in everywhere.... You name it,...



Materials Design-for-Properties : "Alloyed Pleasure"

창의와 도전 - "미래를 여는 연금술사"

차시별 강의 계획									
회차	수업 일시 (강의 장소)	주제 또는 수업 내용	수강생 활동 및 활용자료						
1차	9월 3일(화) 17:00~18:30 33동 230호	금속, 인류의 역사와 함께하다! 역사 속 금속 이야기	수업자료						
2차	9월10일(화) 17:00~18:30 33동 230호	Alloying: Understanding the Basics	수업자료						
3차	9월17일(화) 17:00~18:30 33동 230호	분임 토의	팀 구성 및 각 도전주제 합금설계 브레인스토밍						
4차	9월24일(화) 17:00~18:30 33동 230호	각 팀별 연구계획발표	모든 팀원 협동 발표						
5차	10월15일(화) 17:00~18:30 33동 230호	각 팀별 합금 제조	모 원소 준비/ 아크 용해 주조 실험						
6차	10월29일(화) 17:00~18:30 33동 230호	제조 시편의 미세구조 분석 I	시편 전처리/ 광학현미경 관찰						
7차	10월30일(수) 17:00~18:30 33동 230호	제조 시편의 미세구조 분석 Ⅱ	전자현미경 관찰 실험						
8차	11월05일(화) 17:00~18:30 33동 230호	제조시편 기초 물성 분석	X-선 회절분석,경도 등실험						
9차	11월12일(화) 17:00~18:30 33동 230호	제조시편 타겟 물성 분석	타겟 물성 평가 실험 (강도, 연신 등)						
10차	11월26일(화) 17:00~18:30 33동 230호	최종연구결과 발표 및 토의	개발 합금의 미래첨단기술 적용 아이디어 제안 포함						

Schedule

- week 1 Introduction
- week 2 Atomic Structure and Interatomic Bonding (Chap. 2)
- week 3 Fundamentals of Crystallography (Chap. 3)
- week 4 The Structure of Crystalline Solids (Chap. 4)
- week 5 Imperfections in Solids (Chap. 6)
- week 6 Diffusion (Chap. 7) & Mid-term
- week 7 Mechanical Properties of Metals (Chap. 8)
- week 8 Dislocations and Strengthening Mechanisms (Chap. 9)
- week 9 Failure (Chap. 10)
- week 10 Phase Diagram (Chap. 11)
- week 11 Phase Transformation (Chap. 12)
- week 12 Polymer Structures (Chap. 5)
- week 13 Characteristics, Applications, and Processing of Polymers (Chap. 15)
- week 14 Functional Polymers (Chap. 16)
- week 15 Presentation of Team project and Final Exam

CHAPTER 2: BONDING AND PROPERTIES

ISSUES TO ADDRESS...

- What promotes bonding?
- What types of bonds are there?
- What properties are inferred from bonding?

Contents for today's class

Atomic Structure

2.2 Fundamental concepts

2.3 Electrons in atoms

: atomic models, Quantum #s, Electron configurations

2.4 Periodic table

Atomic Structure (Freshman Chem.)

- atom electrons 9.11 x 10⁻³¹ kg protons neutrons $\left. \right\}$ 1.67 x 10⁻²⁷ kg
- atomic number = # of protons in nucleus of atom (Z)
 = # of electrons of neutral species (N)
- <u>atomic mass</u> unit (A \approx Z+N) = amu = 1/12 mass of ¹²C

Atomic wt = wt of 6.023×10^{23} molecules or atoms

1 amu/atom = 1g/mol

- C 12.011 A H 1.008 A Fe 55.85 amu/atom = **55.85 g/mol** etc.
- isotope same Z, but different N: two or more different A 24

Atomic Structure

- Valence electrons determine following properties
 - 1) Chemical
 - 2) Electrical
 - 3) Thermal
 - 4) Optical
 - 5) Mechanical

Fundamental Concepts

- Atomic Bonding
- It involves the <u>transfer or sharing of electrons</u> between atoms, resulting in electrostatic or mutual attractions.



atomic structures & electronic configurations are important ingredients to understanding bonding.

