Introduction to Materials Science and Engineering 2020

Lecture title: Introduction to Materials Science and Engineering

교과목명: 재료공학원리

Course Code (교과목번호): 445.102A Lecture number (강좌번호): 002

Professor: Park, Eun Soo (박은수)

Office (연구실): 33동 313호

Office ☎ (연락처): 02-880-7221

e-mail (전자우편): espark@snu.ac.kr

Class hour(강의시간): Tuesday, Thursday 12:30 – 13: 45

Lecture room (강의실): Zoom 이용 실시간 비대면 수업

Lecture homepage (강좌관련 홈페이지): *http://etl.snu.ac.kr/*

Office hour(면담시간) : By appointment via email

☐ Textbook and references

Main textbook: William D. Calister, Jr., David G. Rethwisch

“Materials Science and Engineering”, ISBN: 978-1-118-31922-2

9th edition SI Version, John Wiley & Sons Inc., 2014

References: J.F. Shackelford, “Introduction to Materials Science for Engineers”

8th edition, Prentice Hall Inc., 2016

☐ Grade

- Relative grading ((A+B) 70%, (C) 20%, (D-F) 10%)
- Midterm(35%), Final exam (40 %),
- Homework and team project (15%) and Attendance (10 %)
- Note: 1) The weight of each component above could be adjusted up to 5% based on students’ performance. 2) Student who retakes this course will have their final scores adjusted downward by 10% in order to ensure fairness with other students.

“2020년 2학기부터 입학 후 두 번째 등록학기에 수강하는 학생과 그 이후에 처음 수강하는 학생은 별도로 평가할 수 있다”

Schedule

week 1 *Introduction & Atomic Structure and Interatomic Bonding* (Chap.1 & Chap. 2)

week 2 *Fundamentals of Crystallography* (Chap. 3)

week 3 *The Structure of Crystalline Solids* (Chap. 4)

week 4 *Polymer Structures* (Chap. 5)

week 5 *Imperfections in Solids* (Chap. 6)

week 6 *Diffusion* (Chap. 7) & *Mid-term (Face-to-face examination)*

week 7 *Mechanical Properties of Metals* (Chap. 8)

week 8 *Dislocations and Strengthening Mechanisms* (Chap. 9)

week 9 *Failure* (Chap. 10)

week 10 *Phase Diagrams* (Chap. 11)

week 11 *Phase Transformations* (Chap. 12)

week 12 *Properties and Application of Metals & Ceramics* (Chap. 13 & Chap. 14)

week 13 *Properties and Application of Polymers* (Chap. 15)

week 14 *Composite Materials* (Chap. 16)

week 15 *Fabrication and Processing of Eng. Mater*. (Chap. 17) *&*
Final Exam (Face-to-face examination)

Why do I need to study materials?

1. To graduate ㅜ.ㅜ 
2. Professor Park is known to be generous on the grade.
3. To conserve professor's job….
4. Not many class I can take….
5. My girl friend is taking this class …
6. I want to develop new materials…..
7. My parents suggested to take this course…..
8. This is the start of my challenge to the universe…

What are Materials?

- **That’s easy! Look around.**
- Our clothes are made of materials, our homes are made of materials - mostly manufactured. Glass windows, vinyl siding, metal silverware, ceramic dishes…
- **Most things are made from many different kinds of materials.**

Periodic Table of the Elements

KCS 대한화학회
KOREAN CHEMICAL SOCIETY
화학이 지구를 더 푸르게

Current ACS and IUPAC preferred.

[a]Mass number of most stable or best-known isotope
[b]Mass of the isotope of longest half-life

Symbol	**O**
Atomic number	8
Name	Oxygen
Atomic weight	15.9994
Electron arrangement	$2S^22P^4$

Atomic weights are based on carbon-12. Atomic weights in parentheses indicate the most stable or best-known isotope.

← Transition elements →

Period	1 (IA)	2 (IIA)	3 (IIIB)	4 (IVB)	5 (VB)	6 (VIB)	7 (VIIB)	8	9 (VIIIB)	10	11 (IB)	12 (IIB)	13 (IIIA)	14 (IVA)	15 (VA)	16 (VIA)	17 (VIIA)	18 (VIIIA)
1	🟨 **H** 1 Hydrogen 1.00794 $1s^1$																	🟨 **He** 2 Helium 4.002602 $1s^2$
2	🟦 **Li** 3 Lithium 6.941 $2s^1$	🟦 **Be** 4 Beryllium 9.01218 $2s^2$											🟧 **B** 5 Boron 10.81 $2s^22p^1$	🟨 **C** 6 Carbon 12.011 $2s^22p^2$	🟨 **N** 7 Nitrogen 14.0067 $2s^22p^3$	🟨 **O** 8 Oxygen 15.9994 $2s^22p^4$	🟨 **F** 9 Fluorine 18.99840 $2s^22p^5$	🟨 **Ne** 10 Neon 21.1797 $2s^22p^6$
3	🟦 **Na** 11 Sodium 22.98977 $3s^1$	🟦 **Mg** 12 Magnesium 24.305 $3s^2$											🟦 **Al** 13 Aluminum 26.98154 $3s^23p^1$	🟧 **Si** 14 Silicon 28.086 $3s^23p^2$	🟨 **P** 15 Phosphorus 30.97376 $3s^23p^3$	🟨 **S** 16 Sulfur 32.06 $3s^23p^4$	🟨 **Cl** 17 Chlorine 35.453 $3s^23p^5$	🟨 **Ar** 18 Argon 39.948 $3s^23p^6$
4	🟦 **K** 19 Potassium 39.098 $4s^1$	🟦 **Ca** 20 Calcium 40.08 $4s^2$	🟦 **Sc** 21 Scandium 44.9559 $3d^14s^2$	🟦 **Ti** 22 Titanium 47.90 $3d^24s^2$	🟦 **V** 23 Vanadium 50.9415 $3d^34s^2$	🟦 **Cr** 24 Chromium 51.996 $3d^54s^1$	🟦 **Mn** 25 Manganese 54.9380 $3d^54s^2$	🟦 **Fe** 26 Iron 55.845 $3d^64s^2$	🟦 **Co** 27 Cobalt 58.9332 $3d^74s^2$	🟦 **Ni** 28 Nickel 58.69 $3d^84s^2$	🟦 **Cu** 29 Copper 63.546 $3d^{10}4s^1$	🟦 **Zn** 30 Zinc 65.409 $3d^{10}4s^2$	🟦 **Ga** 31 Gallium 69.72 $3d^{10}4s^24p^1$	🟧 **Ge** 32 Germanium 72.61 $3d^{10}4s^24p^2$	🟧 **As** 33 Arsenic 74.9216 $3d^{10}4s^24p^3$	🟨 **Se** 34 Selenium 78.96 $3d^{10}4s^24p^4$	🟨 **Br** 35 Bromine 79.904 $3d^{10}4s^24p^5$	🟨 **Kr** 36 Krypton 83.80 $3d^{10}4s^24p^6$
5	🟦 **Rb** 37 Rubidium 85.4678 $5s^1$	🟦 **Sr** 38 Strontium 87.62 $5s^2$	🟦 **Y** 39 Yttrium 88.9059 $4d^15s^2$	🟦 **Zr** 40 Zirconium 91.22 $4d^25s^2$	🟦 **Nb** 41 Niobium 92.9064 $4d^45s^1$	🟦 **Mo** 42 Molybdenum 95.94 $4d^55s^1$	🟦 **Tc** 43 Technetium 98.9062[b] $4d^55s^2$	🟦 **Ru** 44 Ruthenium 101.07 $4d^75s^1$	🟦 **Rh** 45 Rhodium 102.9055 $4d^85s^1$	🟦 **Pd** 46 Palladium 106.4 $4d^{10}$	🟦 **Ag** 47 Silver 107.868 $4d^{10}5s^1$	🟦 **Cd** 48 Cadmium 112.411 $4d^{10}5s^2$	🟦 **In** 49 Indium 114.82 $4d^{10}5s^25p^1$	🟦 **Sn** 50 Tin 118.71 $4d^{10}5s^25p^2$	🟧 **Sb** 51 Antimony 121.760 $4d^{10}5s^25p^3$	🟧 **Te** 52 Tellurium 127.60 $4d^{10}5s^25p^4$	🟨 **I** 53 Iodine 126.9045 $4d^{10}5s^25p^5$	🟨 **Xe** 54 Xenon 131.293 $4d^{10}5s^25p^6$
6	🟦 **Cs** 55 Cesium 132.9054 $6s^1$	🟦 **Ba** 56 Barium 137.327 $6s^2$	🟦 **La*** 57 Lanthanum 138.9055 $5d^16s^2$	🟦 **Hf** 72 Hafnium 178.49 $4f^{14}5d^26s^2$	🟦 **Ta** 73 Tantalum 180.9479 $4f^{14}5d^36s^2$	🟦 **W** 74 Tungsten 183.84 $4f^{14}5d^46s^2$	🟦 **Re** 75 Rhenium 186.2 $4f^{14}5d^56s^2$	🟦 **Os** 76 Osmium 190.2 $4f^{14}5d^66s^2$	🟦 **Ir** 77 Iridium 192.22 $4f^{14}5d^76s^2$	🟦 **Pt** 78 Platinum 195.078 $4f^{14}5d^96s^1$	🟦 **Au** 79 Gold 196.9665 $4f^{14}5d^{10}6s^1$	🟦 **Hg** 80 Mercury 200.59 $4f^{14}5d^{10}6s^2$	🟦 **Tl** 81 Thallium 204.3833 $4f^{14}5d^{10}6s^26p^1$	🟦 **Pb** 82 Lead 207.2 $4f^{14}5d^{10}6s^26p^2$	🟦 **Bi** 83 Bismuth 208.9804 $4f^{14}5d^{10}6s^26p^3$	🟧 **Po** 84 Polonium (210)[a] $4f^{14}5d^{10}6s^26p^4$	🟨 **At** 85 Astatine (210)[a] $4f^{14}5d^{10}6s^26p^5$	🟨 **Rn** 86 Radon (222)[a] $4f^{14}5d^{10}6s^26p^6$
7	🟦 **Fr** 87 Francium (223)[a] $7s^1$	🟦 **Ra** 88 Radium 226.0254[b] $7s^2$	🟦 **Ac**** 89 Actinium (227)[a] $6d^17s^2$	🟦 **Rf** 104 Rutherfordium (261)[a] $5f^{14}6d^27s^2$	🟦 **Db** 105 Dubnium (262)[a] $5f^{14}6d^37s^2$	🟦 **Sg** 106 Seaborgium (266) $5f^{14}6d^47s^2$	🟦 **Bh** 107 Bohrium (264) $5f^{14}6d^57s^2$	🟦 **Hs** 108 Hassium (269) $5f^{14}6d^67s^2$	🟦 **Mt** 109 Meitnerium (268) $5f^{14}6d^77s^2$	🟦 – 110 – (269) – –	🟦 – 111 – (272) – –							

🟦 Metal 🟧 Semimetal 🟨 Nonmetal

Inner transition elements

Lanthanide series * 6	🟦 **Ce** 58 Cerium 140.116 $4f^15d^16s^2$	🟦 **Pr** 59 Praseodymium 140.90765 $4f^36s^2$	🟦 **Nd** 60 Neodymium 144.24 $4f^46s^2$	🟦 **Pm** 61 Promethium (145)[a] $4f^56s^2$	🟦 **Sm** 62 Samarium 150.4 $4f^66s^2$	🟦 **Eu** 63 Europium 151.964 $4f^76s^2$	🟦 **Gd** 64 Gadolinium 157.25 $4f^75d^16s^2$	🟦 **Tb** 65 Terbium 158.92534 $4f^96s^2$	🟦 **Dy** 66 Dysprosium 162.50 $4f^{10}6s^2$	🟦 **Ho** 67 Holmium 164.93032 $4f^{11}6s^2$	🟦 **Er** 68 Erbium 167.26 $4f^{12}6s^2$	🟦 **Tm** 69 Thulium 168.9342 $4f^{13}6s^2$	🟦 **Yb** 70 Ytterbium 173.04 $4f^{14}6s^2$	🟦 **Lu** 71 Lutetium 174.97 $4f^{14}5d^16s^2$
Actinide series ** 7	🟦 **Th** 90 Thorium 232.0381[b] $6d^27s^2$	🟦 **Pa** 91 Protactinium 231.03588 $5f^26d^17s^2$	🟦 **U** 92 Uranium 238.02891 $5f^36d^17s^2$	🟦 **Np** 93 Neptunium (237) $5f^46d^17s^2$	🟦 **Pu** 94 Plutonium (244) $5f^67s^2$	🟦 **Am** 95 Americium (243) $5f^77s^2$	🟦 **Cm** 96 Curium (247)[a] $5f^76d^17s^2$	🟦 **Bk** 97 Berkelium (247) $5f^97s^2$	🟦 **Cf** 98 Californium (251)[a] $5f^{10}7s^2$	🟦 **Es** 99 Einsteinium (251) $5f^{11}7s^2$	🟦 **Fm** 100 Fermium (257) $5f^{12}7s^2$	🟦 **Md** 101 Mendelevium (258) $5f^{13}7s^2$	🟦 **No** 102 Nobelium (259) $5f^{14}7s^2$	🟦 **Lr** 103 Lawrencium (262) $5f^{14}6d^17s^2$

Kinds of Materials

- **Metals:** are materials that are normally combinations of "metallic elements". Metals usually are good conductors of heat and electricity. Also, they are quite strong but malleable and tend to have a lustrous look when polished.

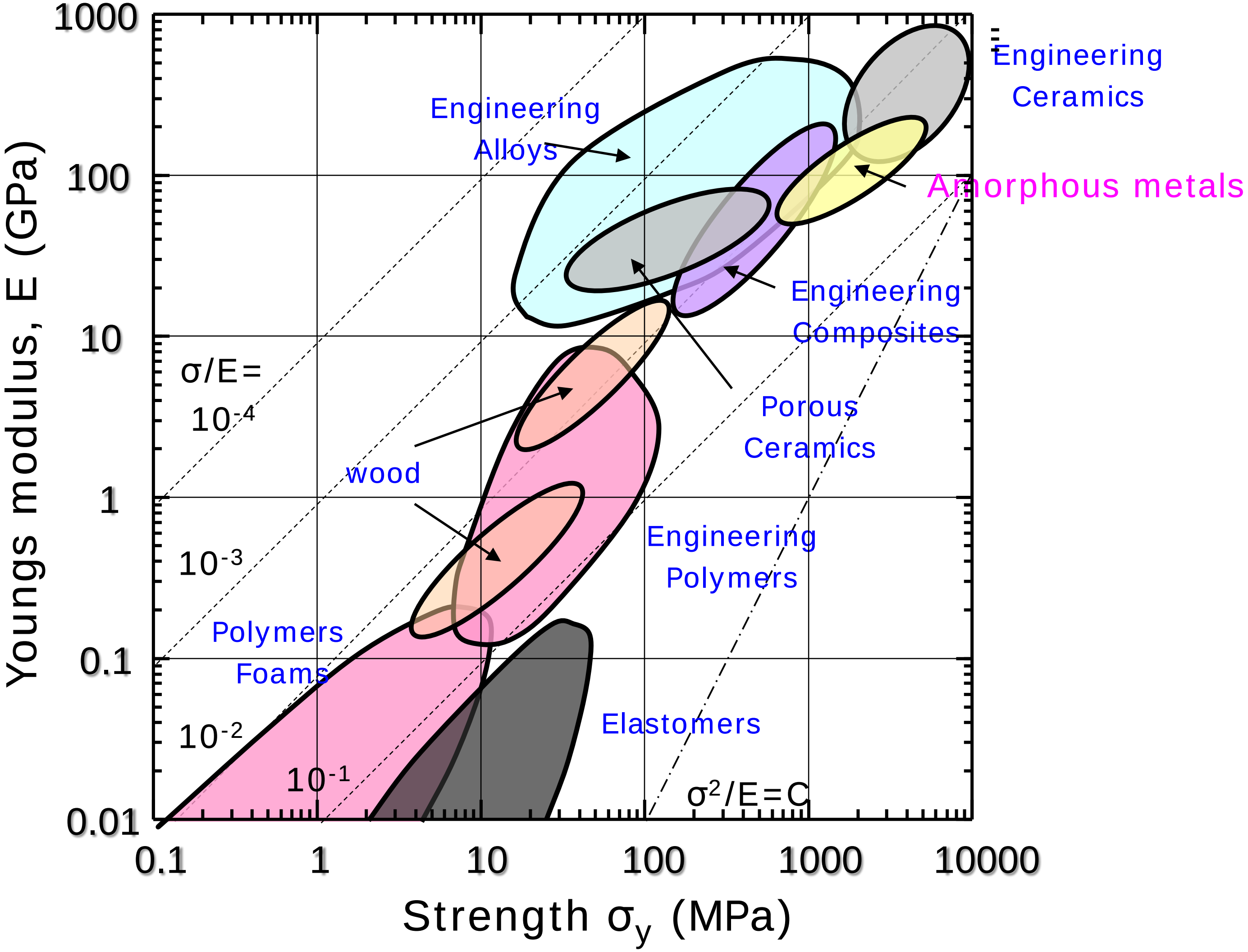
- **Ceramics:** are generally compounds between metallic and nonmetallic elements. Typically they are insulating and resistant to high temperatures and harsh environments.

Kinds of Materials

- **Plastics:** (or polymers) are generally organic compounds based upon carbon and hydrogen. They are very large molecular structures. Usually they are low density and are not stable at high temperatures.

- **Semiconductors:** have electrical properties intermediate between metallic conductors and ceramic insulators. Also, the electrical properties are strongly dependent upon small amounts of impurities.

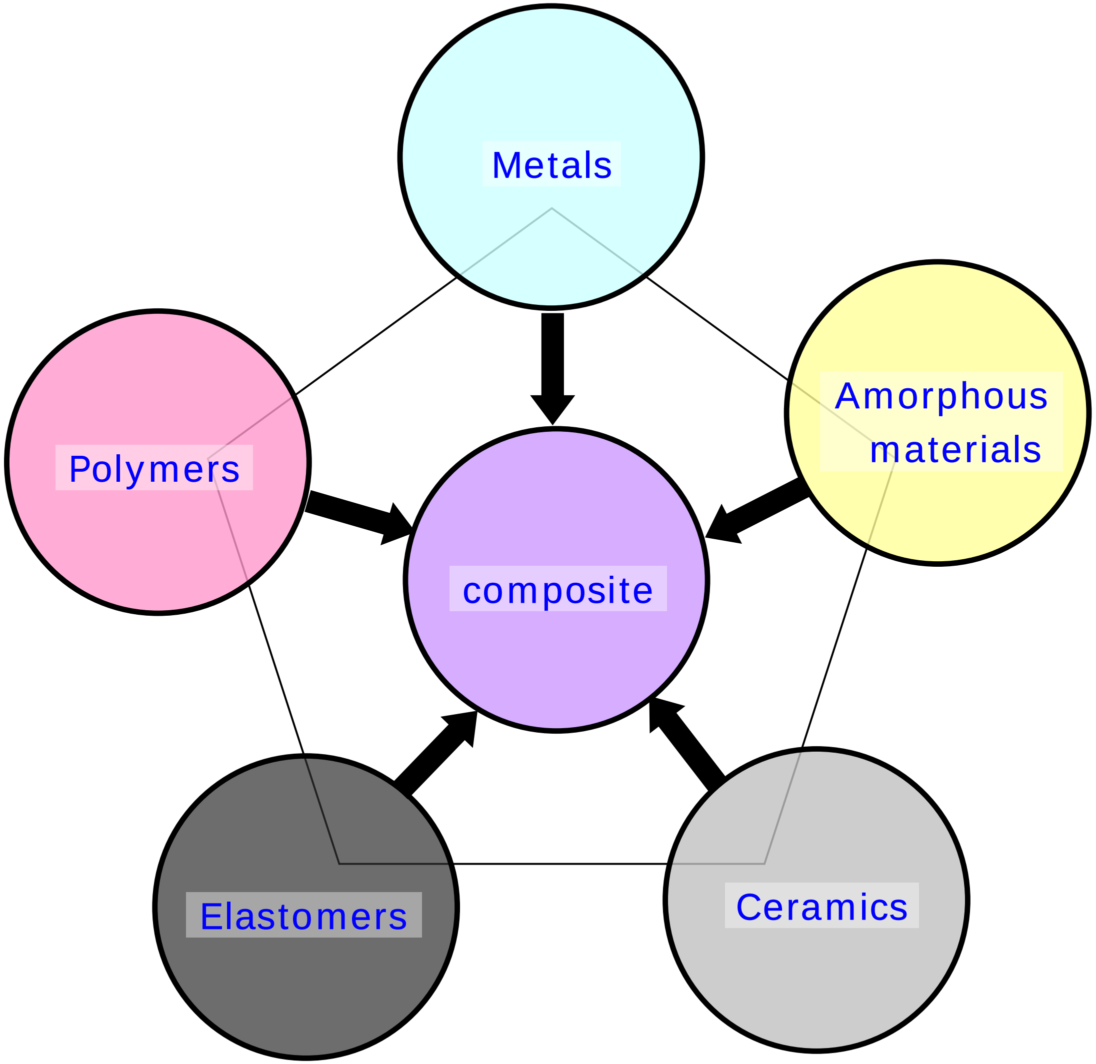
< Ashby map >


1000
100
10
1
0.1
0.01
Youngs modulus, E (GPa)
0.1
1
10
100
1000
10000
Strength σ_y (MPa)
Engineering Ceramics
Engineering Alloys
Amorphous metals
Engineering Composites
Porous Ceramics
wood
Engineering Polymers
Polymers Foams
Elastomers
$\sigma/E=$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
$\sigma^2/E=C$

Kinds of Materials

- **Composites:** consist of more than one material type. Fiberglass, a combination of glass and a polymer, is an example. Concrete and plywood are other familiar composites. Many new combinations include ceramic fibers in metal or polymer matrix.

Menu of engineering materials



Metals

Amorphous materials

Polymers

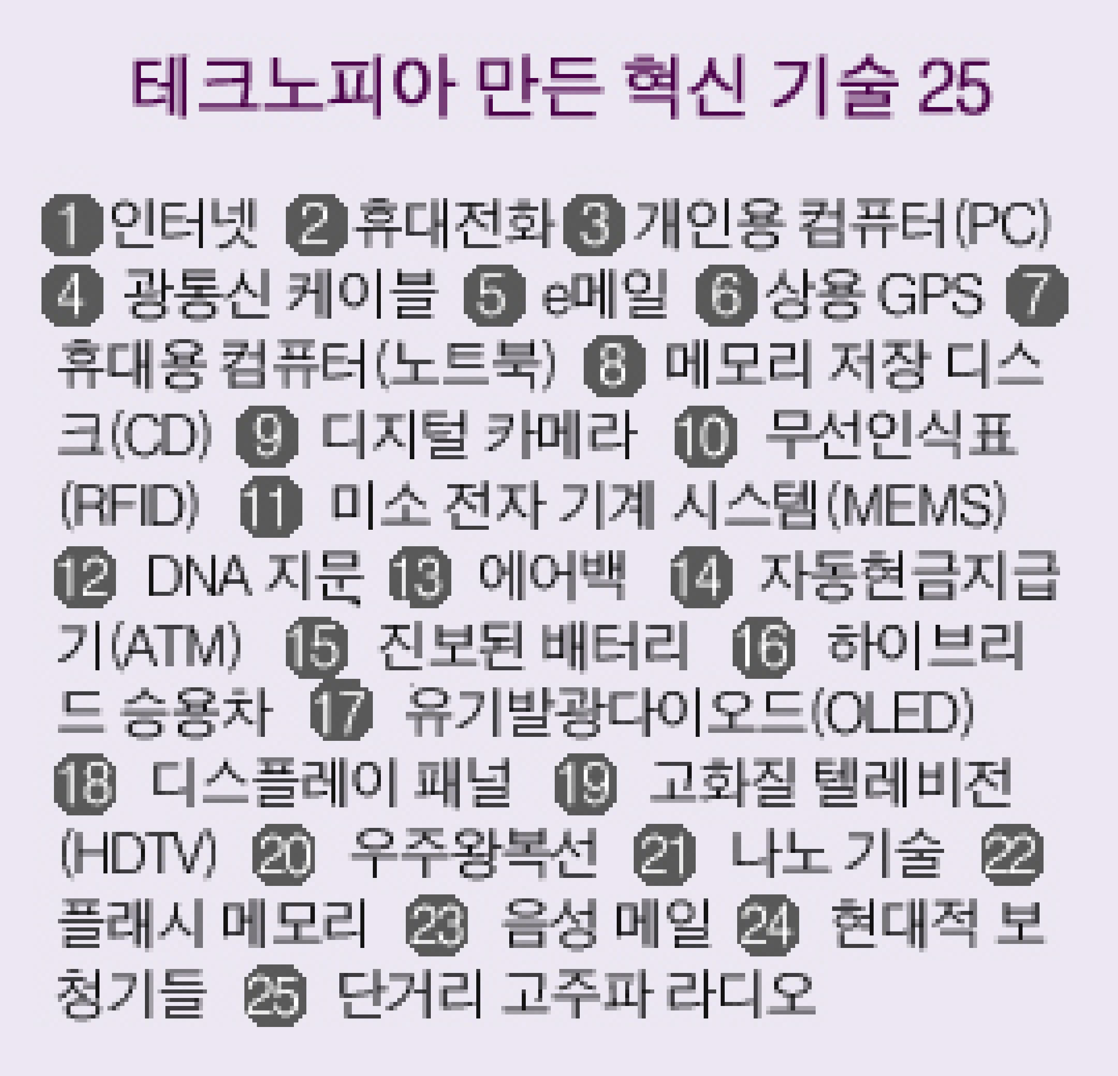
composite

Elastomers

Ceramics

지난 25년 동안 세상을 바꾼 신기술 25가지

러멜슨-MIT 프로그램

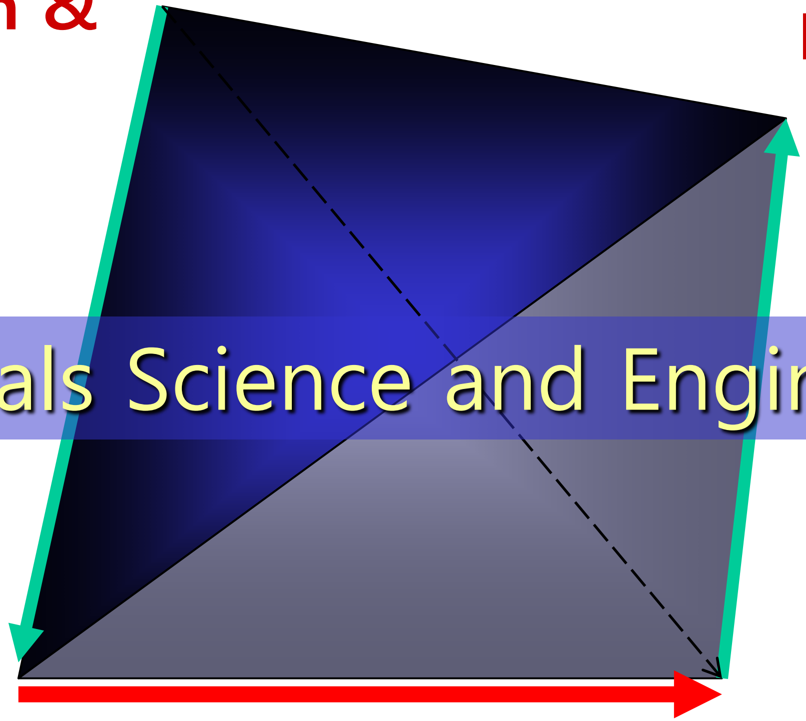


테크노피아 만든 혁신 기술 25

① 인터넷 ② 휴대전화 ③ 개인용 컴퓨터(PC) ④ 광통신 케이블 ⑤ e메일 ⑥ 상용 GPS ⑦ 휴대용 컴퓨터(노트북) ⑧ 메모리 저장 디스크(CD) ⑨ 디지털 카메라 ⑩ 무선인식표(RFID) ⑪ 미소 전자 기계 시스템(MEMS) ⑫ DNA 지문 ⑬ 에어백 ⑭ 자동현금지급기(ATM) ⑮ 진보된 배터리 ⑯ 하이브리드 승용차 ⑰ 유기발광다이오드(OLED) ⑱ 디스플레이 패널 ⑲ 고화질 텔레비전(HDTV) ⑳ 우주왕복선 ㉑ 나노 기술 ㉒ 플래시 메모리 ㉓ 음성 메일 ㉔ 현대적 보청기들 ㉕ 단거리 고주파 라디오

의료 및 의약 분야 기술 제외

Microstructure-Properties Relationships



Alloy design & Processing

Performance

" Materials Science and Engineering"

Microstructure

down to atomic scale

Properties

"Tailor-made Materials Design"

합금설계 + 공정조절 ➡

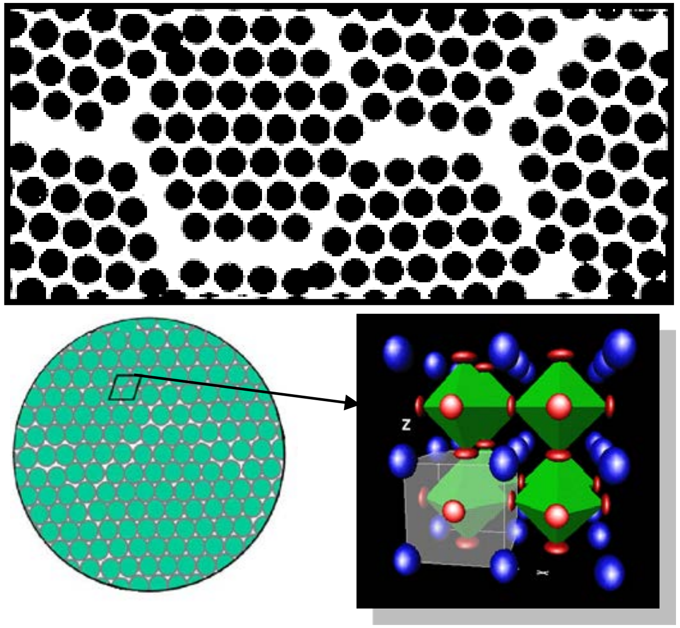
Microstructure Control of Materials

⬇

Better Material Properties

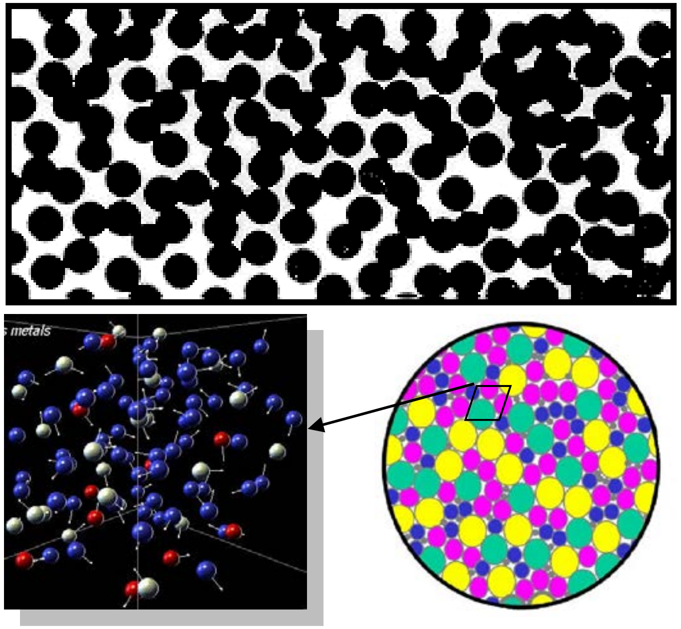
Structure *of crystals, liquids and glasses*

Crystals



- **periodic**
- **grain boundaries**

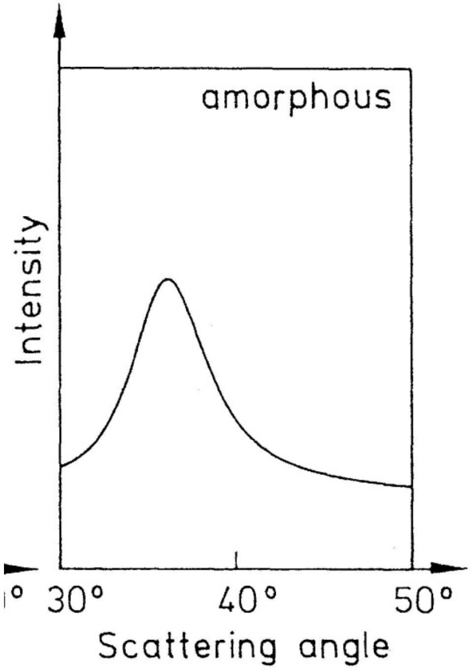
Liquids, glasses

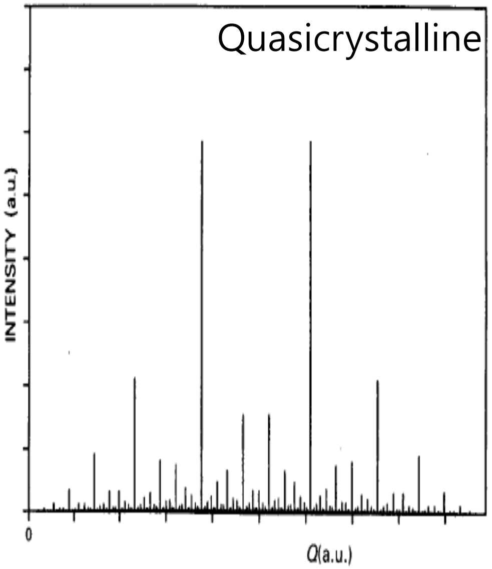


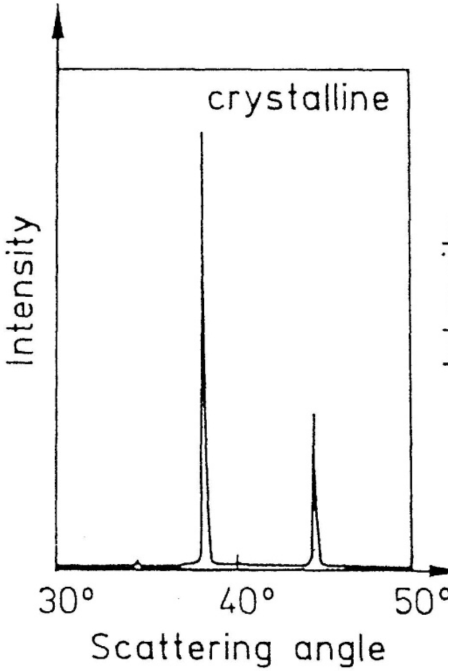
- **amorphous = non-periodic**
- **no grain boundaries**

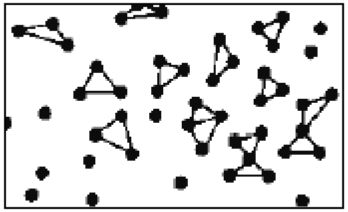
Atomic structure

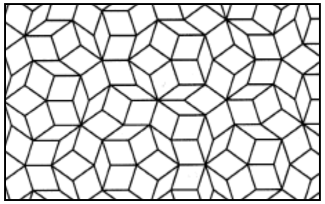
Short-range order ↔ **Periodic order**

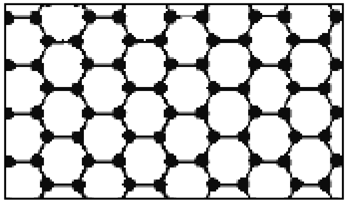












2011 노벨화학상 수상자 대니얼 셰시트먼 박사

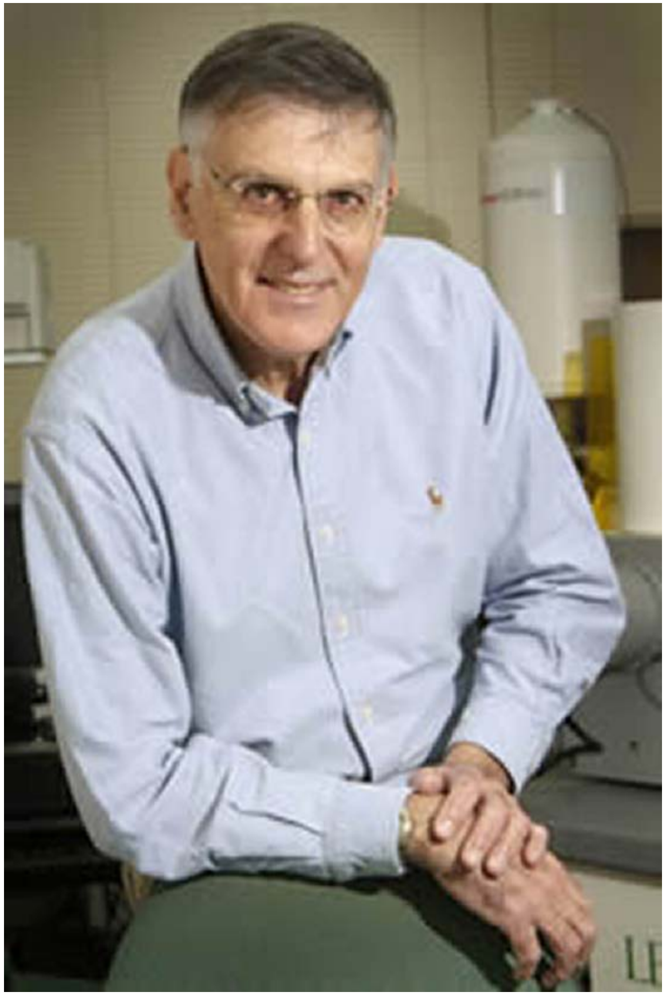
이스라엘 테크니온 공대의 대니얼 셰시트먼 박사(70·사진)가 2011년 노벨 화학상 수상자로 선정됐다.

스웨덴 왕립 과학아카데미는 5일(현지시간) 대니얼 셰시트먼 박사가 준결정(quasicrystal) 발견에 대한 공로를 인정받아 2011년 노벨 화학학상 수상자로 선정했다고 발표했다.

위원회는 "일반적으로 결정(crystal)은 원자가 같은 형태를 반복하면서 이뤄진다"며 "하지만 셰시트먼 박사는 결정 안에 원자들이 반복되지 않는 배열로 존재 할 수 있다는 사실을 발견했다"고 밝혔다.

위원회는 또 "액체와 고체의 중간 상태인 준결정 연구를 통해 고체물질에 대한 이해를 바꿔놨다"고 수상 이유를 밝혔다.

셰시트먼 교수는 지난 1982년 세계 최초로 1982년 4월 특정무늬가 반복되지 않는 배열의 준결정을 발견했다.



2011 노벨 화학상 수상자 대니얼 셰시트먼 박사

What is microstructure?

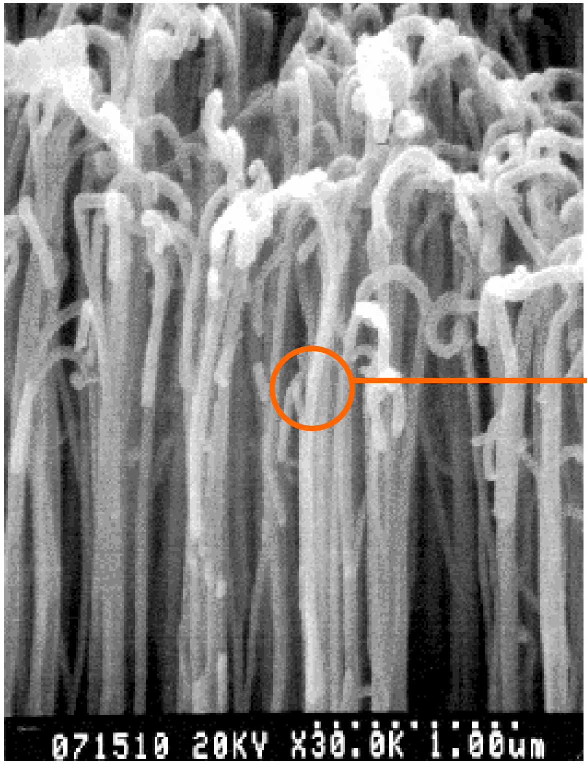
Microstructure originally meant the structure inside a material that could be observed with the aid of a microscope.

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.

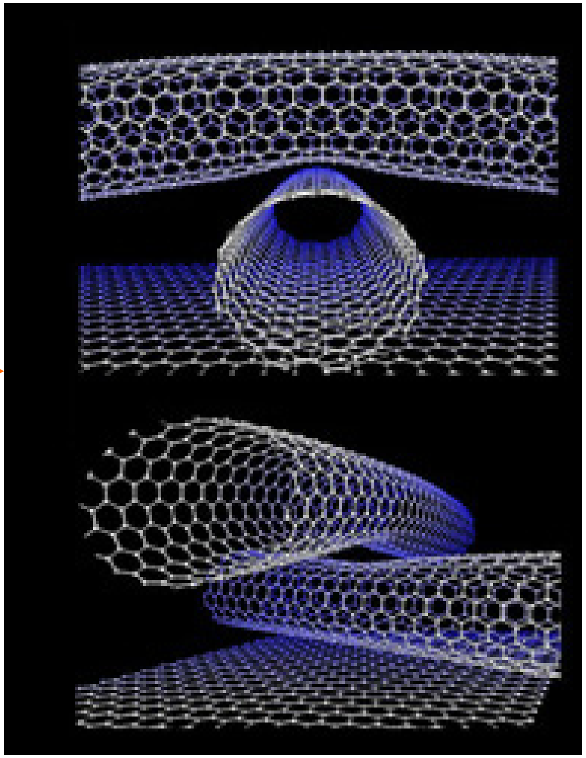
What defects are we interested in?
Interfaces (both grain boundaries and interphase boundaries), which are planar defects,
Dislocations (and other line defects), and
Point defects (such as interstititals and vacancies as well as solute atoms in solution)

미세구조 조절: 1) perfection *vs* imperfection control

Perfect Crystals without Defect



Carbon Nanotubes



High strength, unique magnetic/electrical properties

Perfect Crystal is good in many aspects, But …

☐ 1) ***Imperfection*** in Metallic Materials ;

Point defect : Vacancies, Impurity atoms

Line defect : Dislocations

Plane defect : Grain Boundaries,
Free Surfaces

Bulk defect : Voids, Cracks

☐ 2) ***Second Phase Particles*** in Matrix

Mechanical Properties ;
Magnetic properties
Electrical properties
Etc.

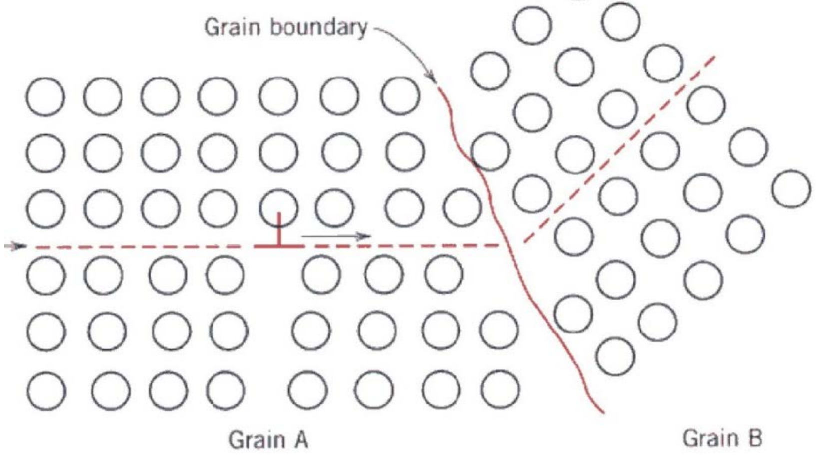
1) *Imperfection:* Grain Boundaries

(Planer defect)

Low Carbon Steel

Optical Microscope

Grain Boundary

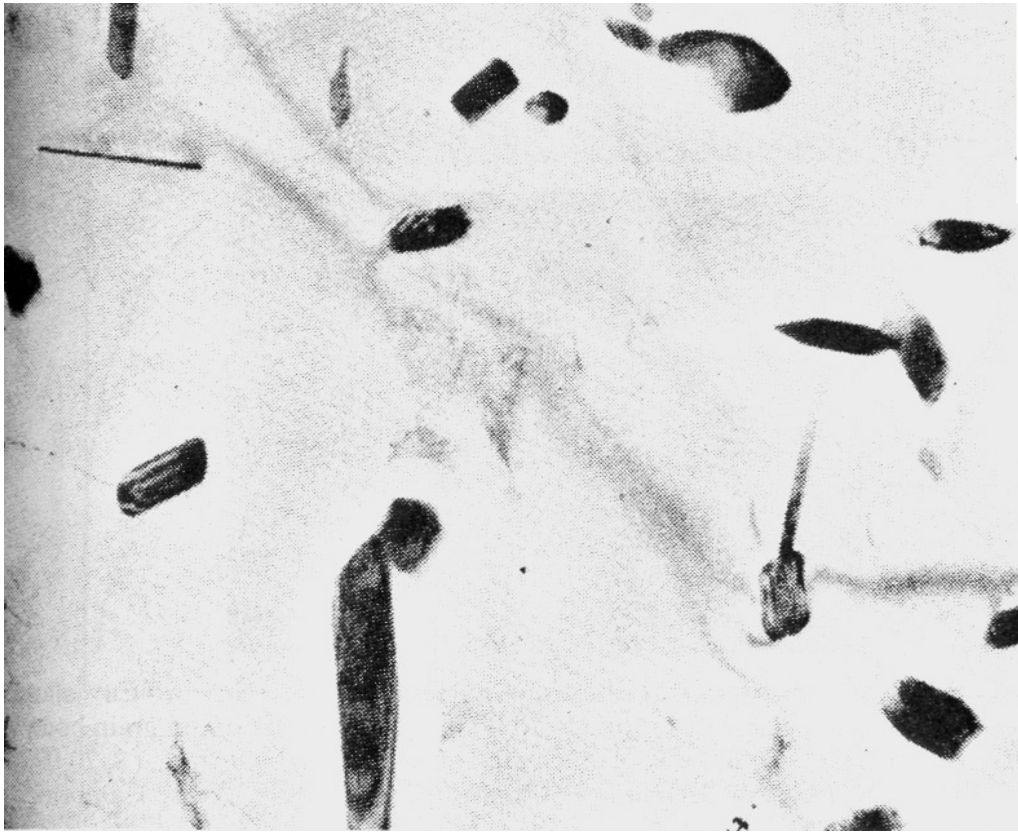


1) *Imperfection:* Phase Boundaries

(Planer defect)

θ of Al-Cu alloys (x 8,000) by SEM

JEOL 7500F-1
scanning electron microcsope

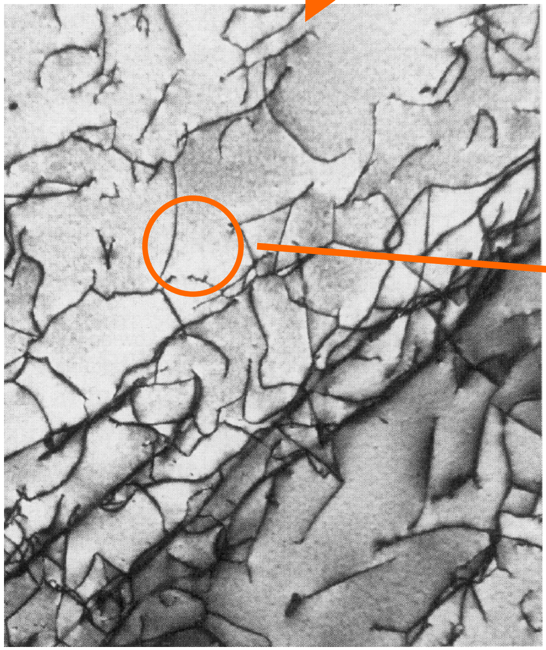


$CuAl_2$: complex body centered tetragonal, incoherent or complex semicoherent

1) *Imperfection:* Dislocations (line defect)

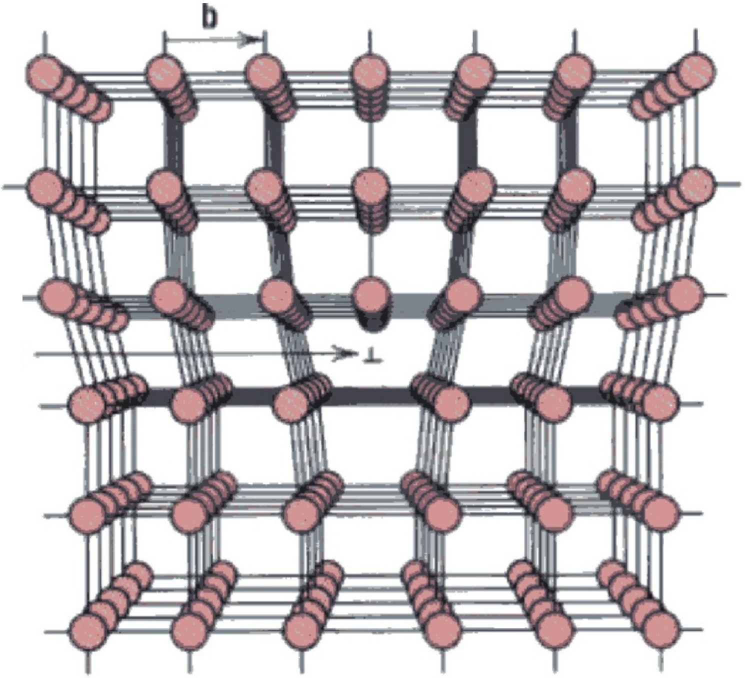
SR-71
with armor of
titanium alloy

It looks perfect.
But….