Fundamental Concepts

Two fundamental types of bonding:

□ primary bonds: strong atom-to-atom attractions produced by <u>changes in</u> <u>electron position of the valence e⁻</u>. *Example : covalent atom between two hydrogen atoms*

strong intramolecular covalent bond

□ secondary bonds: much weaker. It is the attraction due to overall "electric fields", often resulting from electron transfer in primary bonds. *Example: intramolecular bond between* H_2 *molecules* → gas



Fundamental Concepts



Chapter 2.3 고전역학 vs 양자역학 (quantum mechanics: 원자와 원자내 개체거동을 지배)

Early atomic model

- > 1858 : <u>cathode ray</u> identified by Pluker
- > 1869 : <u>negative charge of cathode ray</u> identified by Hittorf
- > 1874 : <u>momentum of cathode ray</u> detected by Crookes
- > 1876 : <u>cathode ray named</u> by Goldstein
- > 1890 : <u>electron named</u> by Stony
- > 1897 : properties of cathode ray → particle-like electron by J. J. Thomson



1958

Louis-Victor Broglie Photoelec



Photoelectric effect – particle Diffraction – wave like



(1895-1975), Nobel Prize in 1937



(1856-1940), Nobel Prize in 1897

Sir George Paget Thomson

Thomson, Sir Joseph John

Bohr Atom:

전자는 <u>정해진 궤도</u>를 가지고 원자주위를 돌고 있다고 가정 (원자내 전자의 위치_'전자궤도'와 에너지_'양자화된 에너지 수준'을 설명)



Atomic mass $A \sim Z + N$

Atomic structure of sodium (Na)



Bohr Atom

- electrons & protons are electrically charged: 1.60 x 10⁻¹⁹ C (기본전하)
- mass-proton = mass-neutron = $1.67 \times 10^{-27} \text{ kg}$
- mass-electron = $9.11 \times 10^{-31} \text{ kg}$
- atomic number (Z) = # protons
- atomic mass (A) = mass-protons (Z) + mass-neutrons (N)
- # of protons: same for all atoms of an element
- # of neutrons is variable ⇒ "isotopes" (elements with 2 or more atomic masses)
- atomic weight = weighted average of the atom's isotopes
- the atomic weight of an element may be specified as mass/mole of material
 - 1 amu = 1/12 atomic mass of carbon 12 (¹²C)
 - 1 mole = 6.023×10^{23} (Avogadro's number) atoms or molecules
 - 1 amu/atom (or molecule) = 1 g/mol

Limitations in Bohr's model

... Classic mechanical theory was employed ...

mr

... What if there are more than two electrons ? ...

... Quantum condition fails ...

Self-contradiction in terms of Heisenberg uncertainty principle ...



ke

$$(\Delta p)(\Delta x) \ge \frac{h}{4\pi}$$

- ✓ Circumferential motion of charged particles should emit <u>EM wave</u>
- Discontinuous emission spectra cannot be understood

Bohr's model + Wave-mechanical model

To resolve the discontinuous emission spectra...

... Therefore, in discussing the motion of an electron of known energy or momentum about a nucleus, it is necessary to speak only in terms of <u>the probability of finding that electron at any particular position</u> ...
(파동역학모델: 전자는 파동성과 입자성을 동시에 갖는다 가정, 전자 = 입자 → 전자의 위치 확률분포 혹은 전자구름)





Electron position is described by a probability distribution or electron cloud Bohr energy levels to be separated into electron subshells described by quantum numbers

Orbital concept

Imagine & take a picture of an electron confined in an atom with single room for it ...



Electronic Structure

- Electrons have wavelike and particulate properties. (원자의 모든 전자는 양자수 (quantum #)라고 하는 4개의 숫자로 정의)
 - This means that electrons are in orbitals defined by a probability.
 - Each orbital at discrete energy level determined by quantum numbers.

<u>Quantum #</u>	<u>Designation</u>
<i>n</i> = principal (energy level-shell)	K, L, M, N, O (1, 2, 3, etc.)
<pre>e = subsidiary (orbitals)</pre>	s, p, d, f (0, 1, 2, 3,, n-1)
m_l = magnetic	1, 3, 5, 7 (- <i>ℓ</i> to + <i>ℓ</i>)
$m_{\rm s}$ = spin	1/2, -1/2

Quantum numbers (양자수)

- *n* principal quantum number 1, 2, 3, 4, --- (K, L, M, N, ---)
 - Determines the effective volume of an electron orbital
 - Distance of an electron from the nucleus, position of an electron
- *l* Angular (azimuthal) quantum number 0, 1, 2, 3, 4, ---, (n-1) (s, p, d, f)
 - Determines the angular momentum of the electron
 - Shape of electron subshell, shape of electron distribution
- m_l magnetic quantum number 0, ±1, ±2, ---, ±1
 - Determines the orientation of the orbital
- m_s spin quantum number $\frac{1}{2}, -\frac{1}{2}$
- Pauli exclusion principle (파울리의 배타원리: 하나의 준위에 최대 스핀방향이 다른 2개 이하의 전자포함)
 - No two interacting entities can have the same set of the quantum numbers ...

→ Each orbital will hold up to two electrons There can never be more than one electron in the same quantum state

- Only one electron can be in a particular quantum state at a given time
- Each electron state cannot hold more than two electrons with opposite spins

Meaning of quantum numbers

n determines the size *l* determines the shape m_l determines the orientation



3-dimensional view of electron orbitals



Additional quantum number



Electron spin : $m_s = \pm \frac{\hbar}{2}$

Therefore, complete description of an electron requires <u>4 quantum numbers</u>

Pauli exclusion principle

... No two interacting entities can have the same set of the quantum # ...