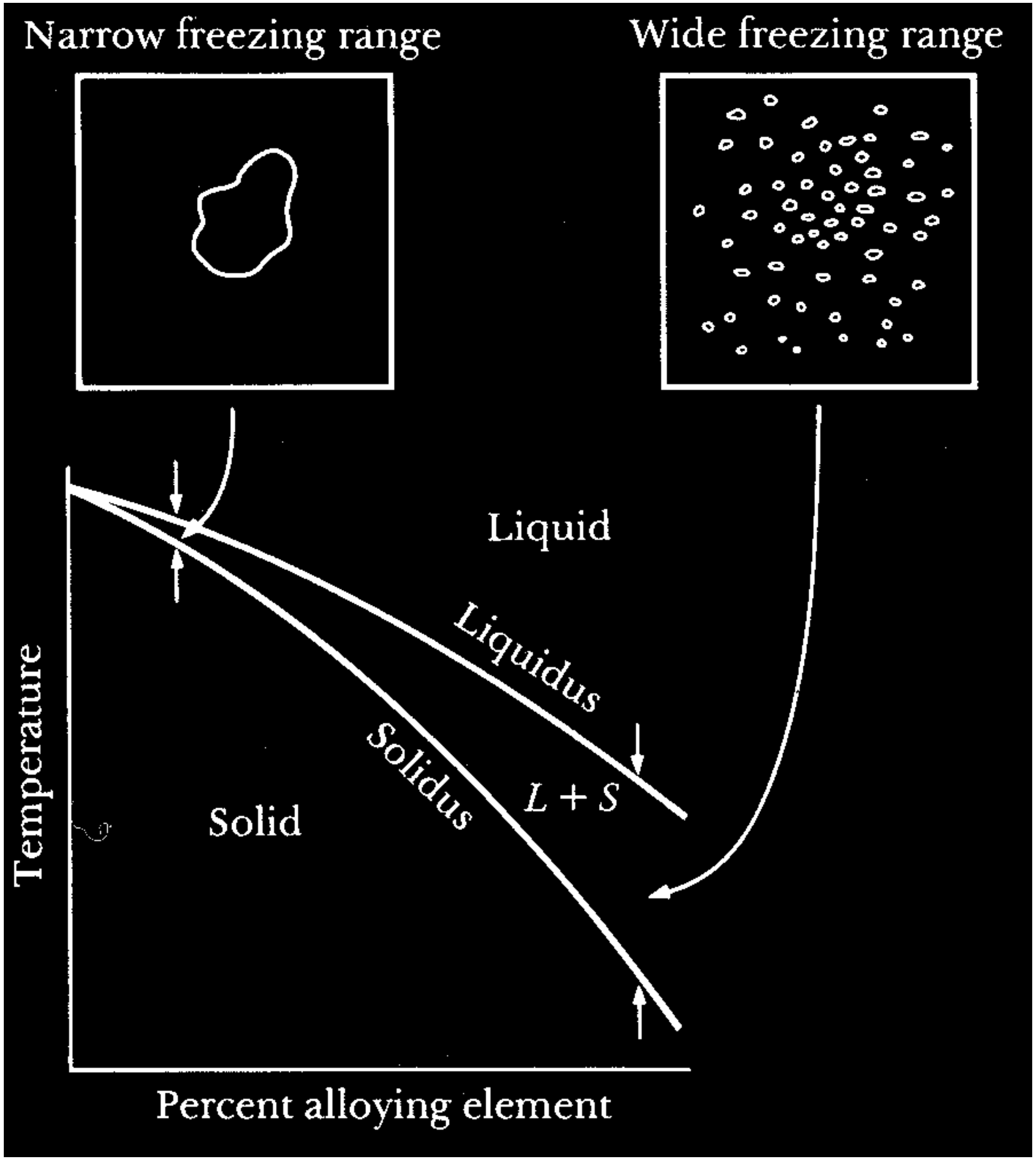
Edge
Dislocation
Line

Burgers vector

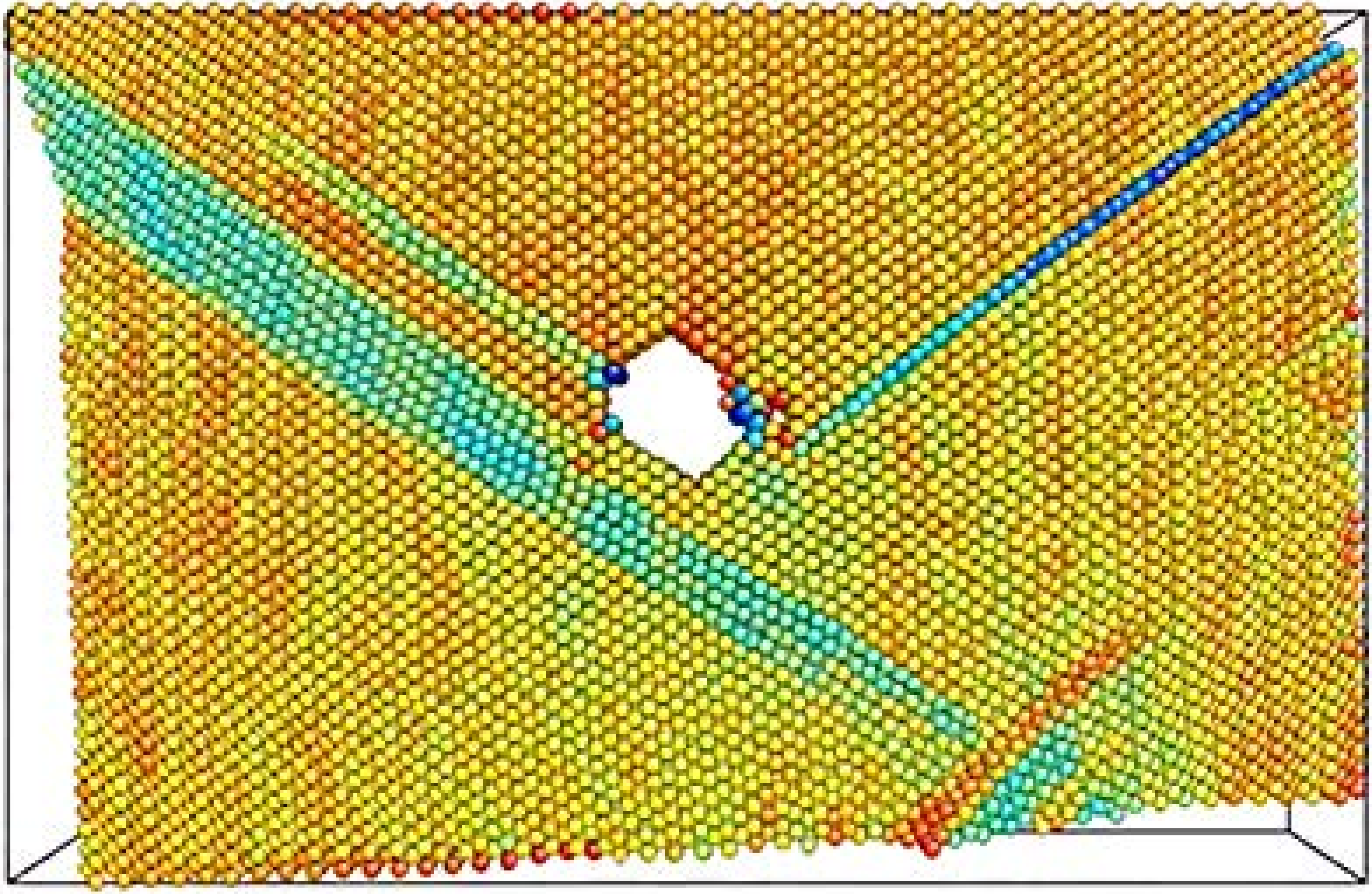


1) *Imperfection:* Voids during solidification

Shrinkage effect

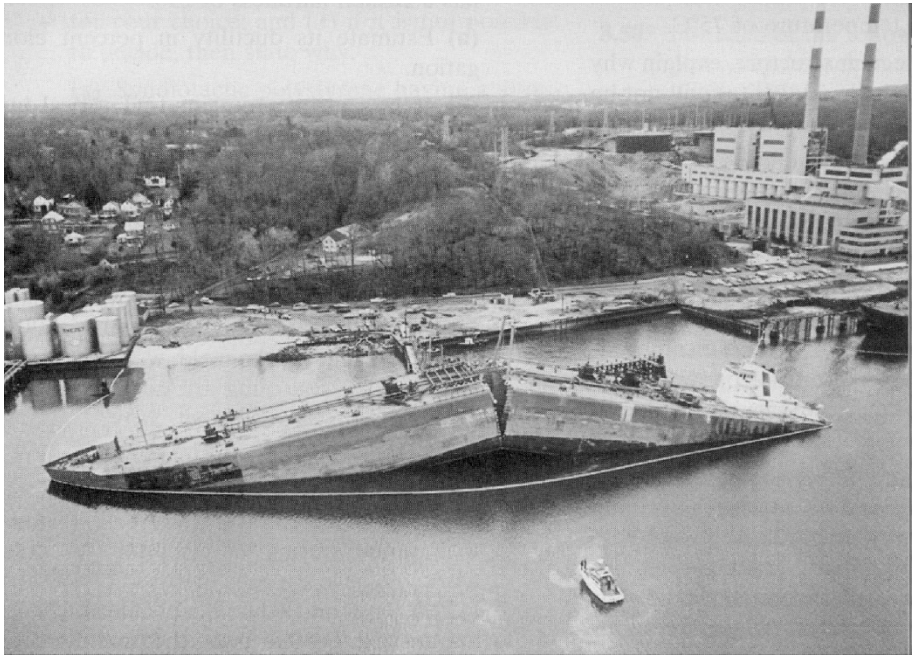


1) *Imperfection:* Voids during deformation



Using of Materials with *Improper Microstructure*

Failures

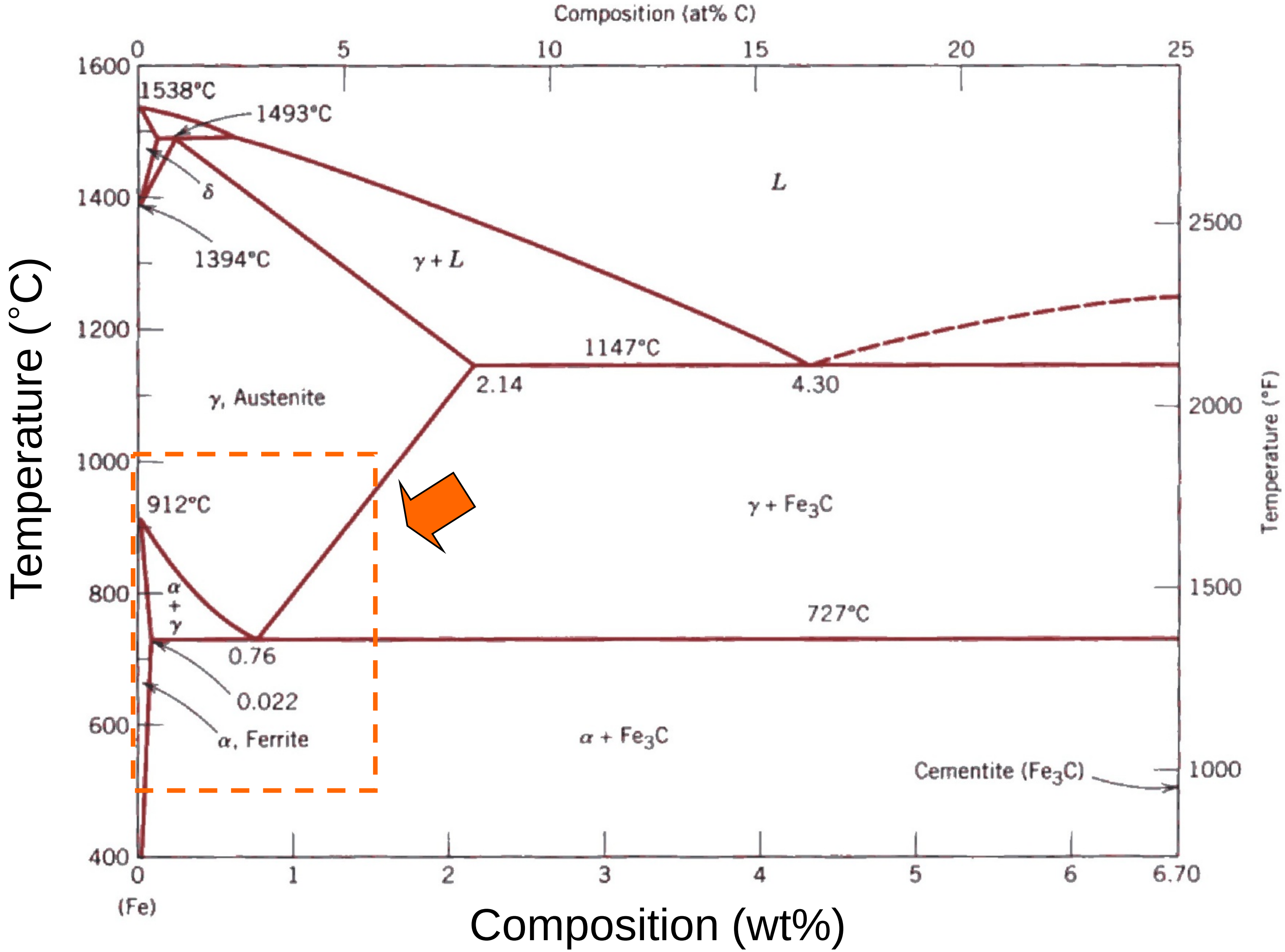


Oil tanker
fractured in a brittle manner

성수대교 붕괴 (1994.10.21)

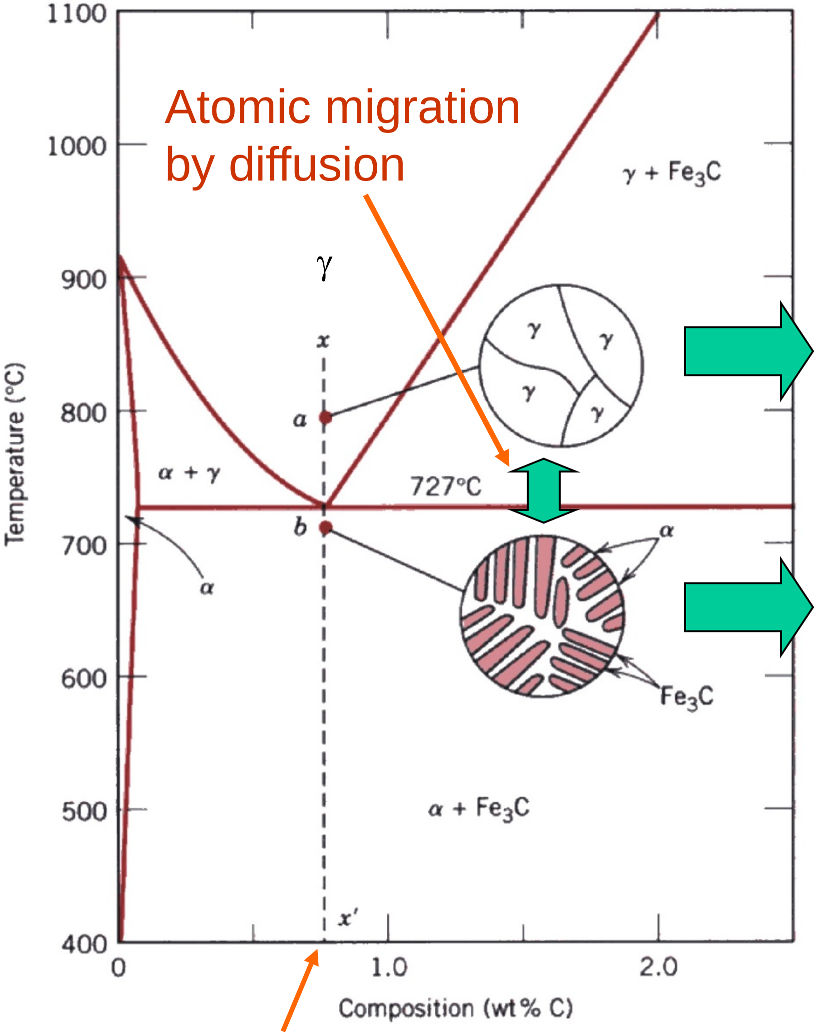
미세구조 조절: 2) Secondary phase control during solidification

Phase Diagram of Iron–Carbon Alloy



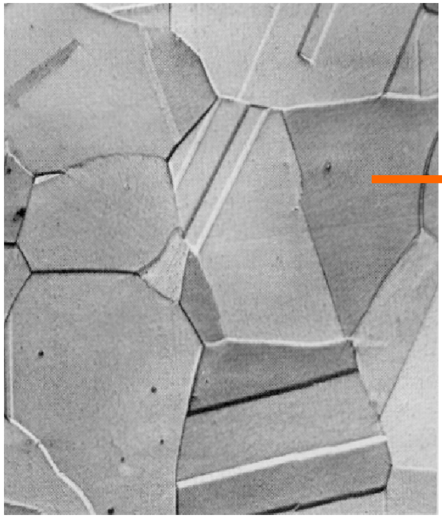
미세구조 조절: 2) Secondary phase control during solidification

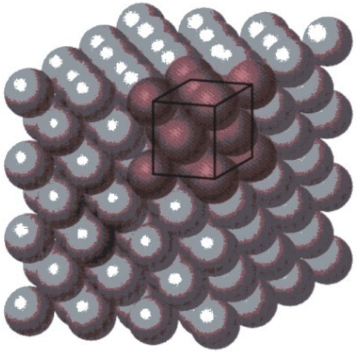
Equilibrium Phases of Iron-Carbon Alloy



Atomic migration by diffusion

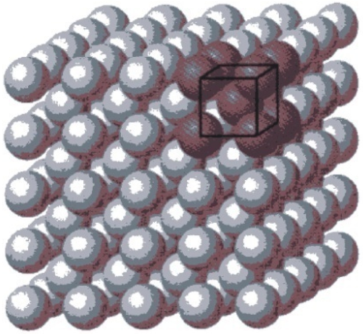
Eutectoid composition





γ phase (FCC)

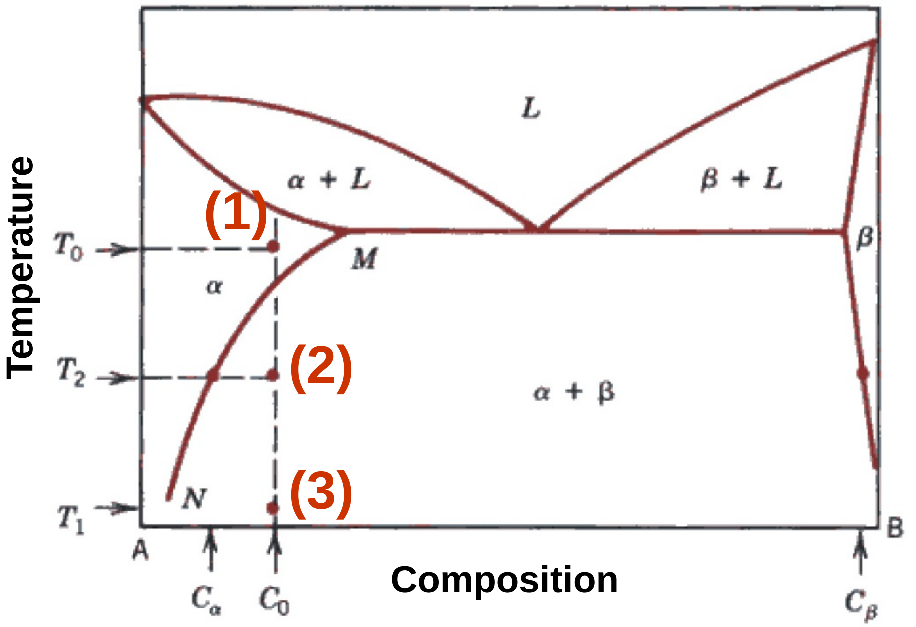
Fe$_3$C phase

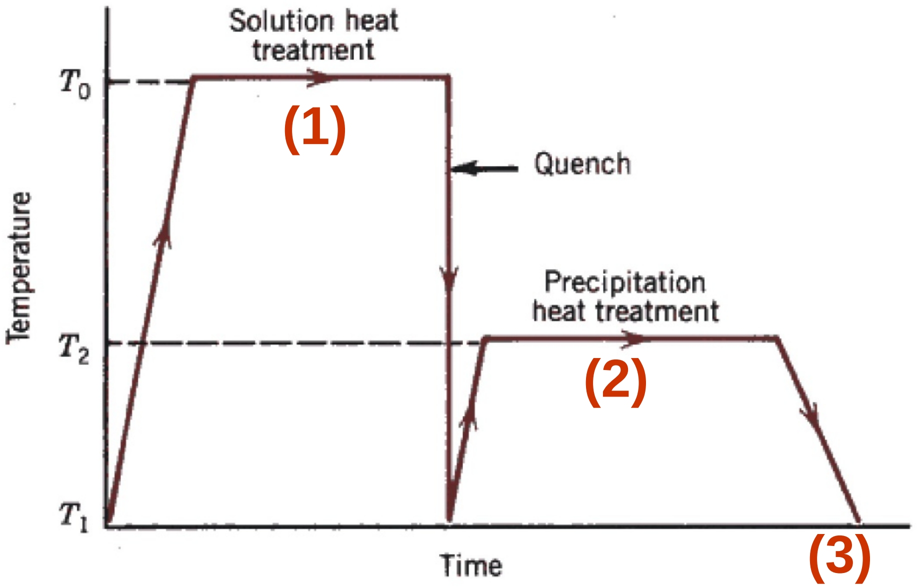


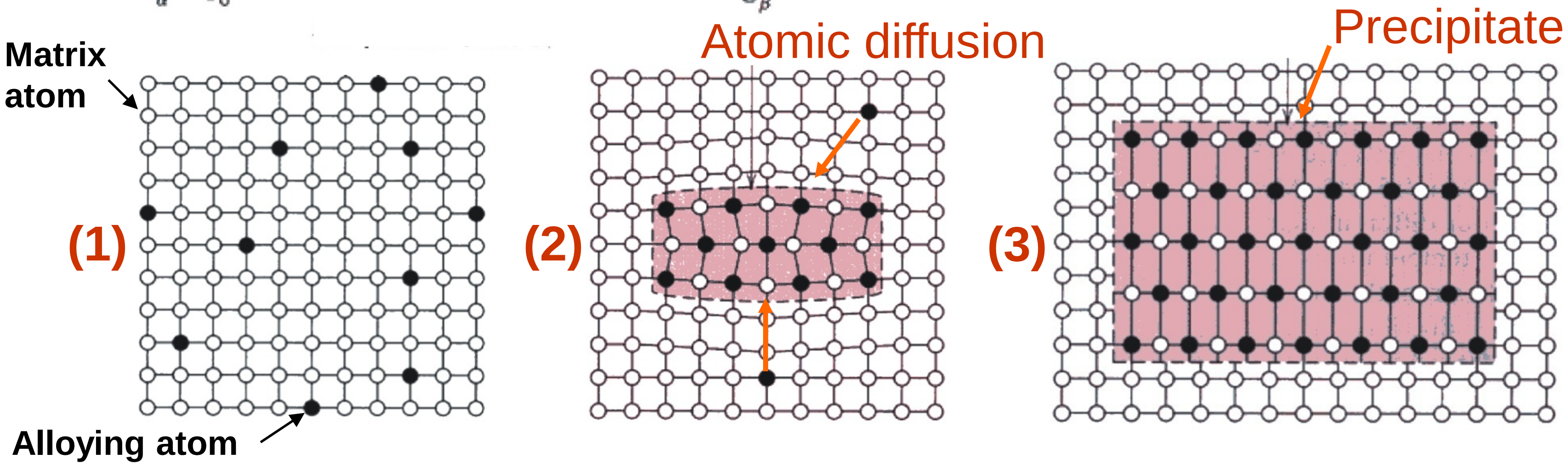
α phase (BCC)

미세구조 조절: 2) Secondary phase control during annealing

Mechanism of Precipitation







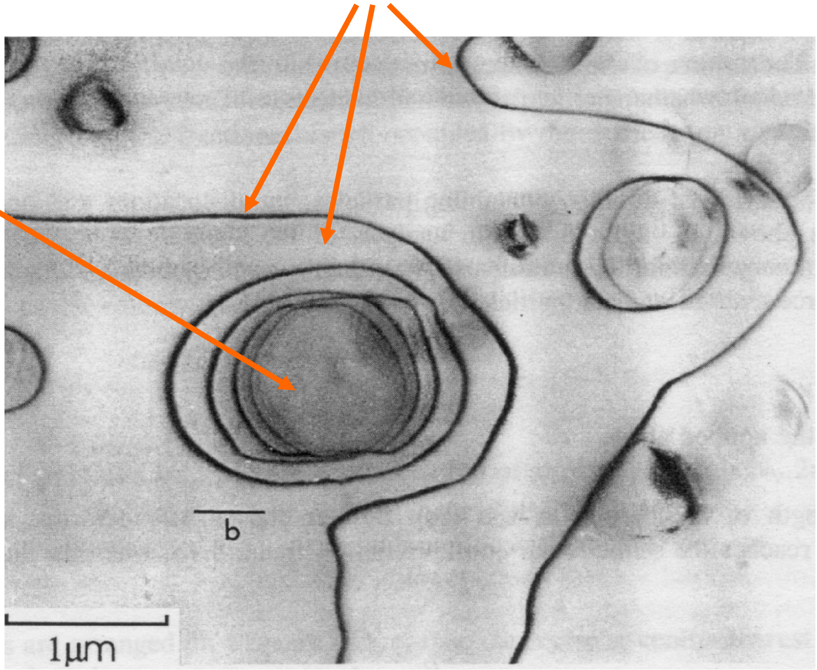
미세구조 조절: 2) Secondary phase control

Effect of Second Phase Particle on Mechanical Property

Second phase particle in matrix material

Obstacle of dislocation slip & grain growth

High strength

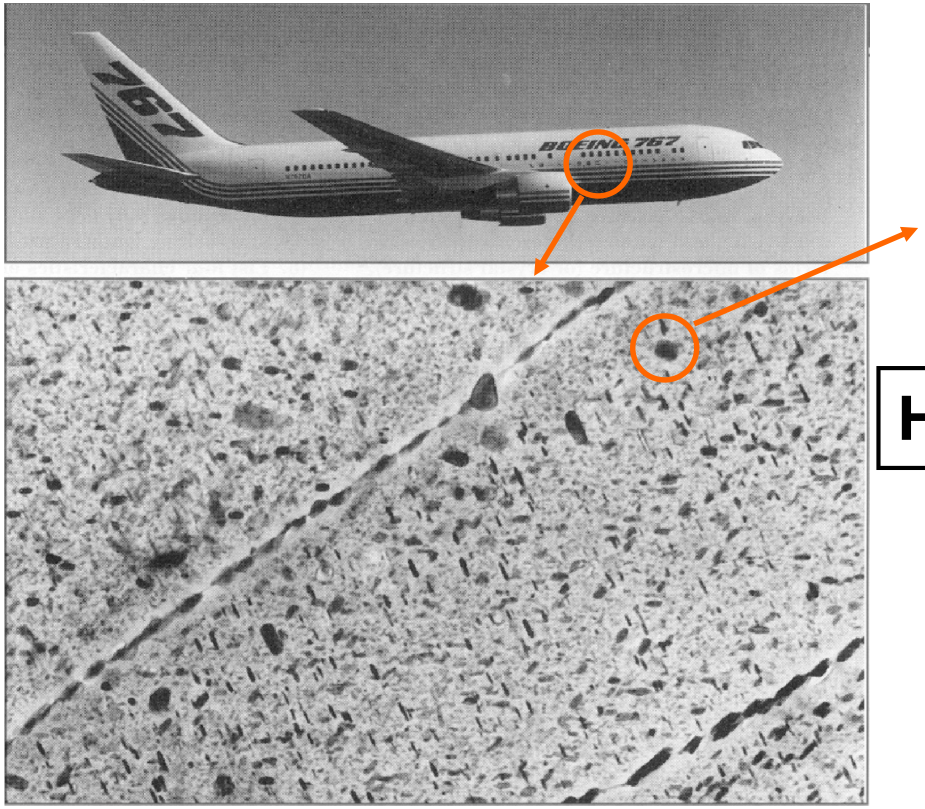


Ni_3Si particles in Ni-6%Si single crystal

미세구조 조절: 2) Secondary phase control

Control of Microstructures by Precipitation Transformation in Aluminum Alloy

Boeing 767 by AA7150 T651 alloy



Precipitates in aluminum matrix

↓

Hindering dislocation slip

↓

High strength

미세구조 조절: 2) Secondary phase control during processing

Control of Microstructures ;

*Cold Work*_압력을 가해 성형하고 인성을 증가시키는 과정

김홍도 "대장간"

조선시대

현대의 단조기

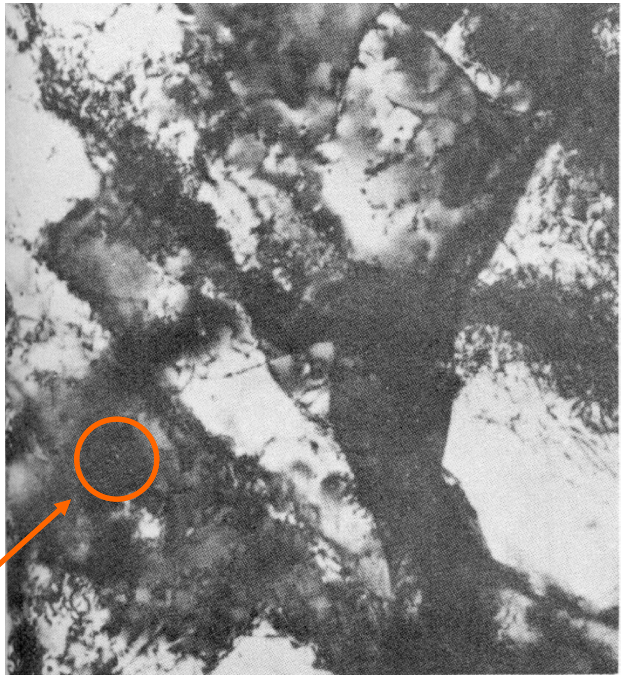
미세구조 조절: 2) Secondary phase control during processing

Hardening Mechanism by Cold Working

Before cold work

Deformation
or
Cold work

Aluminum alloy

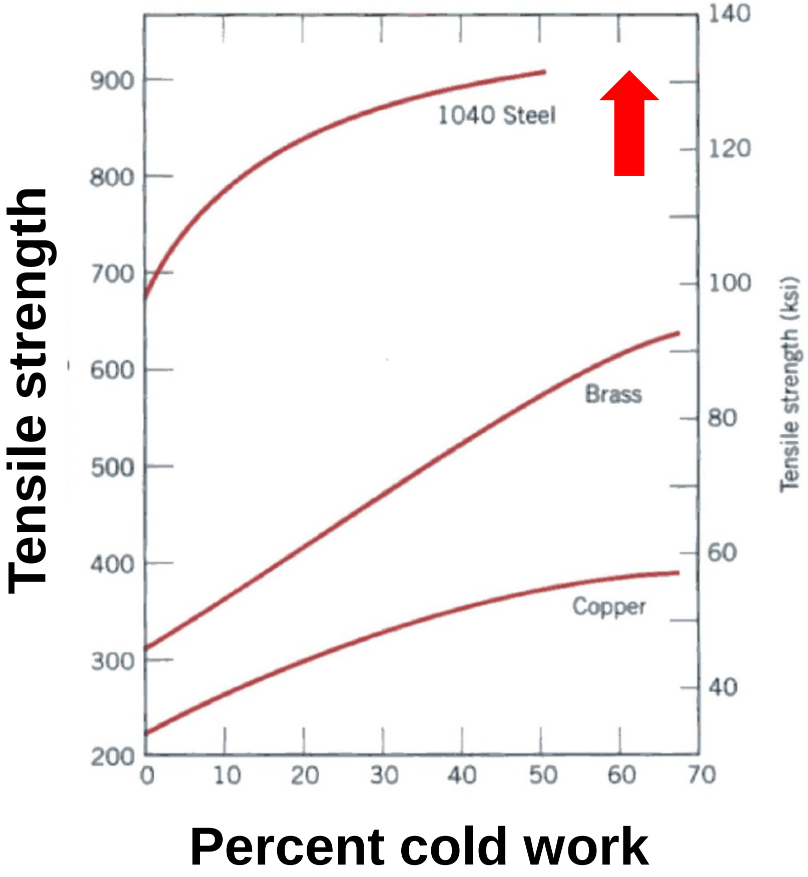


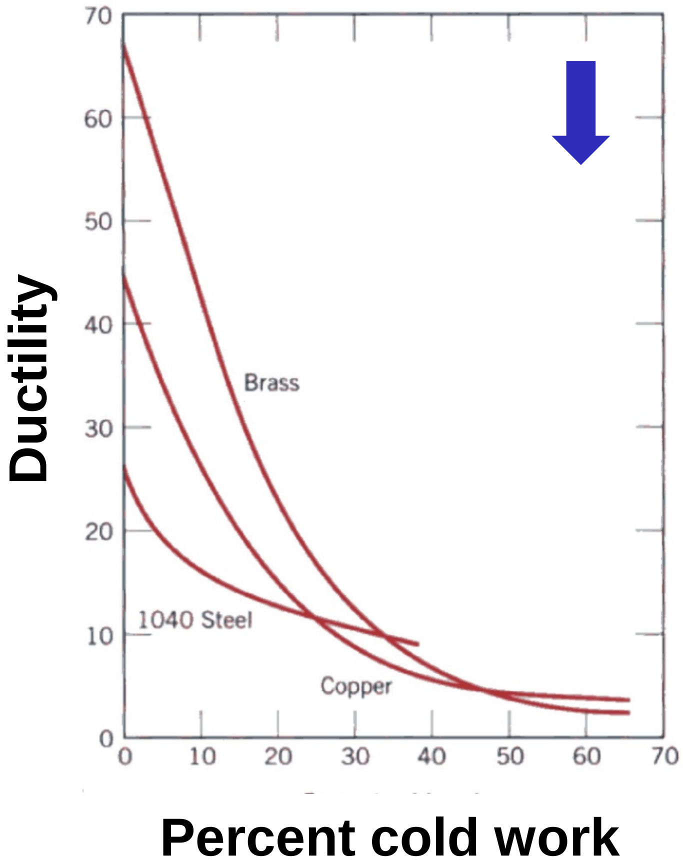
Dislocation tangle

Accumulation of dislocations

미세구조 조절: 2) Secondary phase control during processing

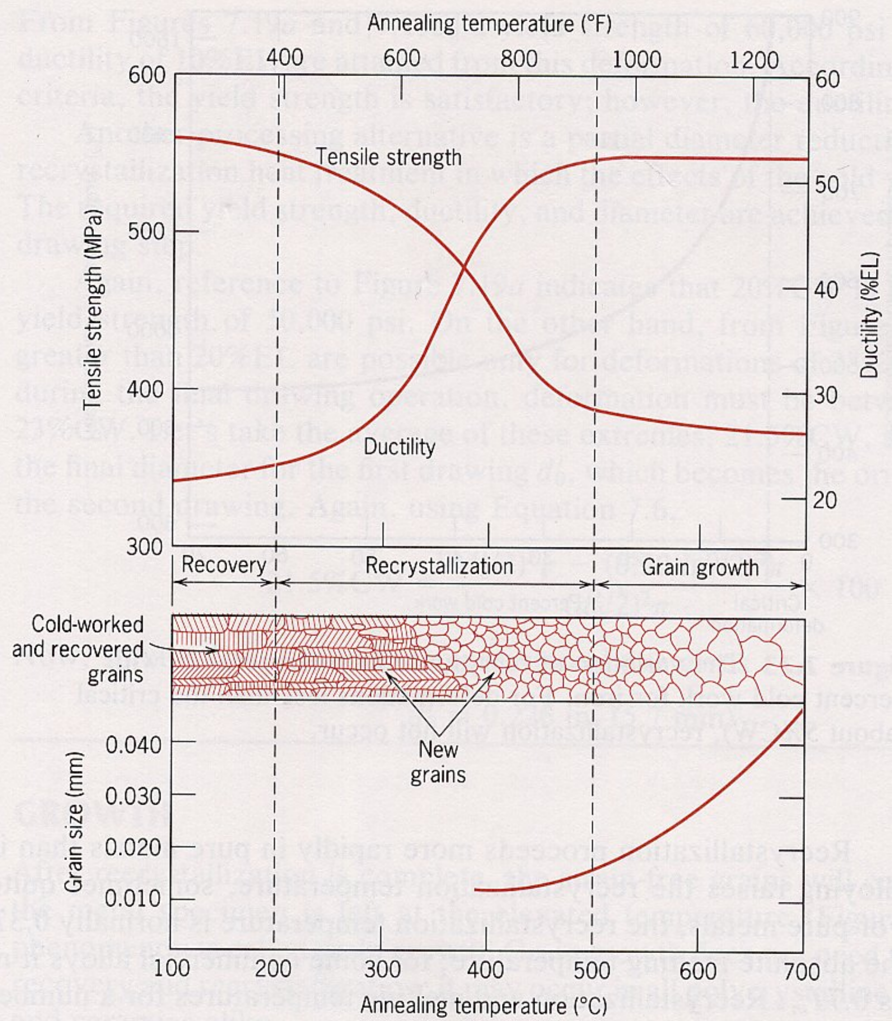
Changes of Strength and Ductility by Cold Working





미세구조 조절: 2) Secondary phase control during processing

Changes of Microstructure & Mechanical Properties during Annealing



Cold working → recovery → recrystallization → grain growth

내부 변형률 에너지 제거 낮은 전위밀도 (변형률이 없는) 결정립

합금설계 + 공정조절 → 특성 최적화

Production and Application of Electrical Steel

Hot rolling - cold rolling – 1st annealing – 2nd annealing

Coils

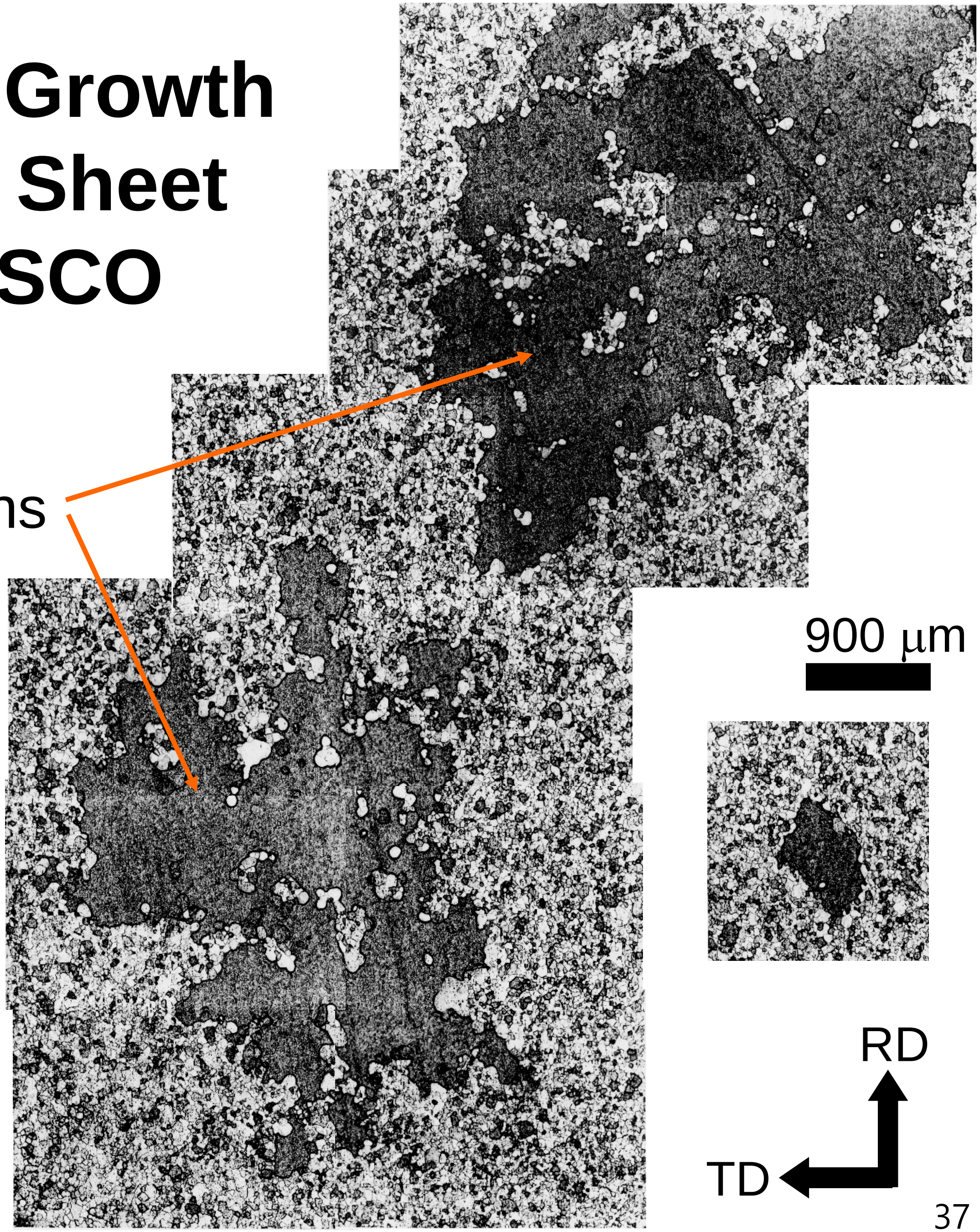
Stacked transformer core

Transformer
Motor
Etc.

Soft magnetization property

Abnormal Grain Growth In Fe-3%Si Steel Sheet produced by POSCO

Abnormally grown grains
with Goss texture



Control of grain growth

Control of magnetic property

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 ($S \rightarrow S_1 + S_2$)
   - etc.

2) **Diffusionless transformation ;**

   Short-distance atomic migration

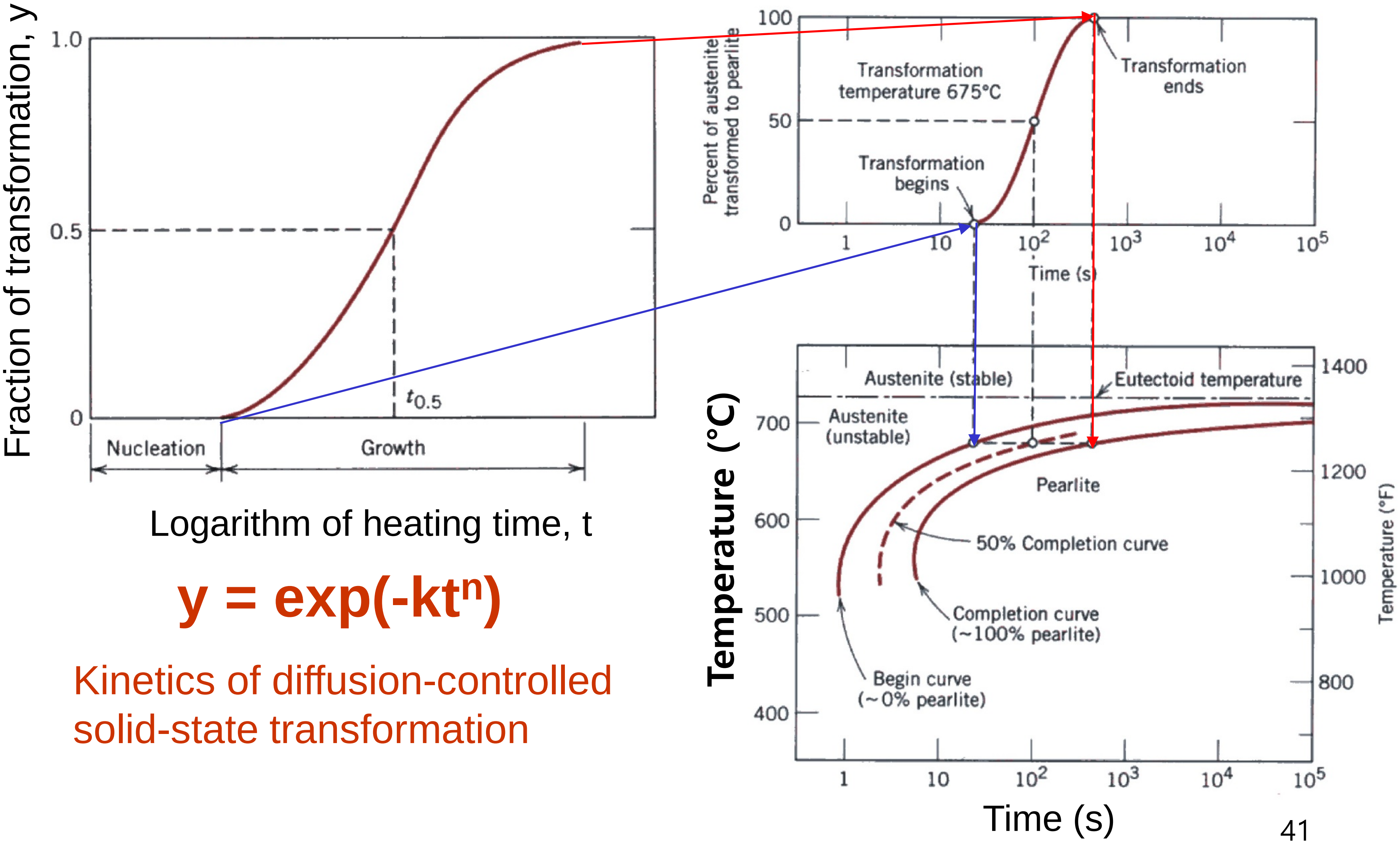
   - Martensitic transformation

Diffusion-Controlled Phase Transformation
time dependency

Non-Equilibrium Phases

Need of Controlling
not only *Temperature* & *Composition*
but *Process conditions* (Cooling Rate)

Transformation Kinetics and Isothermal Transformation Diagram



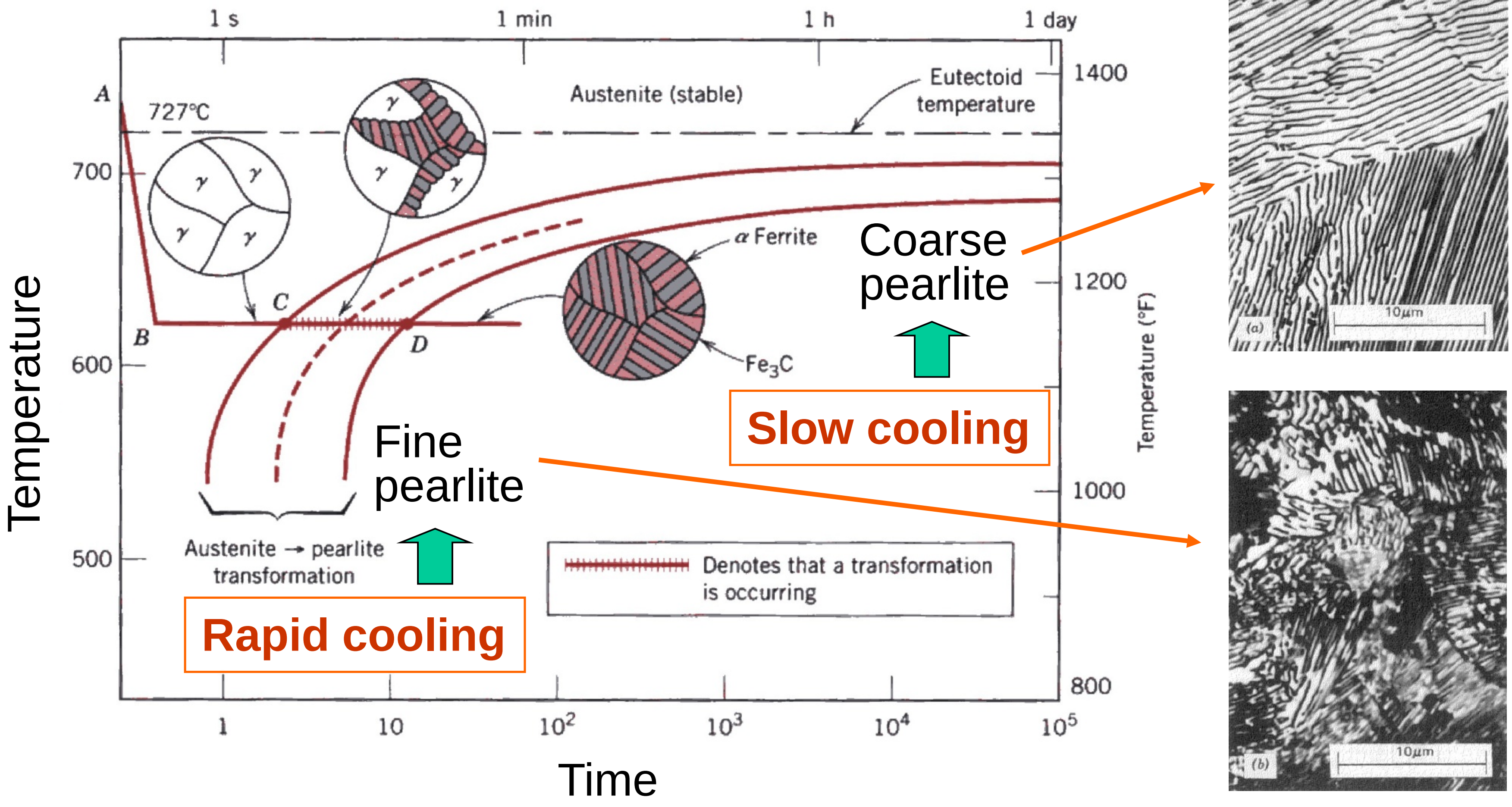
$$y = \exp(-kt^n)$$

Kinetics of diffusion-controlled solid-state transformation

TTT diagram ➡ **Isothermal transformation diagram**

Isothermal Transformation Diagram of a Eutectoid Iron-Carbon Alloy

γ Austenite ➡ **α Ferrite + Fe_3C graphite**



Coarse pearlite

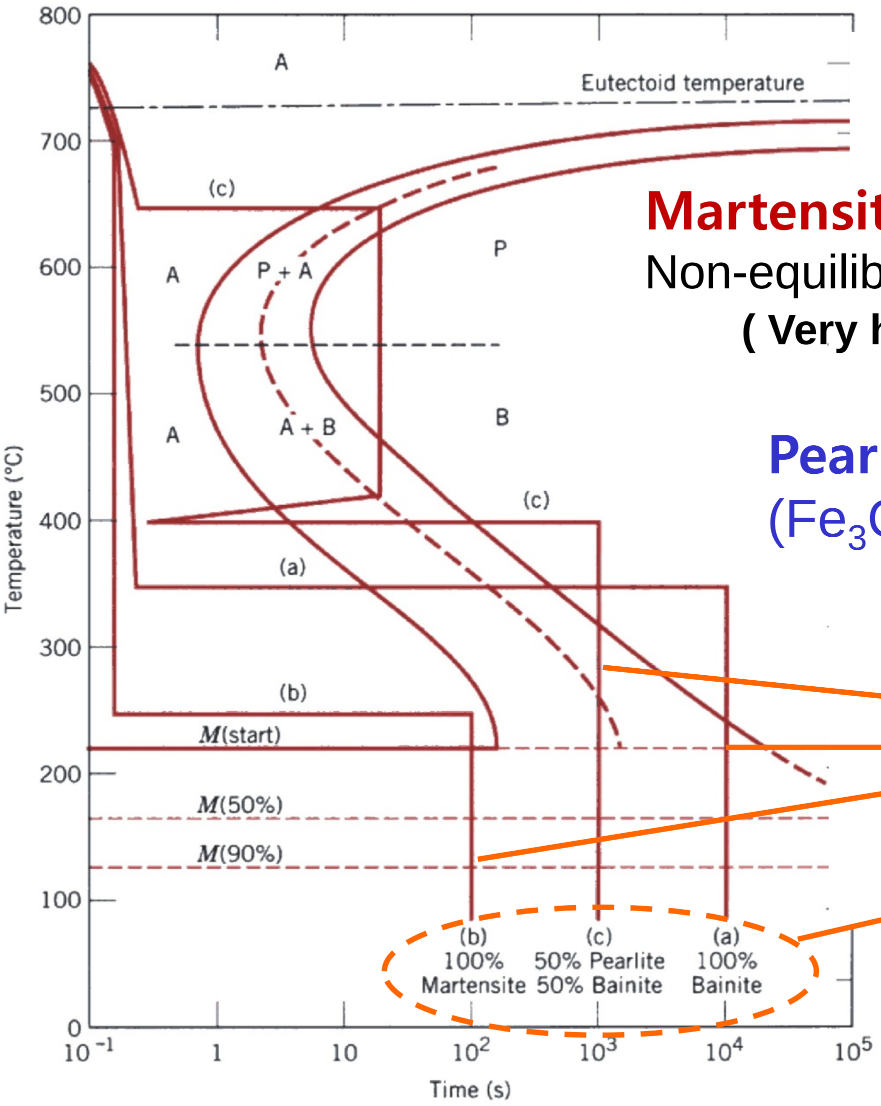
Slow cooling

Fine pearlite

Rapid cooling

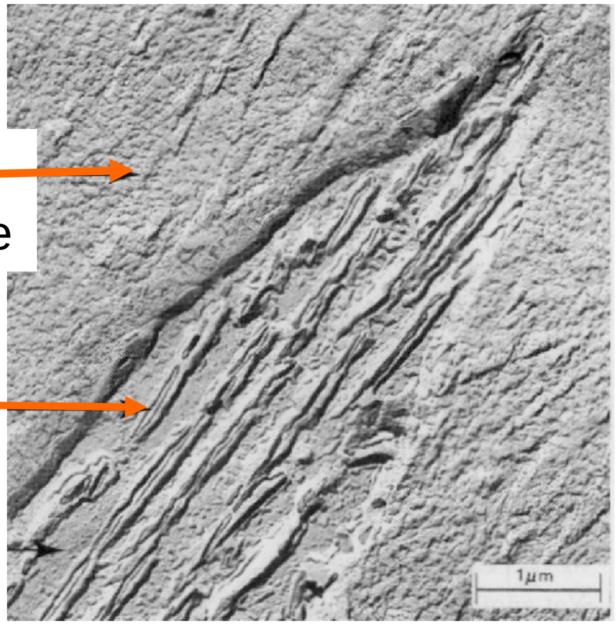
➡ ***Phase Transformation* 제어을 통한 *microstructure*의 조절 가능**