 \rightarrow Each orbital will hold up to two electrons

Electron Configurations (원자의 전자배위 혹은 전자구조)

- Valence electrons those in unfilled shells
- Filled shells more stable
- Valence electrons (원자가전자) are most available for bonding and tend to control the chemical properties

– example: C (atomic number = 6)



Electron Energy States

Electrons...

- have discrete energy states
- tend to occupy lowest available energy state.



Electronic Configurations ex: Fe - atomic # = 26 $1s^2$ $2s^2 2p^6$ $3s^2 3p^6$ $3d^{6} 4s^{2}$ valence *N*-shell n = 4**4***p* electrons 3*d* **4**s 3p 3s *M*-shell n = 3Energy Adapted from Fig. 2.4, Callister 7e. 2*p L*-shell n = 22s **1**s K-shell n = 1

The complete set of quantum numbers for each of the 11 electrons in sodium

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Stable Electron Configurations

• Stable electron configurations...

have complete s and p subshells

- tend to be non-reactive (불활성).

- **Z** Element Configuration
- 2 He 1s²
- 10 Ne $1s^22s^22p^6$
- 18 Ar 1s²2s²2p⁶3s²3p⁶
- $36 \quad \text{Kr} \qquad 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

 $1s^{1}$ 1*s*² $2s^{1}$ $2s^2$ S $2p^{I}$ Ś $2p^6$ $3s^1$ $3s^2$ S 4f *4d 3p 4s 3d 4p*

SURVEY OF ELEMENTS

• Most elements: Electron configuration not stable.

<u>Element</u>	<u>Atomic #</u>	Electron configuration	
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	Adapted from Table 2.2,
Carbon	6	1s ² 2s ² 2p ²	Callister 7e.
Neon	10	1s ² 2s ² 2p ⁶ (sta	able)
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 ¹	$^{0}4s^{2}4p^{6}$ (stable)

• Why? Valence (outer) shell usually not filled completely.

Chapter 2.4 모든 원소는 주기율표 상의 전자 배위에 의해 분류

Periodic Table of the Elements



	(Ce 58	Pr 59	Nd 60	Pm 61	Sm 62	Eu 63	Gd 64	Tb 65	Dy 66	Ho 67	Er 68	Tm 69	Yb 70	Lu 71
Lanthanide series 6		Cerium 140,116	Praseodymium 140,90765	Neodymium 144,24	Promethium (145P	Samarium 150,4	Europium 151,964	Gadolinium 157,25	Terbium 158,92534	Dysprosium 162,50	Holmium 164,93032	Erbium 167.26	Thulium 168,9342	Ytterbium 173.04	Lutetium 174,97
	4	115d16s2	4136s2	4f ⁴ 6s ²	41 ⁵ 6s ²	4166s ²	4f ⁷ 6s ²	4f75d16s2	4196s ²	4f106s2	4f ¹¹ 6s ²	4f126s2	4f136s2	4f ¹⁴ 6s ²	4f145d16s2
	1	Γh 90	Pa 91	U 92	Np 93	Pu 94	Am 95	Cm 96	Bk 97	Cf 98	Es 99	Fm 100	Md 101	NO 102	Lr 103
Actinide series ** 7		Thorium 232,0381b	Protactinium 231,03588	Uranium 238,02891	Neptunium (237)	Plutonium (244)	Americium (243)	Curium (247) ^a	Berkelium (247)	Californium (251) ⁸	Einsteinium (251)	Fermium (257)	Mendelevium (258)	Nobelium (259)	Lawrencium (262)
		6d ² 7s ²	5f26d17s2	5f36d17s2	5f46d17s2	5f ⁶ 7s ²	5f77s2	5t76d17s2	5f ⁹ 7s ²	5f107s2	5f ¹¹ 7s ²	5f127s2	51137s2	5f ¹⁴ 7s ²	5f146d17s2

Inner transition elements

Chapter 2.4 The Periodic Table

• **Columns**: Similar Valence Structure_비슷한 화학적 물리적 특성



Electronegativity (전기음성도)

- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.



Smaller electronegativity



Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

Contents for today's class

Atomic Structure

2.2 Fundamental concepts

 atom – electrons – 9.11 x 10⁻³¹ kg protons neutrons } 1.67 x 10⁻²⁷ kg

2.3 Electrons in atoms

a. atomic models

Bohr's model + Wave-mechanical model 전자는 파동성과 입자성을 동시에 갖는다 가정= 전자구름

b. Quantum #s



c. Electron configurations

2.4 Periodic table

모든 원소는 주기율표 상의 전자 배위에 의해 분류 : 특성의 규칙적인 변화 양상 확인 가능