Control of Phases by Heat Treatment



Martensite ;
Non-equilibrium phase
(Very hard)

Pearlite
(Fe_3C+ferrite)



Heat Treatment 공정조절

Phase & Microstructure

Properties of Material

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

Martensite

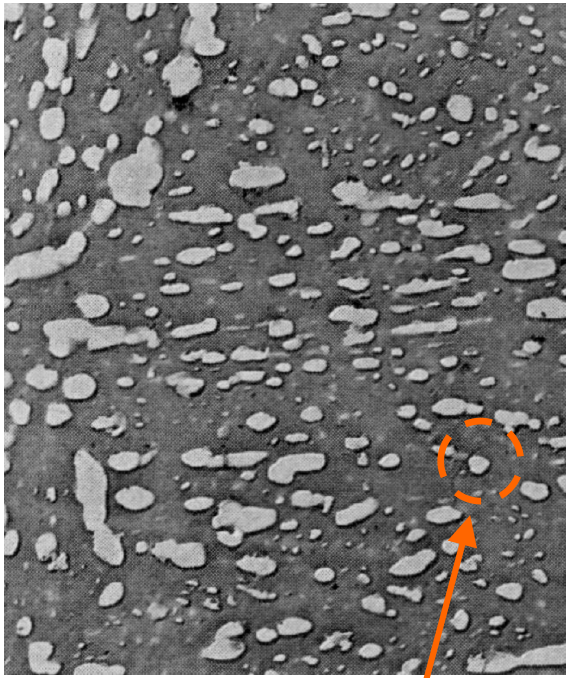
Tip of needle shape grain

Nucleation site of fracture

Brittle

공정조절

Proper heat treatment (tempering)



Tempered martensite

Very small & spherical shape grain

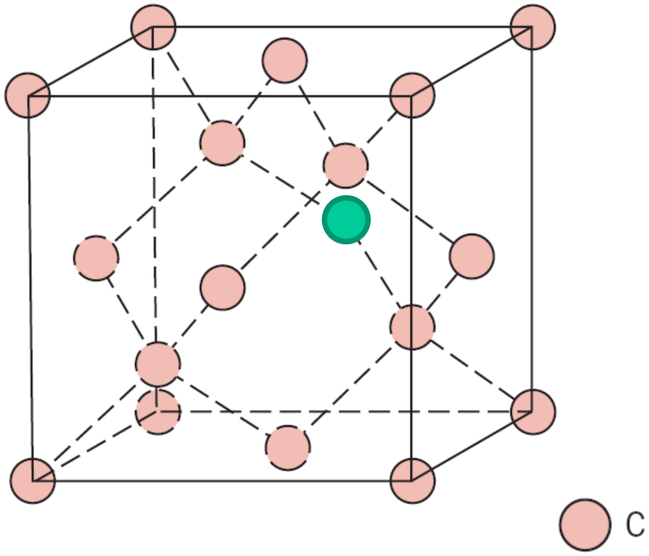
Good strength, ductility, toughness

High performance materials

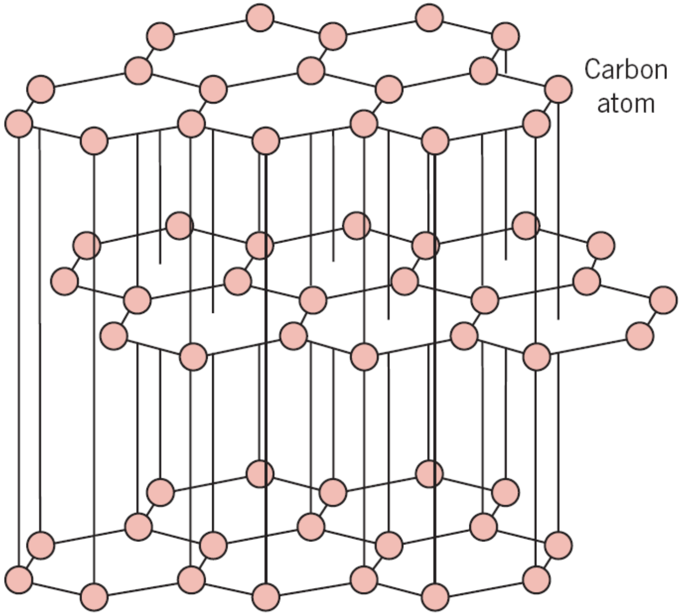
- High/low temperature
- High specific strength (strength/weight)
- High electrical performance
  - High/low dielectric, Ferroelectric, Superconductor
- Nano materials
- Bio-materials
- High performance coatings
- Structural materials
- Optical materials (LED, OLED, Fluorescent)
- Magnetic/Superconducting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

1) Same element, but different structure

diamond



graphite



10	Hardness	2
3.5 g/cm^3	density	2.2 g/cm^3
1.54 Å	bond length	3.4/1.48 Å
(111)	cleavage	(001)
cubic	crystal structure	hexagonal

Top 10 most expensive diamonds (1/2)

Allnatt Diamond
101 carat, $ 3M. 20 g

Moussaieff Red Diamond
14 carat, $ 7M. 2.78 g

The Heart of Eternity
14 carat, $ 16 M. 5.5 g

Wittelsbach Diamond
35.6 carat, $ 16.4 M.

The Steinmetz Pink
60 carat, $ 25 M.

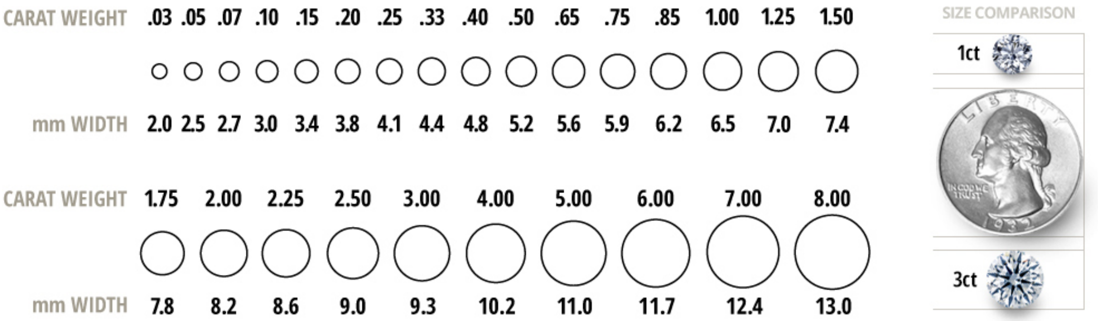
De Beers Centenary Diamond
274 carat, $ 100 M.

The Hope Diamond
45 carat, $ 350 M.

The Cullinan
3100 carat, $ 400 M.

Anything strange? Difference from the typical diamond?

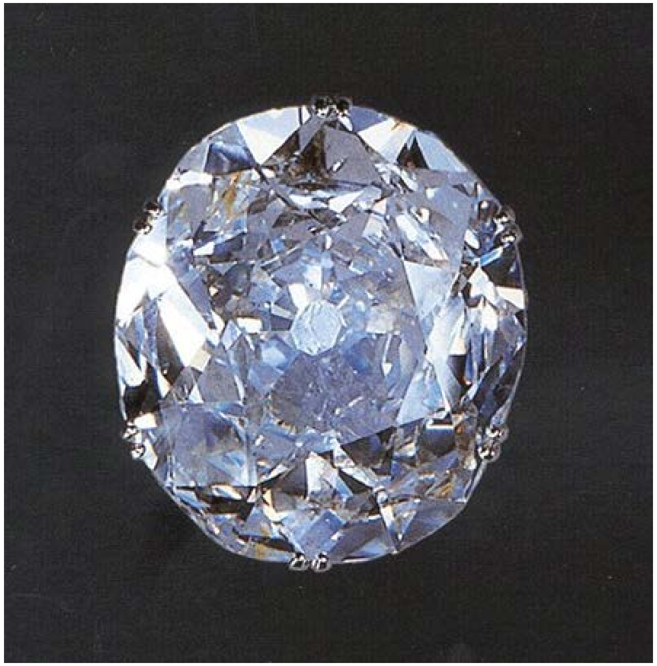
Top 10 most expensive diamonds (2/2)



CARAT WEIGHT	.03	.05	.07	.10	.15	.20	.25	.33	.40	.50	.65	.75	.85	1.00	1.25	1.50
mm WIDTH	2.0	2.5	2.7	3.0	3.4	3.8	4.1	4.4	4.8	5.2	5.6	5.9	6.2	6.5	7.0	7.4

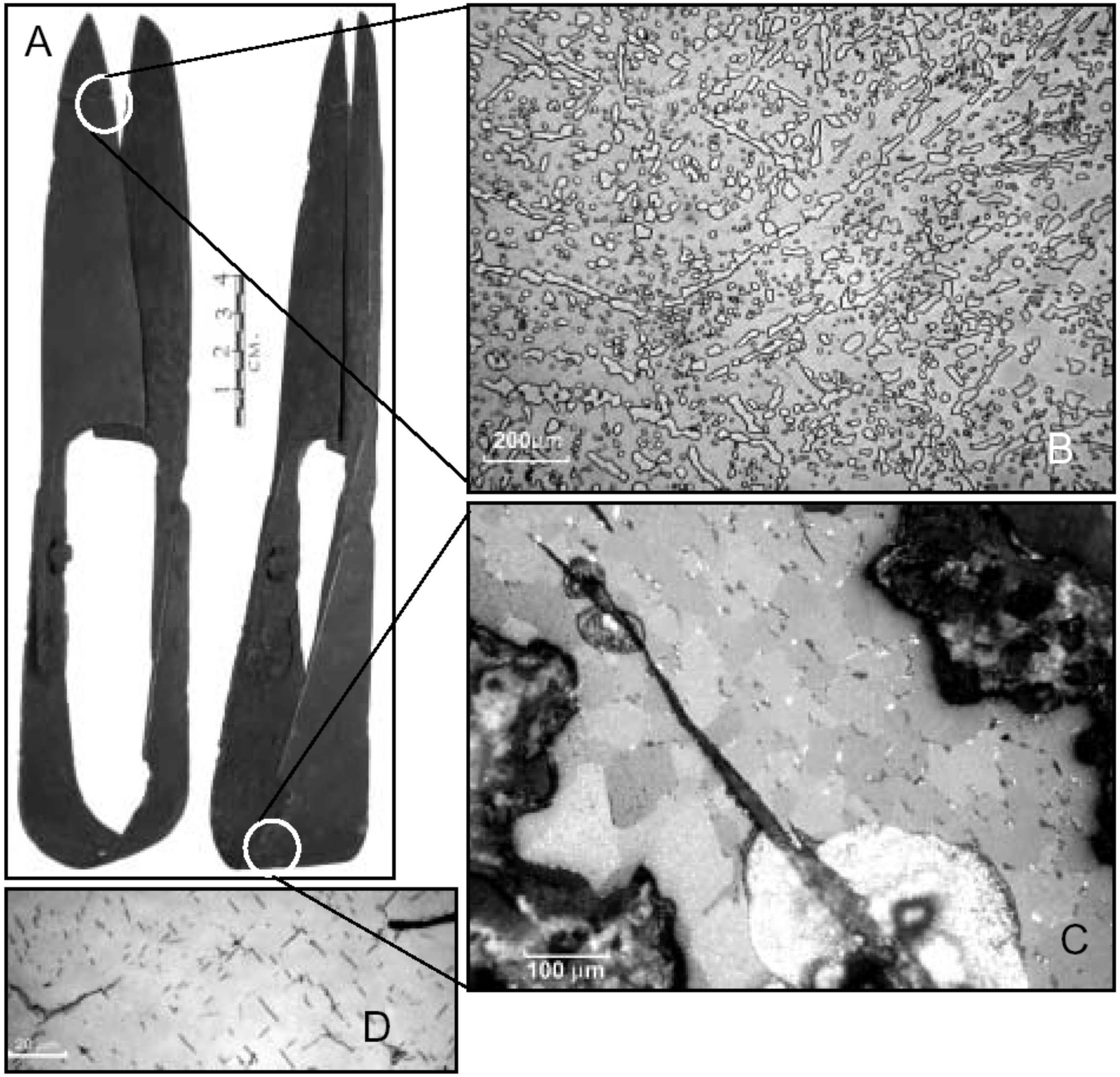
CARAT WEIGHT	1.75	2.00	2.25	2.50	3.00	4.00	5.00	6.00	7.00	8.00
mm WIDTH	7.8	8.2	8.6	9.0	9.3	10.2	11.0	11.7	12.4	13.0

Sancy Diamond
55 carat, $ not estimated.
The great Mughal of India

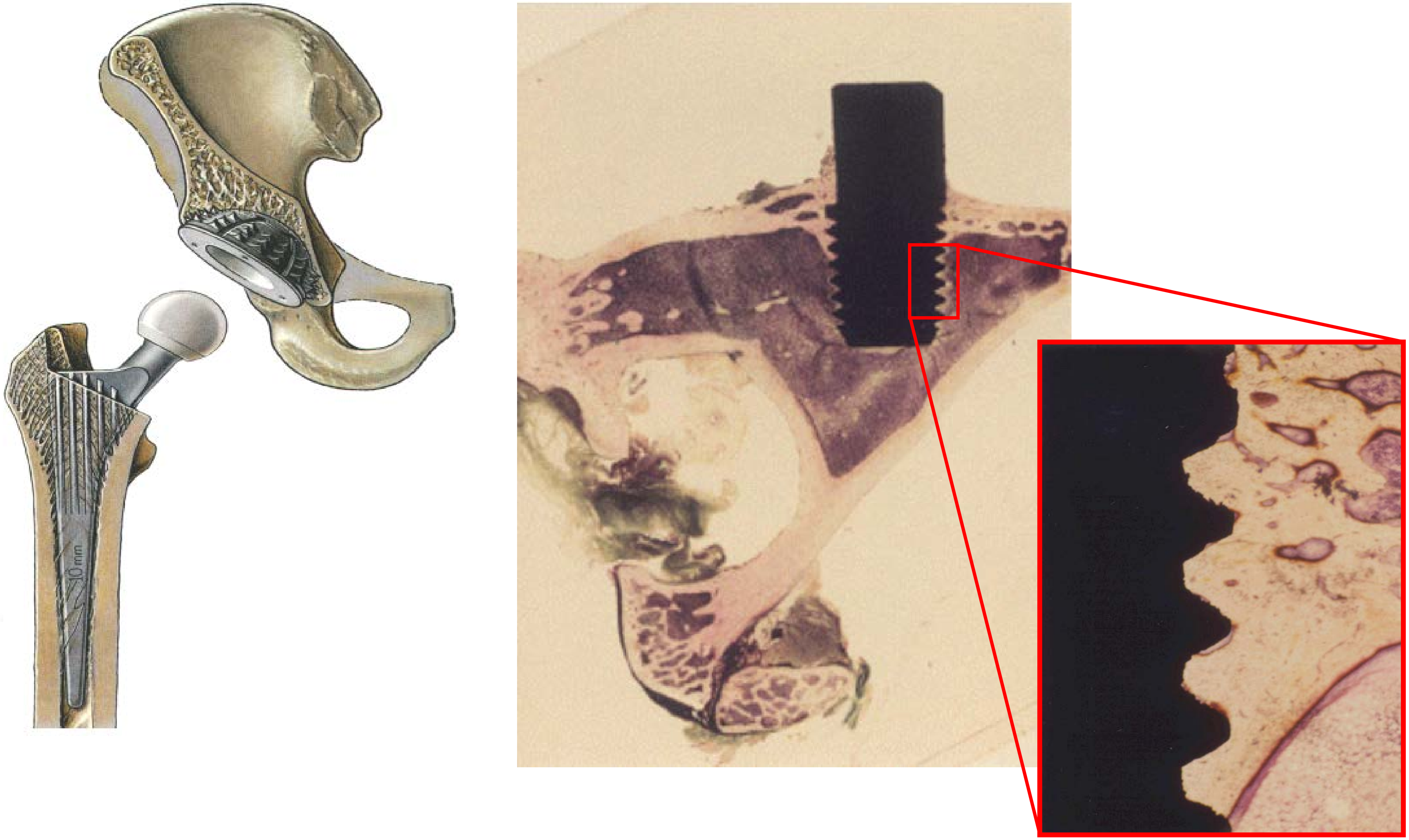


Kohinoor
105 carat, $ not estimated
Purest form of diamond

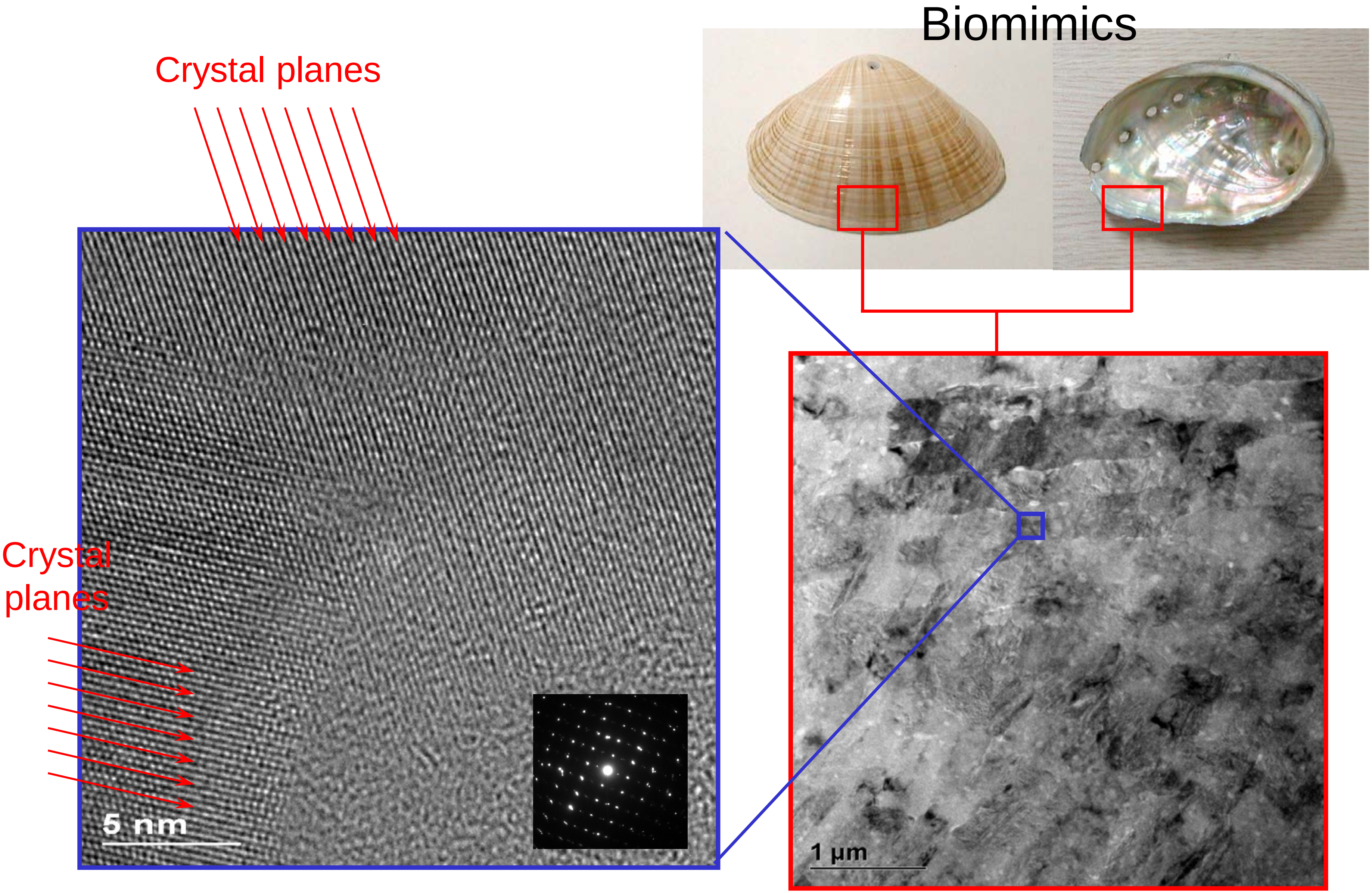
2) Improvement – Microstructure Control



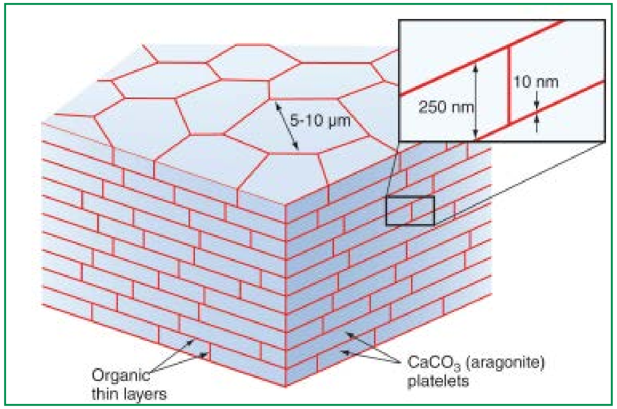
2) Materials for Bio-Medical Application
-Should be failure-proof



Copying from the Nature



Development of ultra-high tough composites



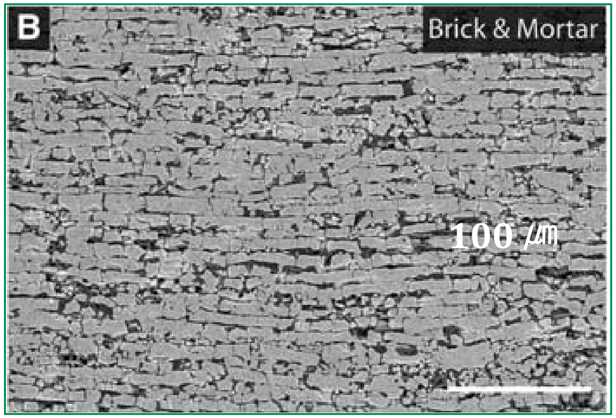
Biological materials

Organic materials / $CaCo_3$

$V_{f.CaCo3}$ ~ 95 vol.%
Thickness δ : < ~ 0.5 ㎛
Wavelength λ < ~ 0.5 ㎛

Bio-inspired materials

Ceramic Brick & PMMA mortar



PMMA / Al_2O_3

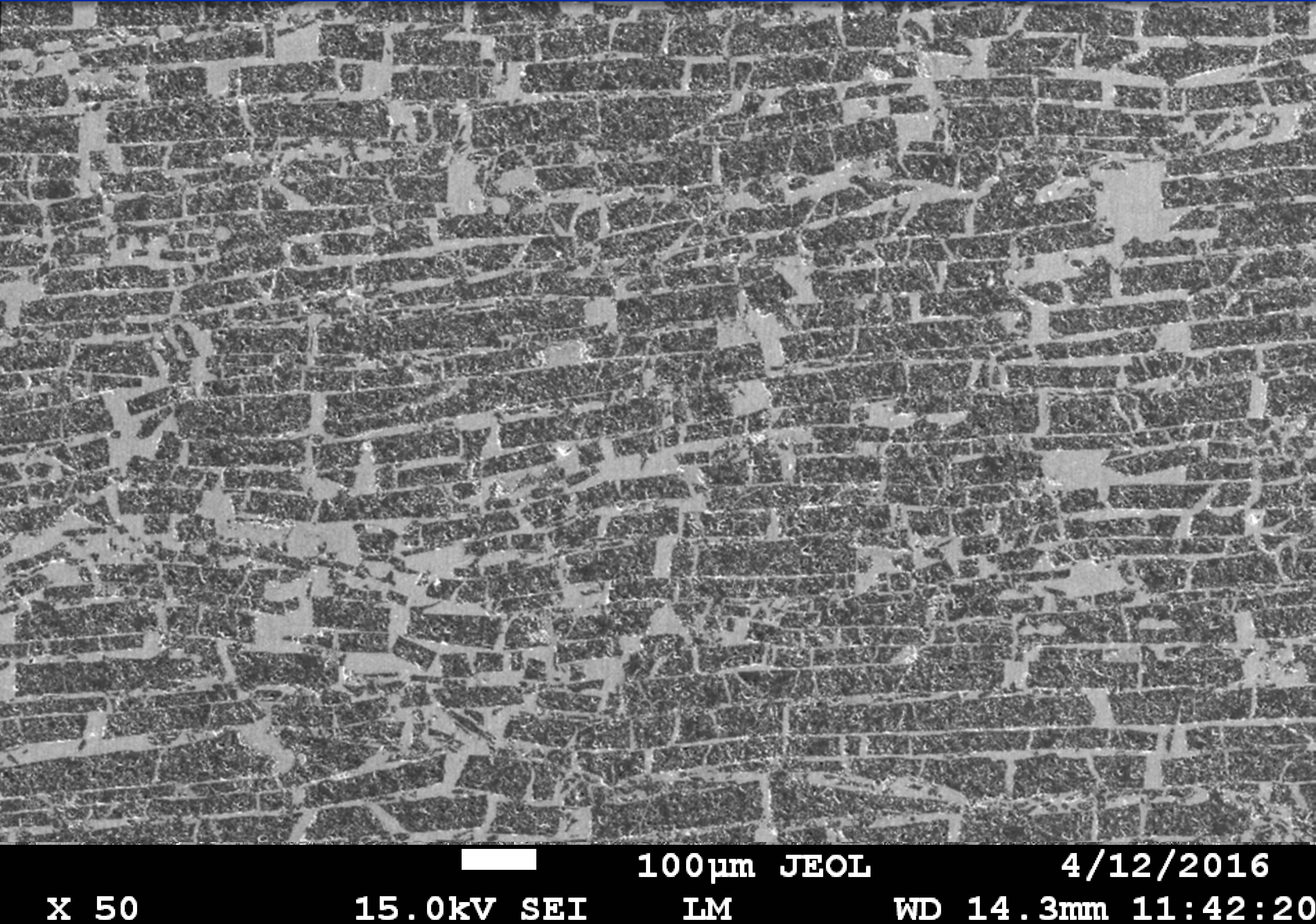
$V_{f.Al2O3}$ ~ 80 vol.%
Thickness δ : < 5 ~ 10 ㎛
Wavelength λ < 11 ~ 12 ㎛

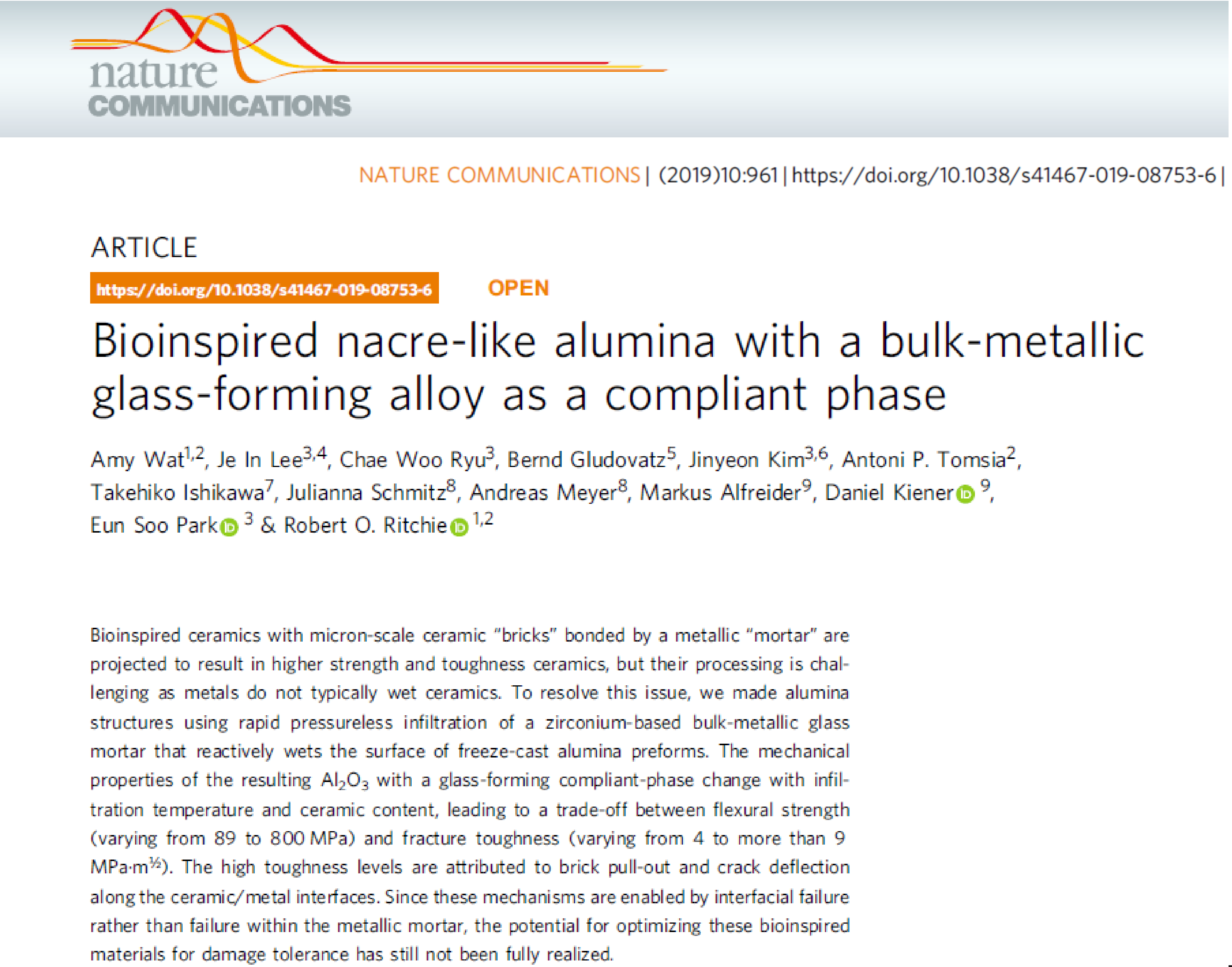
Ceramic Brick & Metal mortar
structure

BMG / Al_2O_3

High strength: > 2 GPa
Large elastic limit: ~ 2 %

Al_2O_3 Ceramic Brick & Zr-BMG mortar composites





nature COMMUNICATIONS

NATURE COMMUNICATIONS | (2019)10:961 | https://doi.org/10.1038/s41467-019-08753-6 |

ARTICLE

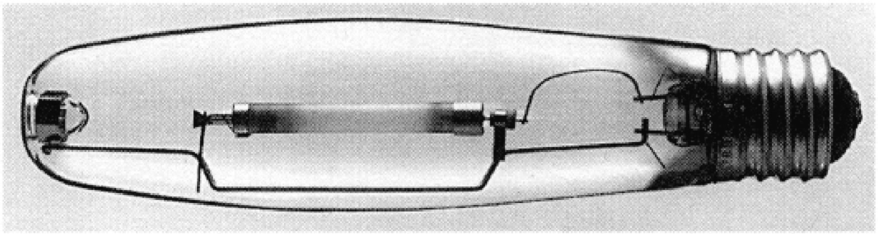
https://doi.org/10.1038/s41467-019-08753-6 OPEN

Bioinspired nacre-like alumina with a bulk-metallic glass-forming alloy as a compliant phase

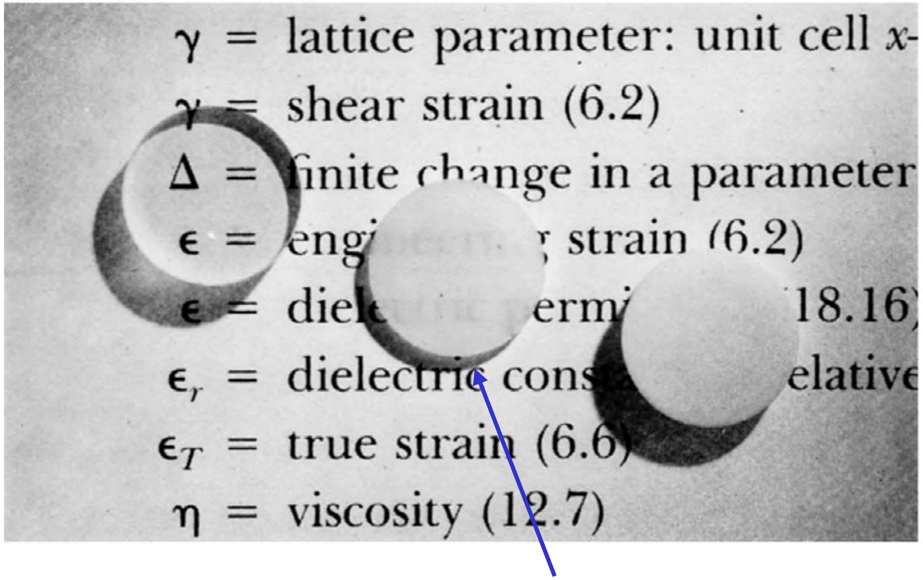
Amy Wat[1,2], Je In Lee[3,4], Chae Woo Ryu[3], Bernd Gludovatz[5], Jinyeon Kim[3,6], Antoni P. Tomsia[2], Takehiko Ishikawa[7], Julianna Schmitz[8], Andreas Meyer[8], Markus Alfreider[9], Daniel Kiener [9], Eun Soo Park [3] & Robert O. Ritchie [1,2]

Bioinspired ceramics with micron-scale ceramic "bricks" bonded by a metallic "mortar" are projected to result in higher strength and toughness ceramics, but their processing is challenging as metals do not typically wet ceramics. To resolve this issue, we made alumina structures using rapid pressureless infiltration of a zirconium-based bulk-metallic glass mortar that reactively wets the surface of freeze-cast alumina preforms. The mechanical properties of the resulting Al_2O_3 with a glass-forming compliant-phase change with infiltration temperature and ceramic content, leading to a trade-off between flexural strength (varying from 89 to 800 MPa) and fracture toughness (varying from 4 to more than 9 MPa·m$^{1/2}$). The high toughness levels are attributed to brick pull-out and crack deflection along the ceramic/metal interfaces. Since these mechanisms are enabled by interfacial failure rather than failure within the metallic mortar, the potential for optimizing these bioinspired materials for damage tolerance has still not been fully realized.

2) Microstructure of optical fiber

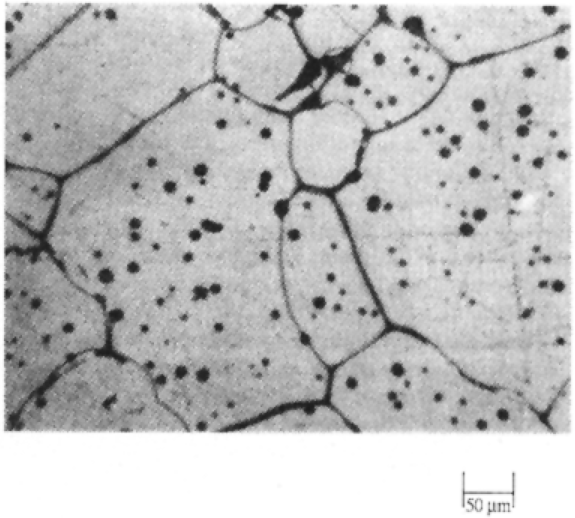


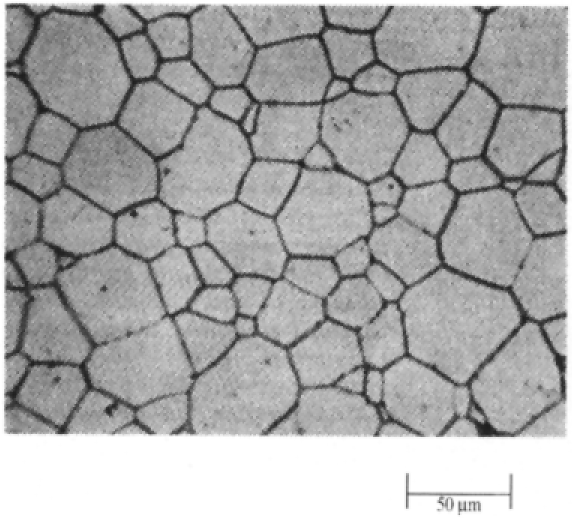
high temp
sodium vapor lamp
Al_2O_3



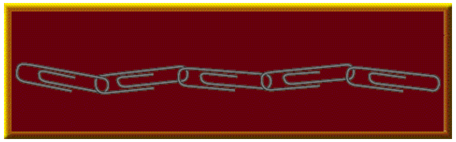
opaque

translucent

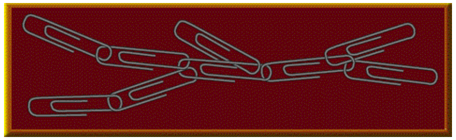




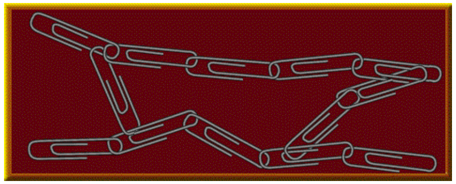
2) Improvement : Lighter and Stronger



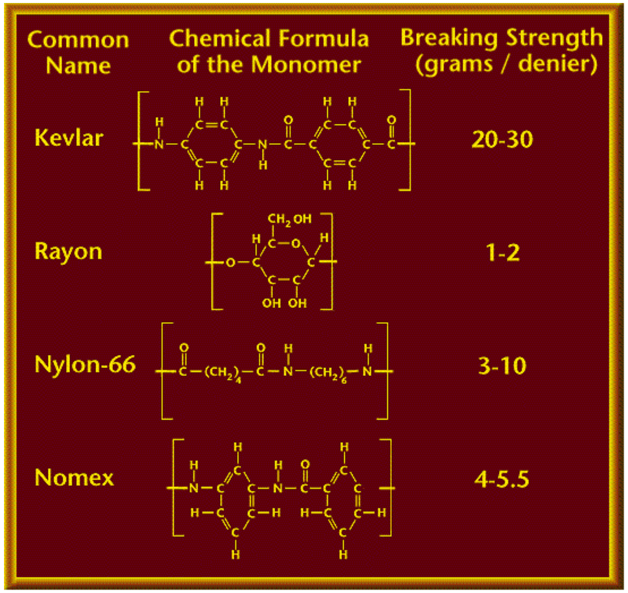
Linear polymer : Microwaveable food containers, Dacron carpets and Kevlar ropes



Branched polymers : flexible shampoo bottles and milk jugs



Cross-linked polymers : Car tires and bowling balls



Common Name	Chemical Formula of the Monomer	Breaking Strength (grams / denier)
Kevlar		20-30
Rayon		1-2
Nylon-66	$-\overset{O}{\overset{\|}{C}}-(CH_2)_4-\overset{O}{\overset{\|}{C}}-\overset{H}{\overset{\|}{N}}-(CH_2)_6-\overset{H}{\overset{\|}{N}}-$	3-10
Nomex		4-5.5

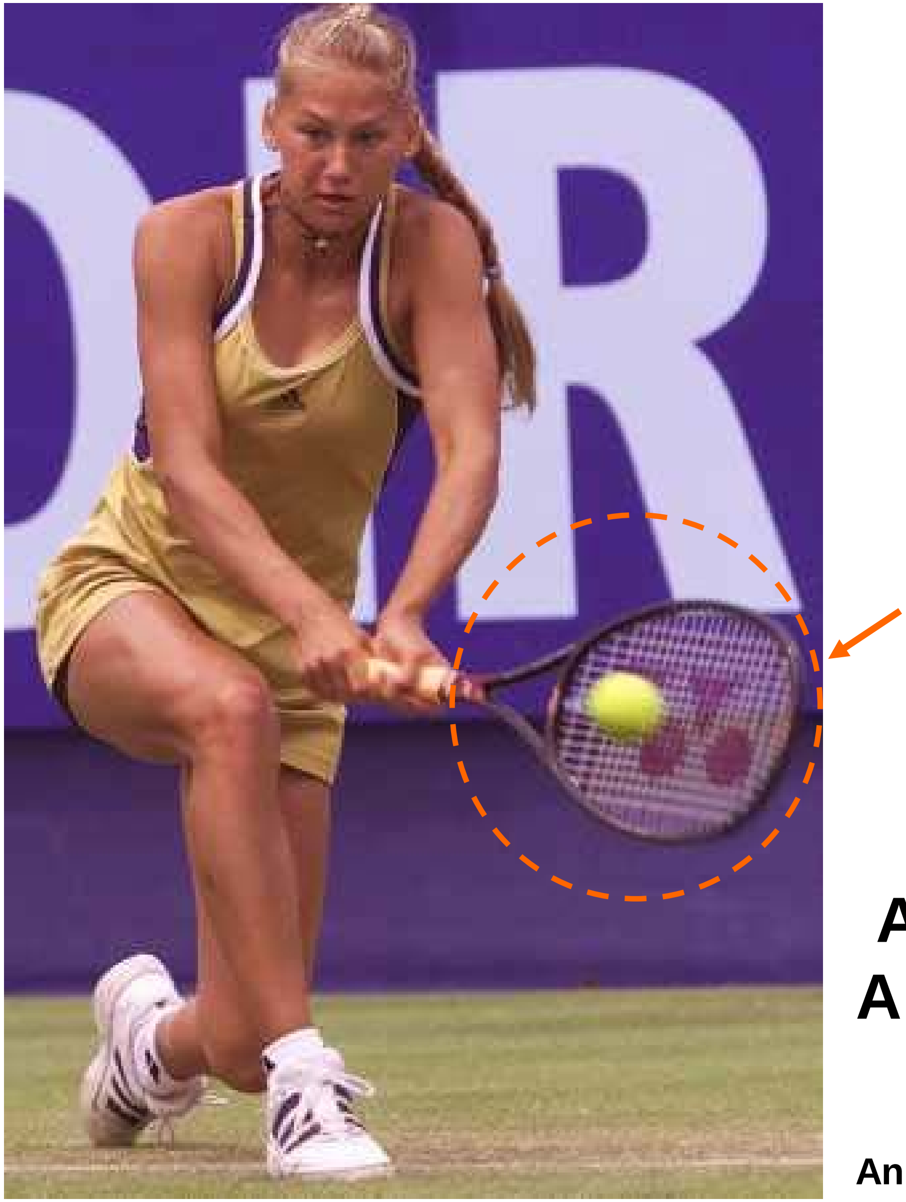
3) Improvement : Phase transformation

Boeing 777

이륙 전 (47 °C)

이륙 후 지상 10000m 높이
외부 온도 영하 38°C

> 섭씨 80도 이상의 온도 차이에서도 안정된 날개



Look !!

Not Anna,
But Racket

Moment of Impact

If the racket is weak
or Its head is small,
…

Anna cannot win alone.
A good racket is needed.

Anna Kournikova

4) Improvement : Composite & Design

a.**Tennis Racket**

Stronger and lower density material → **Bigger head** → **More comfortable to play**

1700’s

1970’s

today

b. **Fighters ;**

Most strong, light, and tough Materials

FW-190

1940's Aluminum alloy

F-22 Raptor

2000's Titanium alloy + Carbon fiber Composites

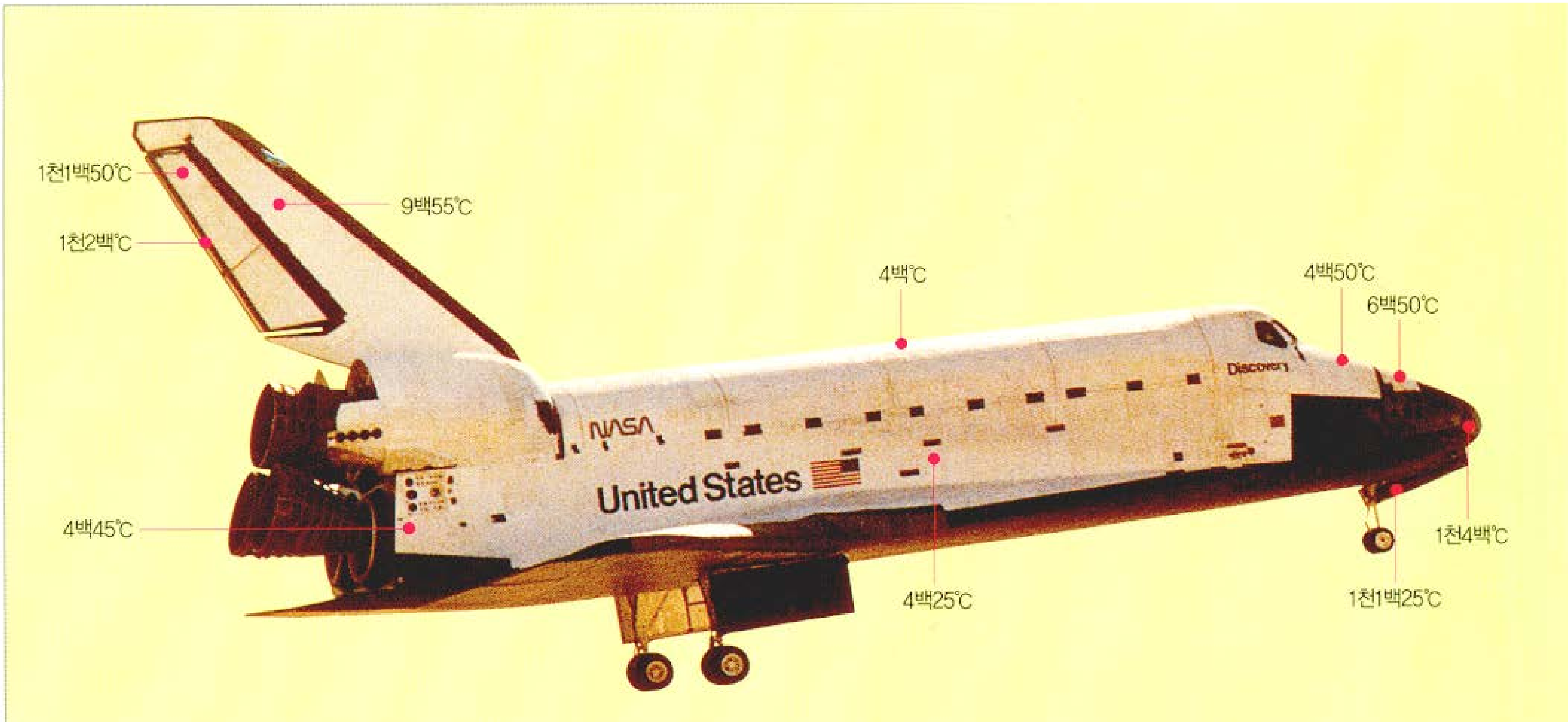
Voker Dr I

1910's wood, canvas

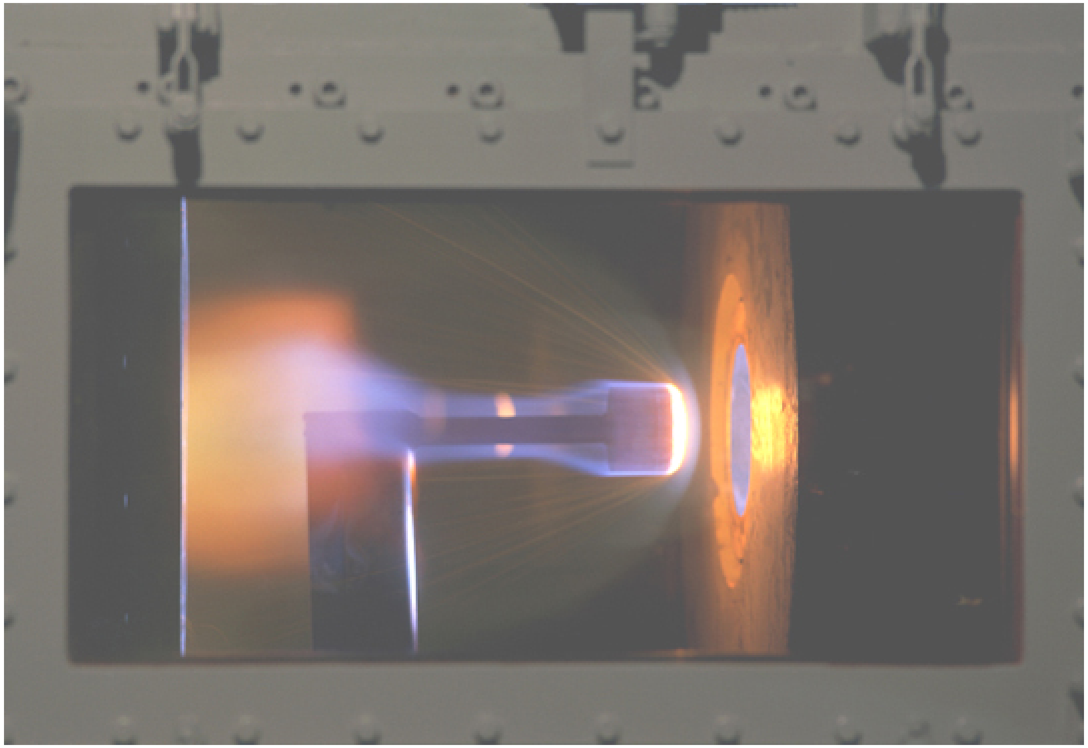
F-14 Tomcat

1970's Steel + Titanium alloy

c. Space Shuttle



c-i) 내열 재료

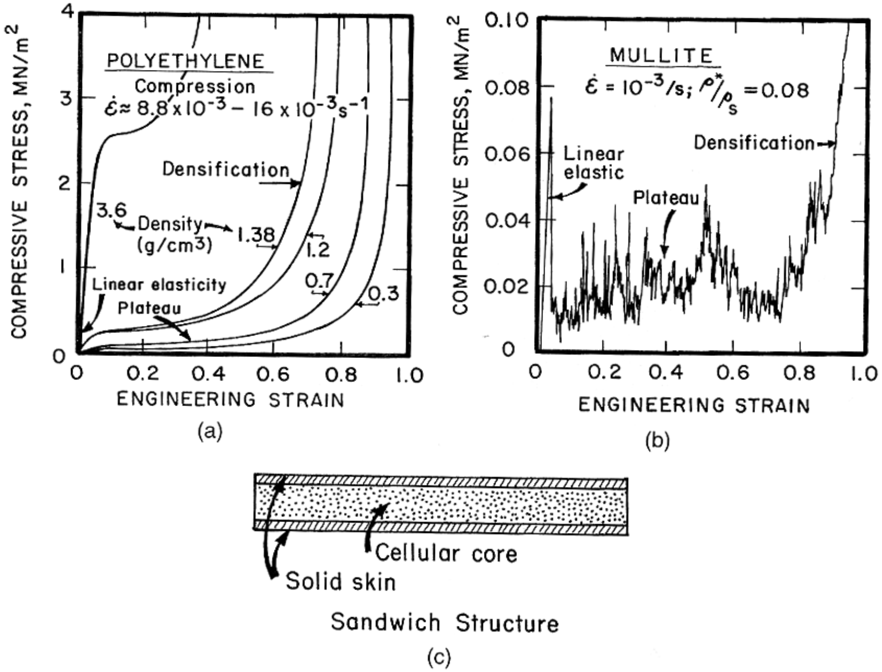


The high temperatures that were to be encountered by the Space Shuttle were simulated in the wind tunnels at Langley in this 1975 test of the thermal insulation materials that were used on the Space Shuttle Orbiter.

Credits - NASA

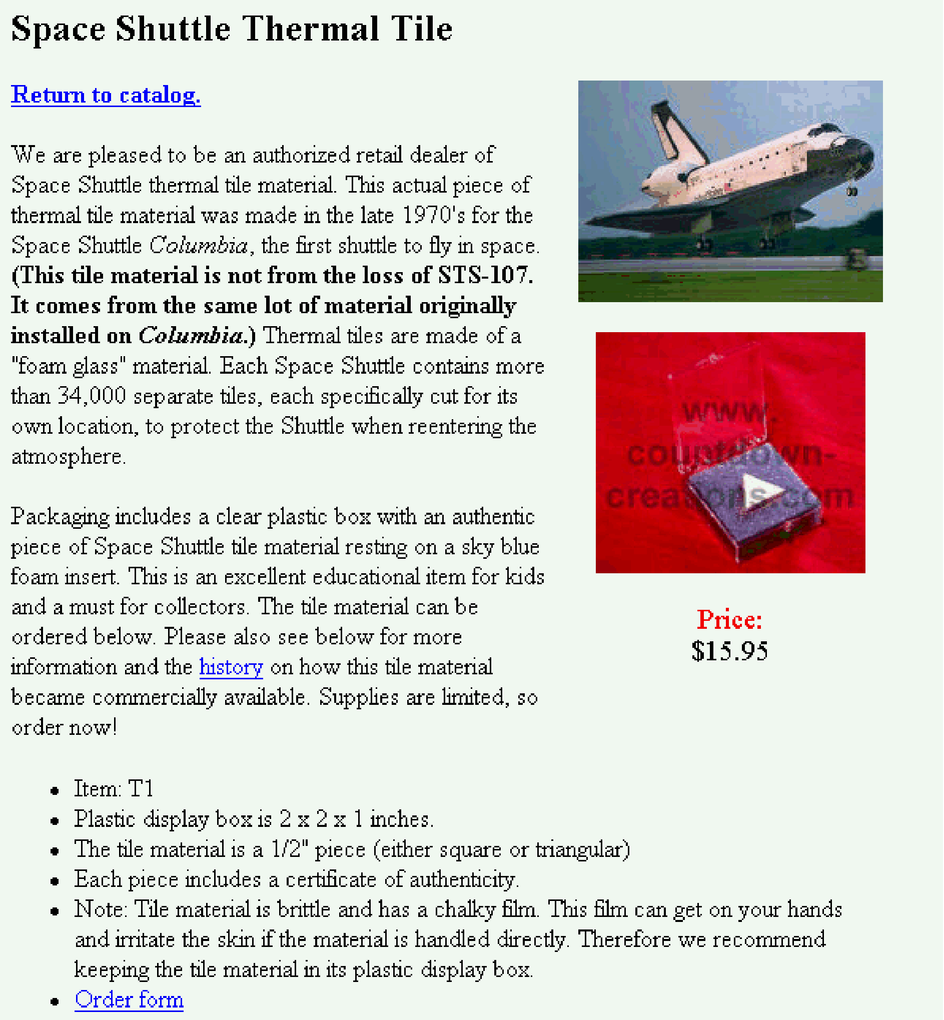
c-ii) Other forms of materials

Porous and Cellular Materials



(a) (b) (c)

Figure 1.31 Compressive stress–strain curves for foams. (a) Polyethylene with different initial densities. (b) Mullite with relative density P^x / Ps = 0.08 (adapted from L. J. Gibson and M. F. Ashby, *Cellular Solids: Structure and Properties* (Oxford, UK: Pergamon Press 1988), pp. 124, 125). (c) Schematic of a sandwich structure.



Space Shuttle Thermal Tile

Return to catalog.

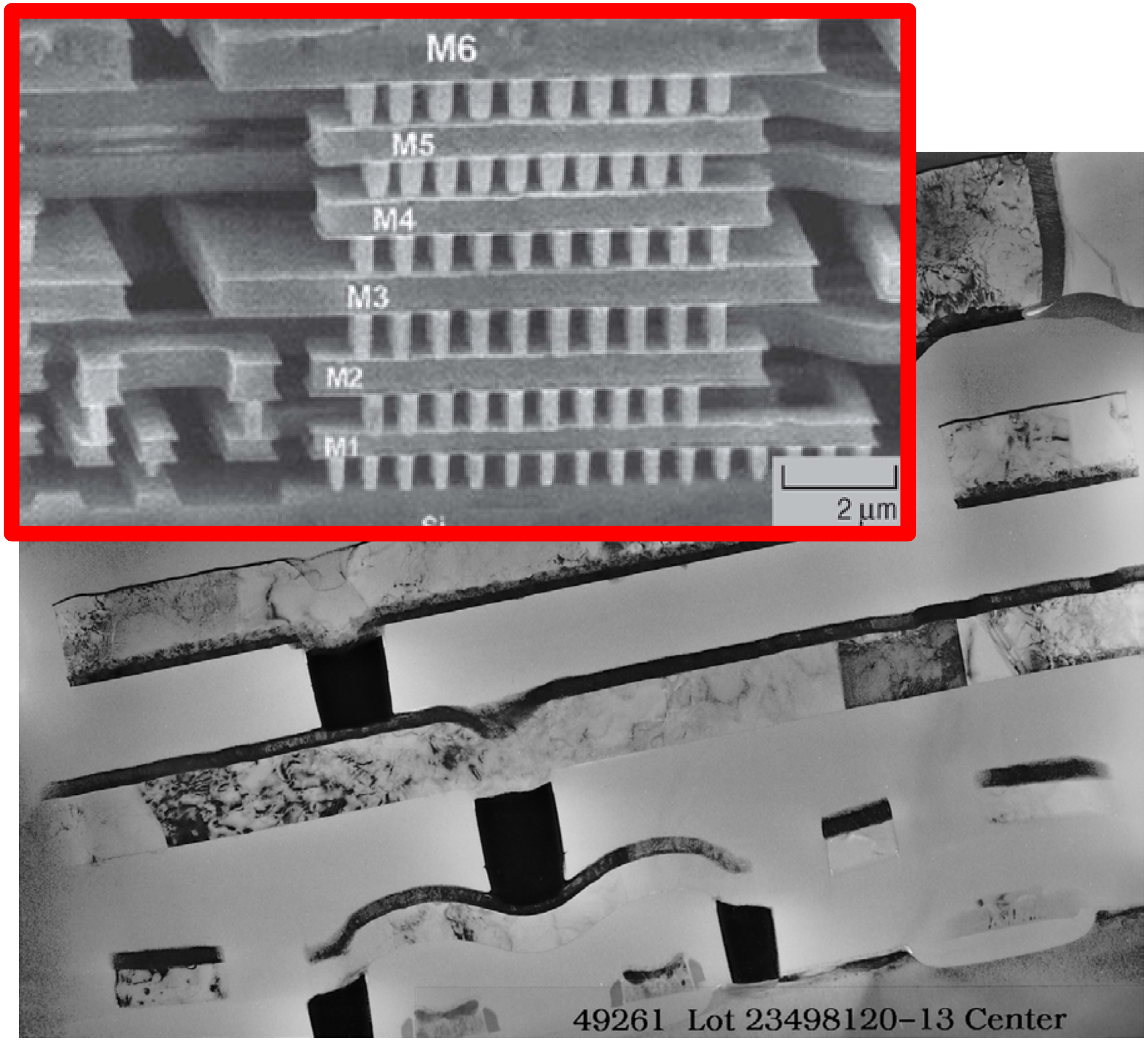
We are pleased to be an authorized retail dealer of Space Shuttle thermal tile material. This actual piece of thermal tile material was made in the late 1970's for the Space Shuttle *Columbia*, the first shuttle to fly in space. **(This tile material is not from the loss of STS-107. It comes from the same lot of material originally installed on *Columbia*.)** Thermal tiles are made of a "foam glass" material. Each Space Shuttle contains more than 34,000 separate tiles, each specifically cut for its own location, to protect the Shuttle when reentering the atmosphere.

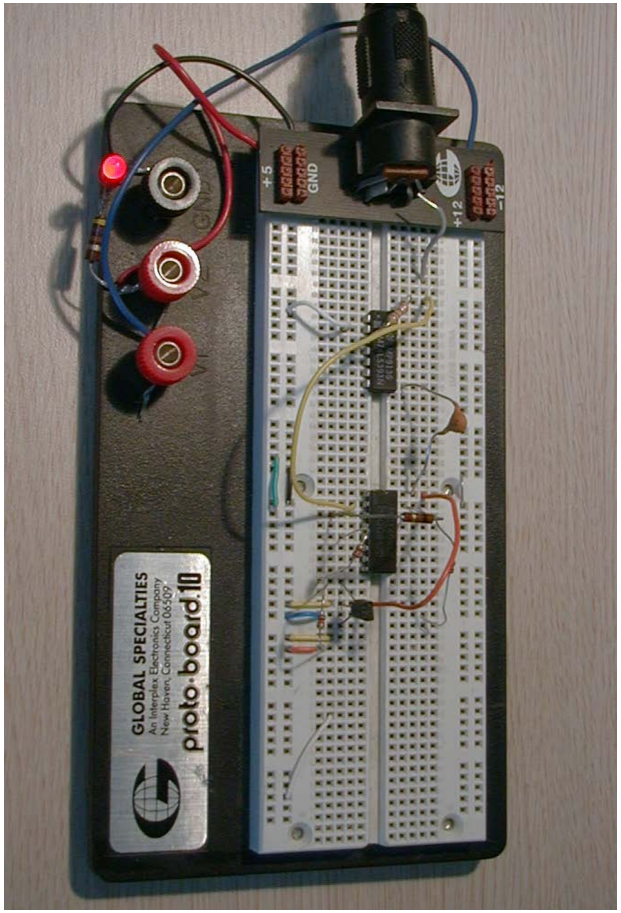
Packaging includes a clear plastic box with an authentic piece of Space Shuttle tile material resting on a sky blue foam insert. This is an excellent educational item for kids and a must for collectors. The tile material can be ordered below. Please also see below for more information and the history on how this tile material became commercially available. Supplies are limited, so order now!

Price:
$15.95

- Item: T1
- Plastic display box is 2 x 2 x 1 inches.
- The tile material is a 1/2" piece (either square or triangular)
- Each piece includes a certificate of authenticity.
- Note: Tile material is brittle and has a chalky film. This film can get on your hands and irritate the skin if the material is handled directly. Therefore we recommend keeping the tile material in its plastic display box.
- Order form

d) Combination of Materials

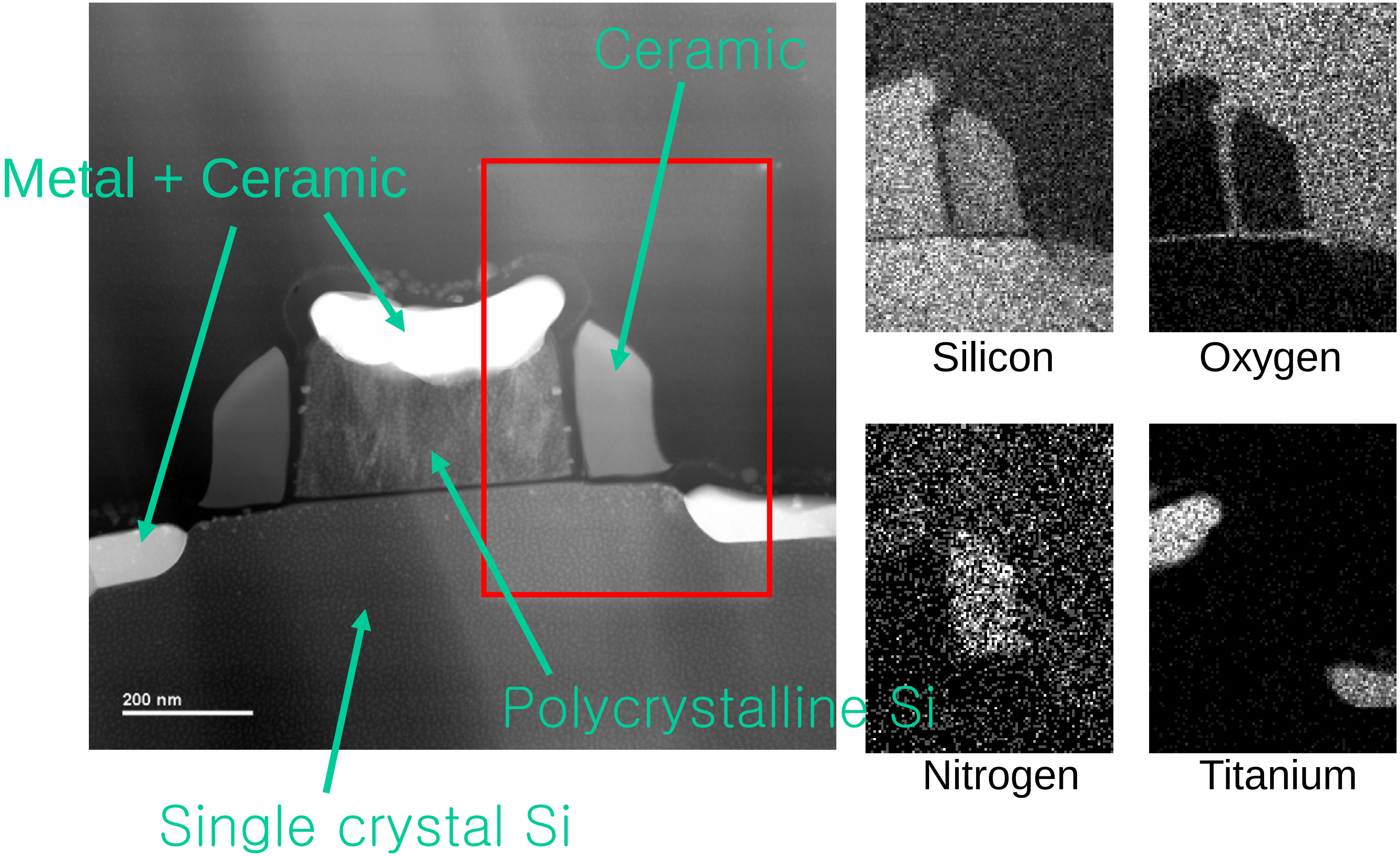




Detailed view of transistor

ADF image

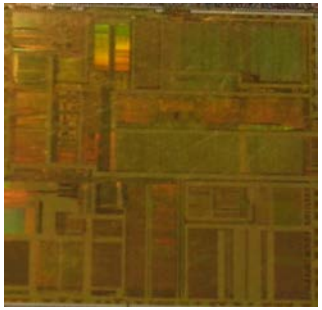
EDS mapping



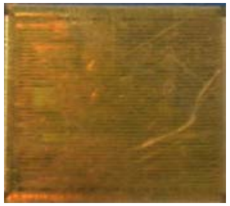
Moore’s Law

“The number of transistors incorporated in a chip will approximately double every ~~24~~ 18 months”

10 mm

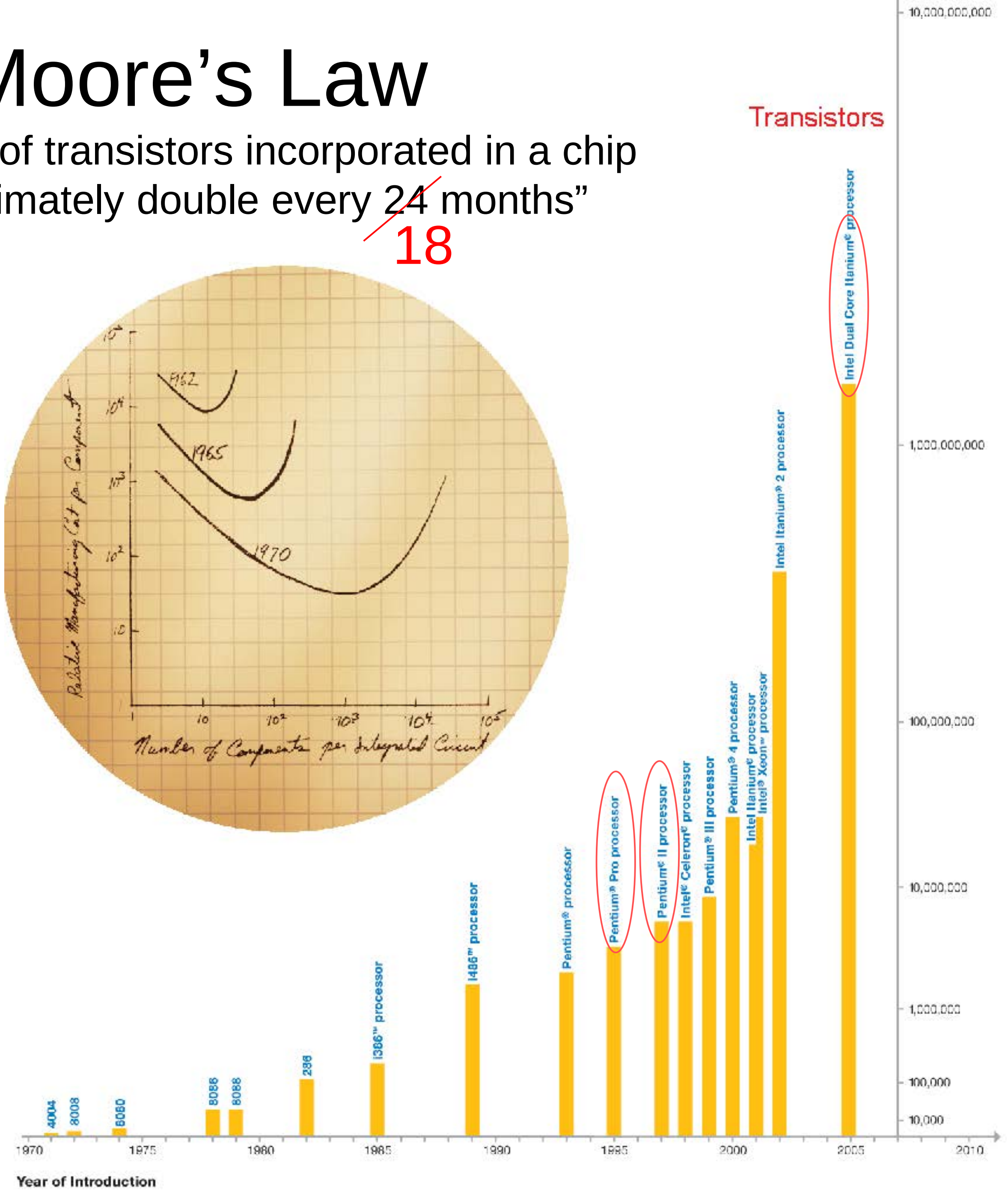


Pentium, 0.8 μm line width

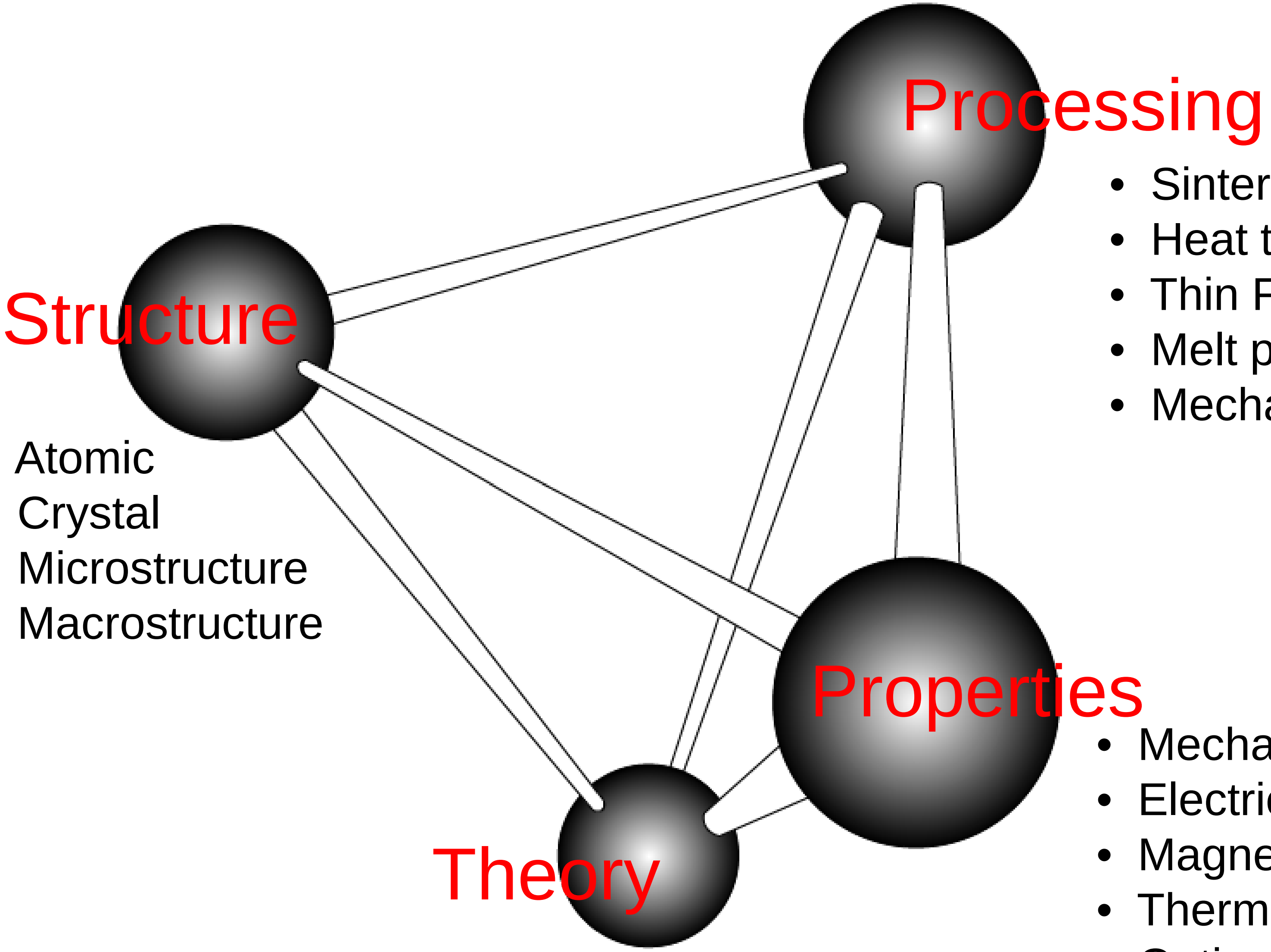


Pentium, 0.5 μm line width

Pentium II, 0.25 μm line width



Materials Science and Engineering



Structure

- Atomic
- Crystal
- Microstructure
- Macrostructure

Processing

- Sintering
- Heat treatment
- Thin Film
- Melt process
- Mechanical

Properties

- Mechanical
- Electrical
- Magnetic
- Thermal
- Optical

Theory

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 1일(화) 17:00~18:30 비대면 실시간 수업	**금속, 인류의 역사와 함께하다! 역사 속 금속 이야기**	수업자료
2차	9월8일(화) 17:00~18:30 비대면 실시간 수업	**Alloying: Understanding the Basics**	수업자료
3차	9월15일(화) 17:00~18:30 비대면 실시간 수업	**분임 토의**	팀 구성 및 각 도전주제 합금설계 브레인스토밍
4차	9월29일(화) 17:00~18:30 비대면 실시간 수업	**각 팀별 연구계획발표**	모든 팀원 협동 발표
5차	10월6일(화) 17:00~18:30 30동 218-1호	**각 팀별 합금 제조**	모 원소 준비/ 아크 용해 주조 실험
6차	10월13일(화) 17:00~18:30 30동 218-1호	**제조 시편의 미세구조 분석 I**	시편 전처리/ 광학현미경 관찰
7차	10월27일(화) 17:00~18:30 30동 218-1호	**제조 시편의 미세구조 분석 II**	전자현미경 관찰 실험
8차	11월03일(화) 17:00~18:30 30동 218-1호	**제조시편 기초 물성 분석**	X-선 회절분석, 경도 등 실험
9차	11월10일(화) 17:00~18:30 30동 218-1호	**제조시편 타겟 물성 분석**	타겟 물성 평가 실험 (강도, 연신 등)
10차	11월24일(화) 17:00~18:30 30동 218-1호	**최종연구결과 발표 및 토의**	개발 합금의 미래첨단기술 적용 아이디어 제안 포함

▣ 5주차-9주차 실험의 경우, 각 팀의 동선이 충돌되지 않도록 순환 실험진행 예정

2020 Fall

Introduction to Materials Science and Engineering

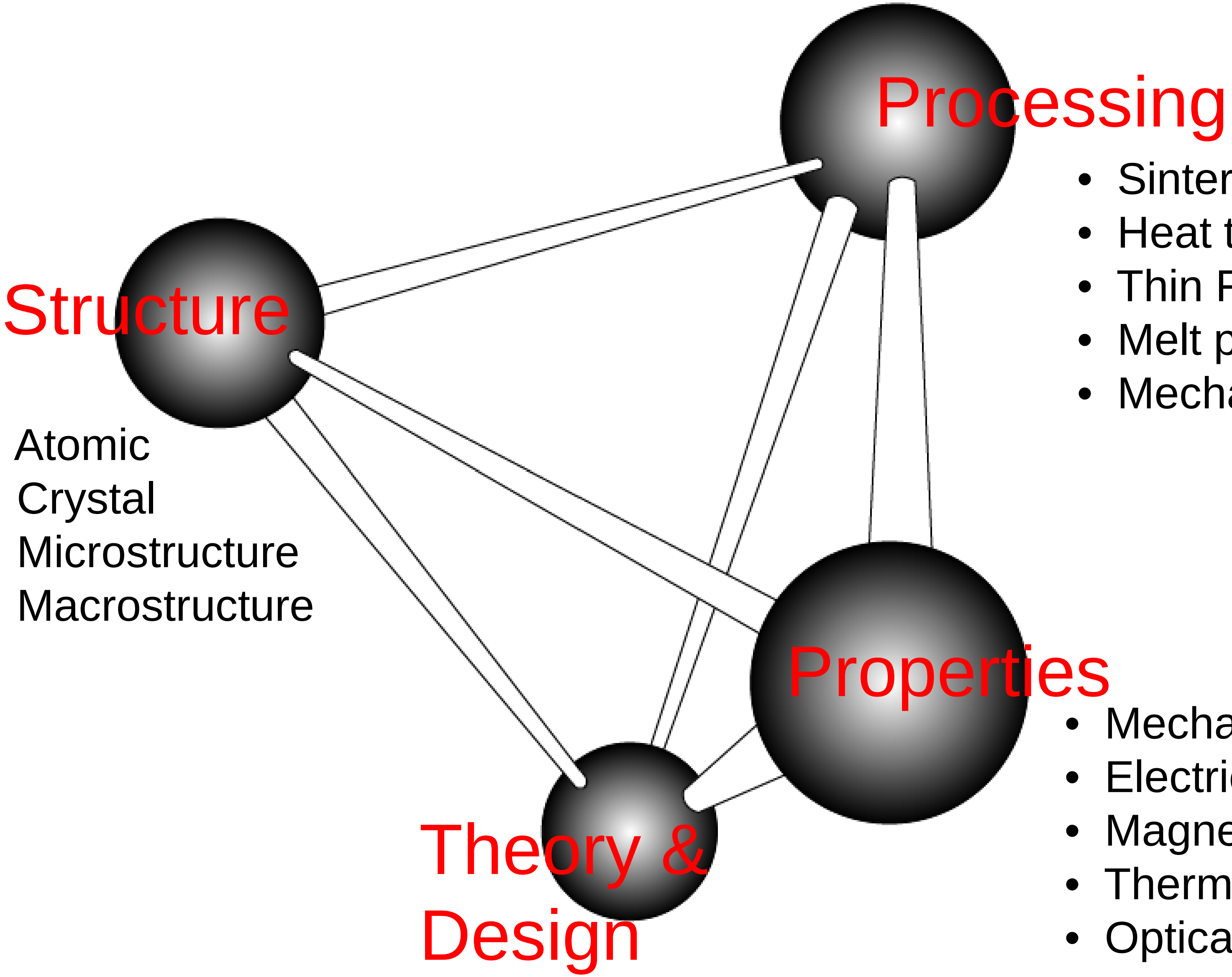
09. 03. 2020

Eun Soo Park

Office: 33-313
Telephone: 880-7221
Email: espark@snu.ac.kr
Office hours: by appointment

Contents for previous class

Materials Science and Engineering



Processing

- Sintering
- Heat treatment
- Thin Film
- Melt process
- Mechanical

Structure

- Atomic
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- Microstructure
- Macrostructure

Properties

- Mechanical
- Electrical
- Magnetic
- Thermal
- Optical

Theory & Design

Materials Science and Engineering

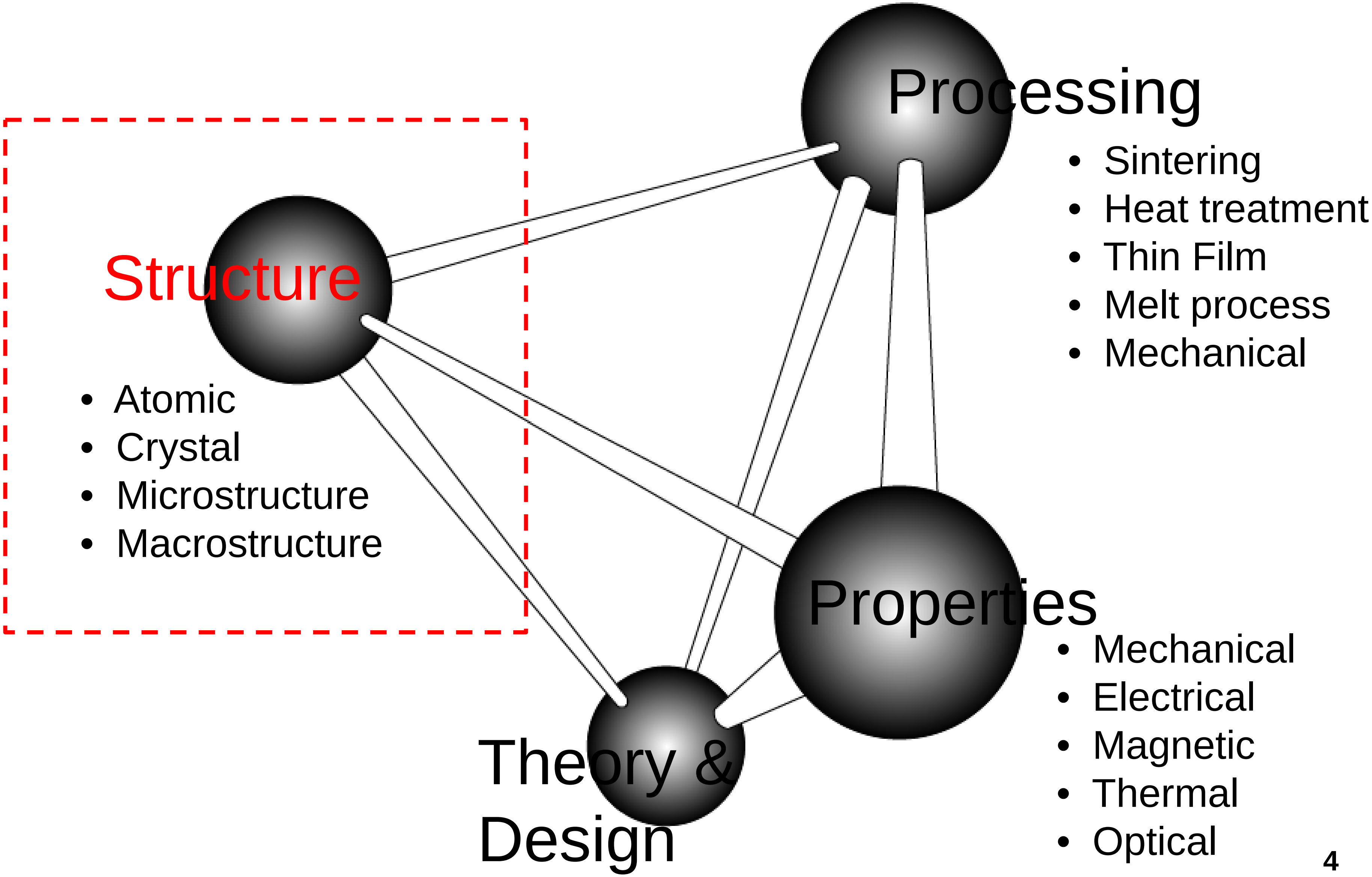
합금설계 + 공정조절 ➡

Microstructure Control of Materials

⬇

Better Material Properties

Materials Science and Engineering



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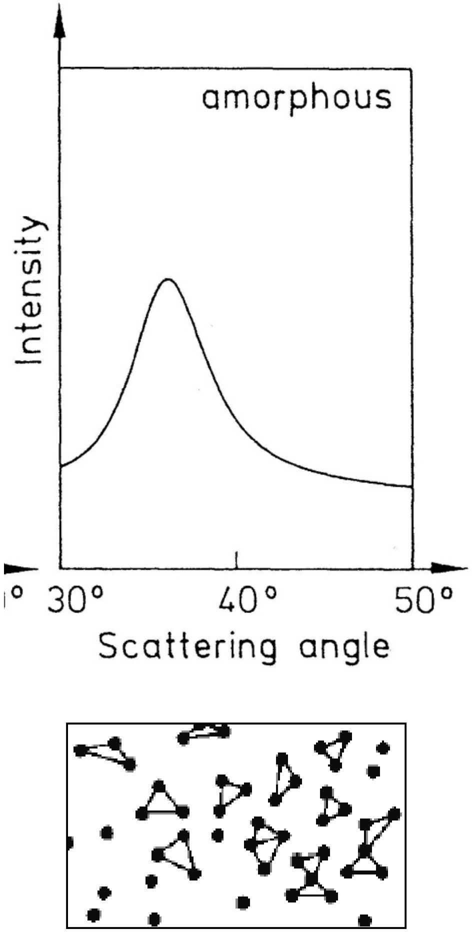
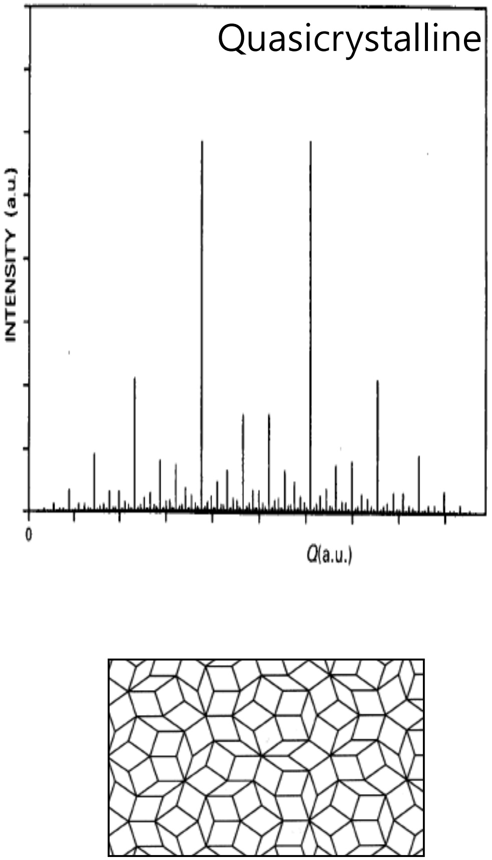
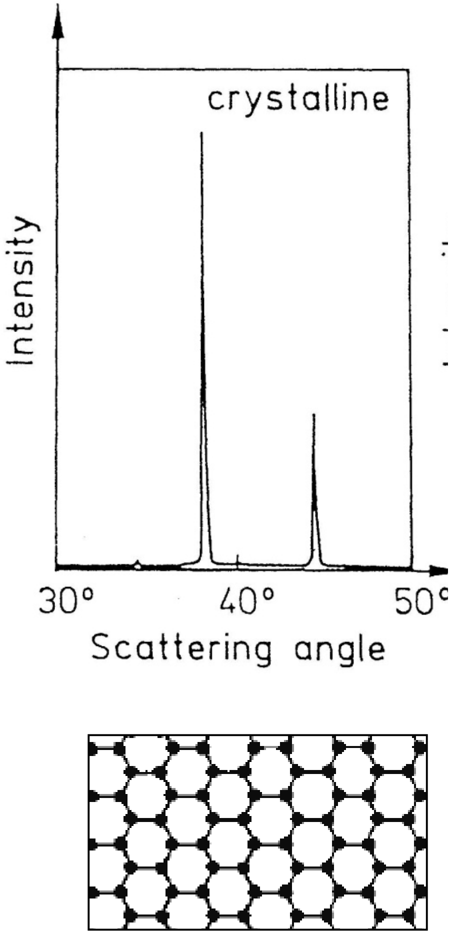
Theory & Design

Atomic structure

Short-range order ⟷ **Periodic order**

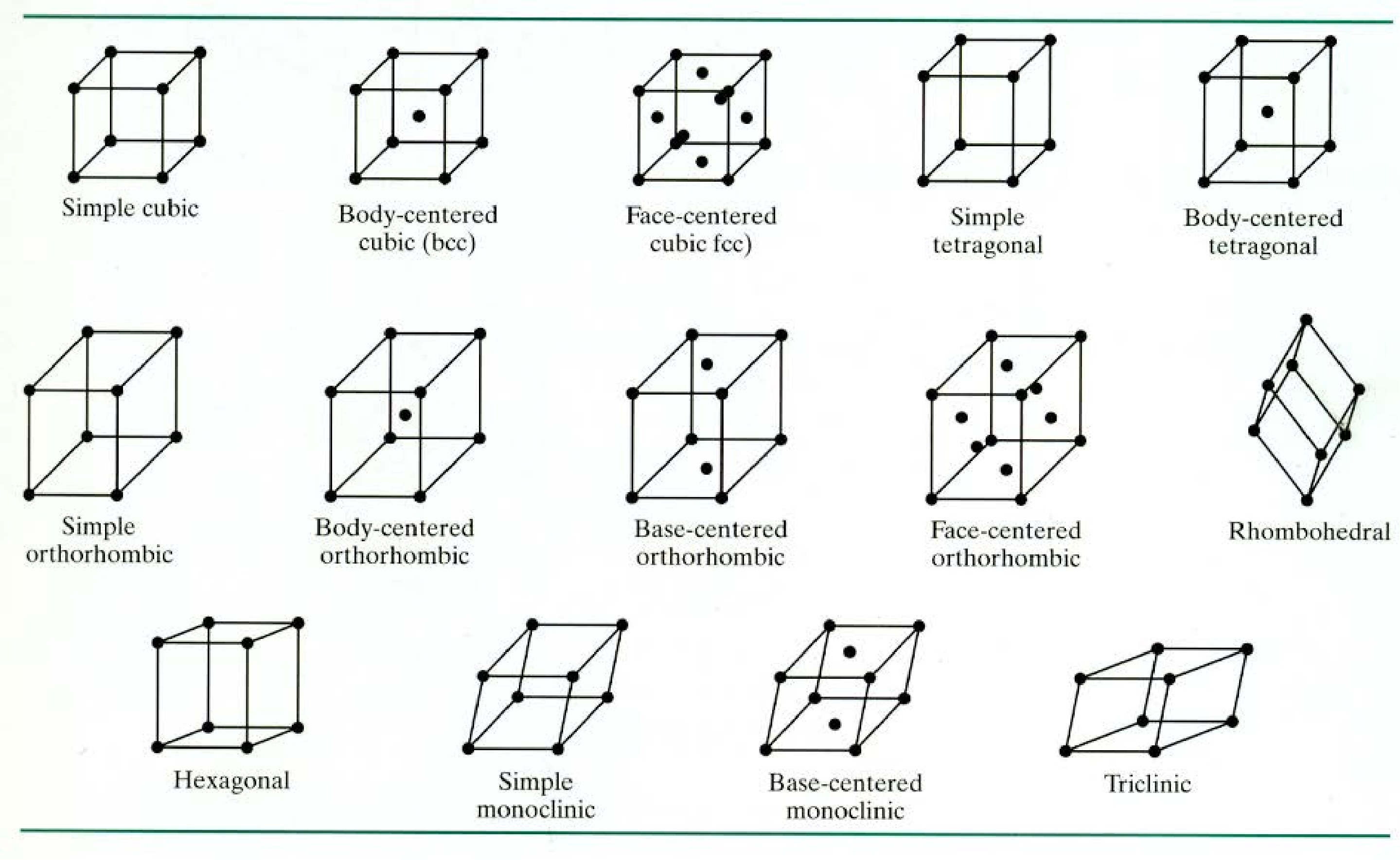






Crystal structure

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)

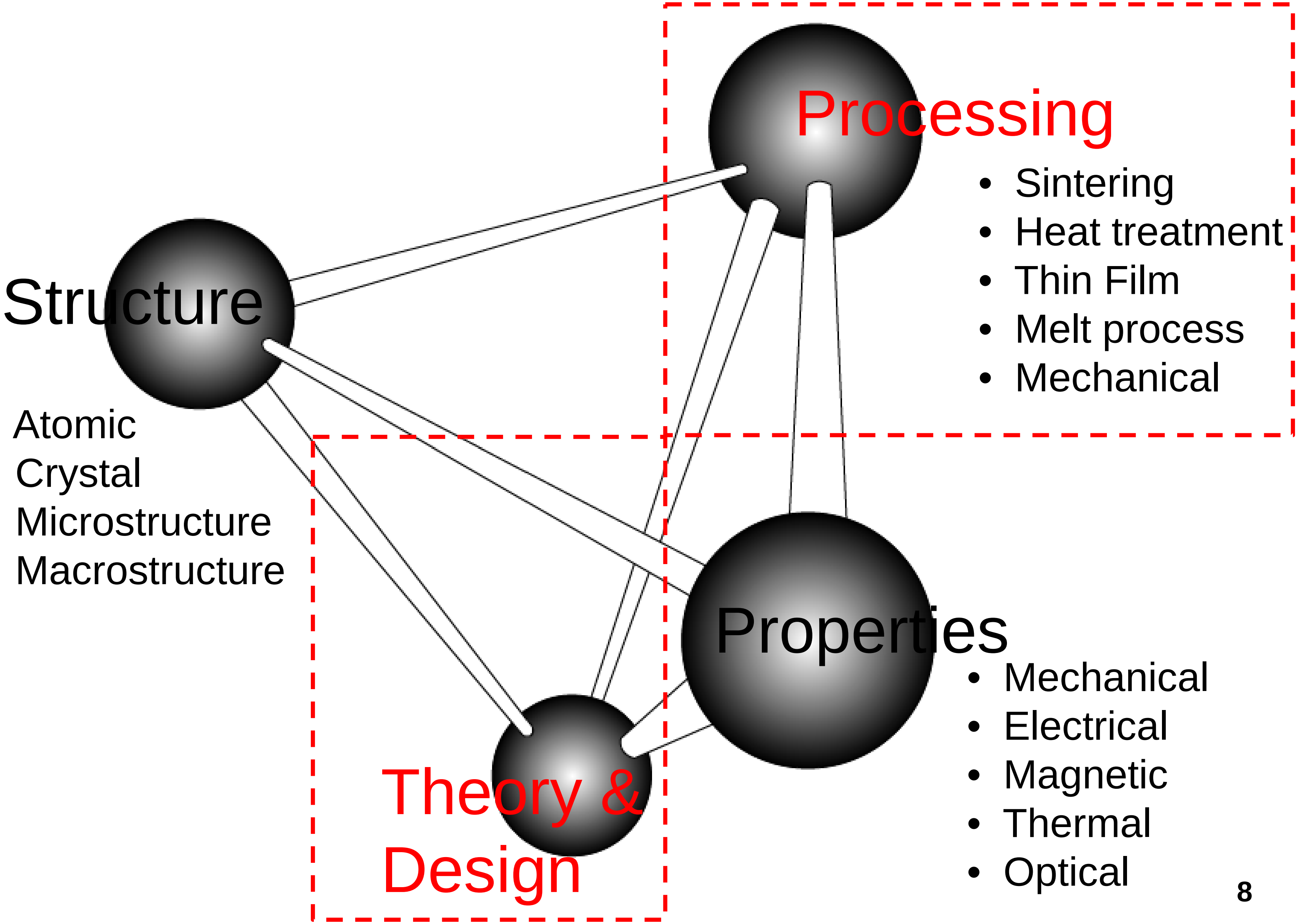
What is microstructure?

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)

Materials Science and Engineering



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Theory & Design

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 → S_1 + S_2)
- etc.

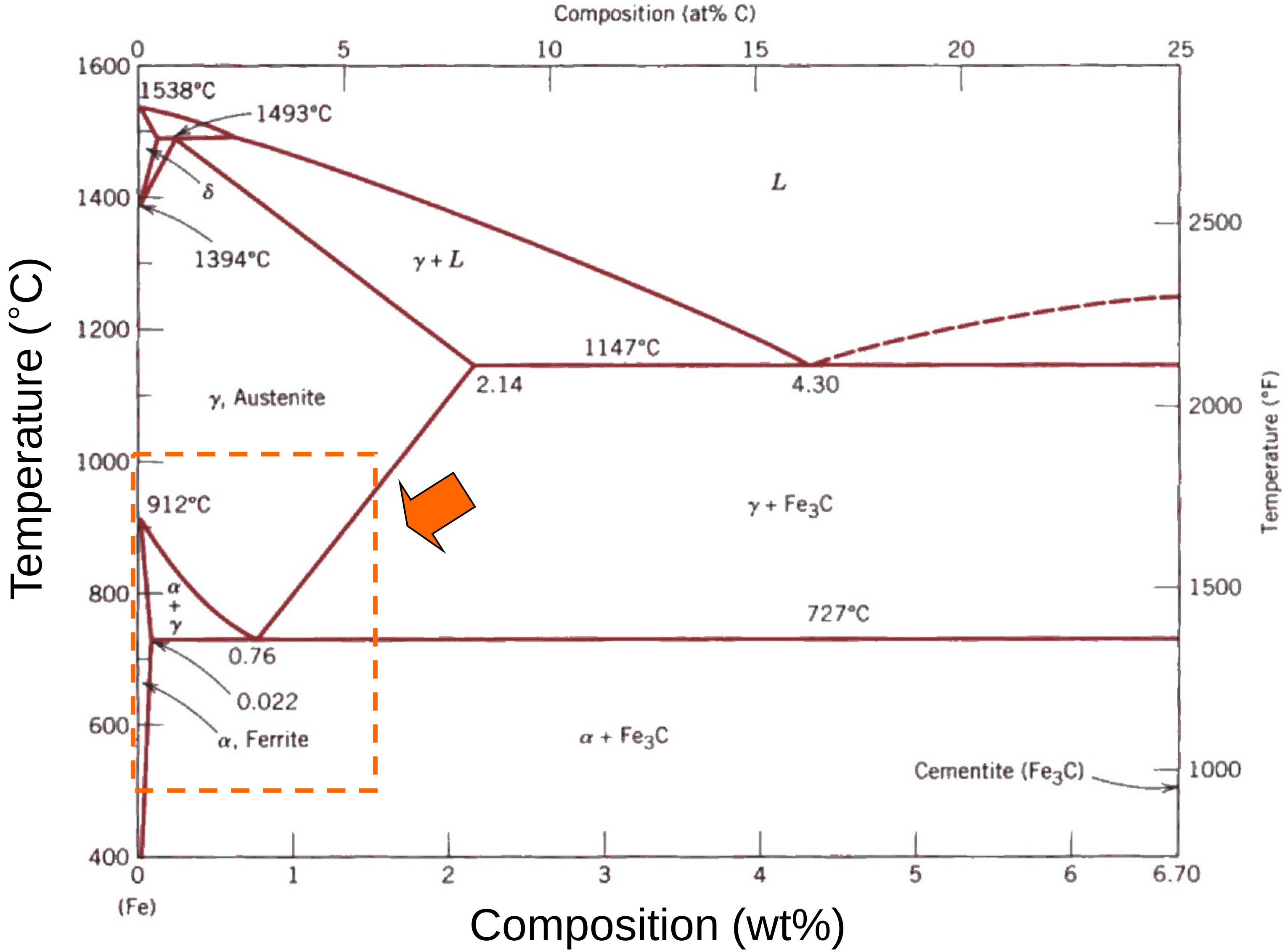
2) Diffusionless transformation ;

Short-distance atomic migration

- Martensitic transformation

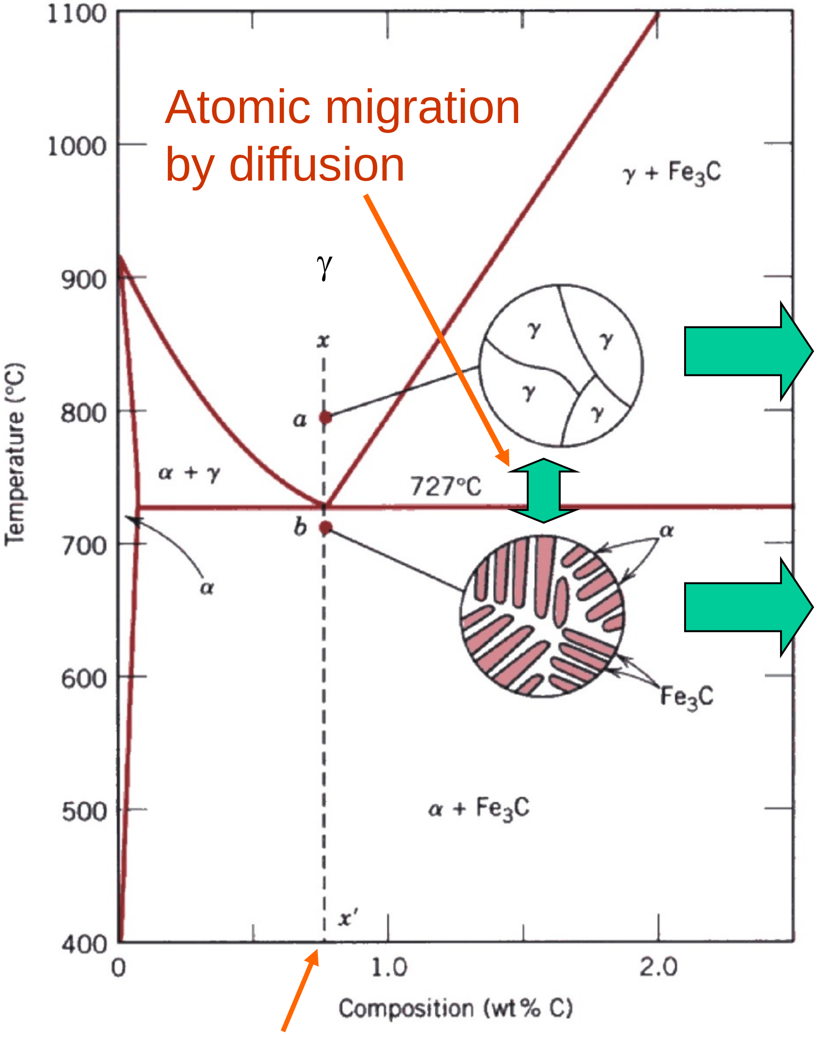
미세구조 조절: 2) Secondary phase control during solidification

Phase Diagram of Iron–Carbon Alloy



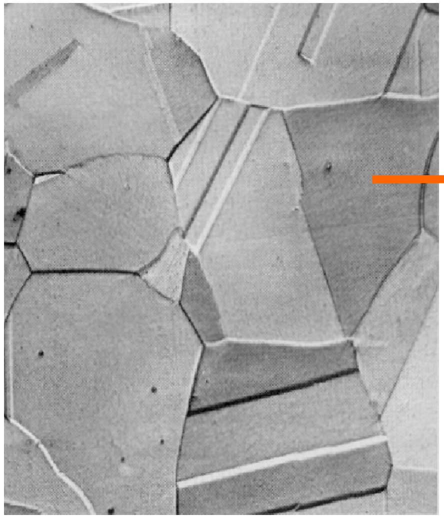
미세구조 조절: 2) Secondary phase control during solidification

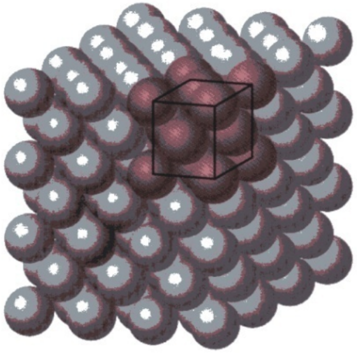
Equilibrium Phases of Iron-Carbon Alloy



Atomic migration by diffusion

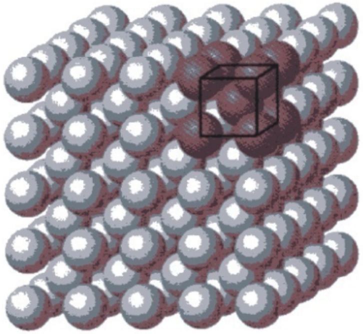
Eutectoid composition





γ phase (FCC)

Fe$_3$C phase



α phase (BCC)

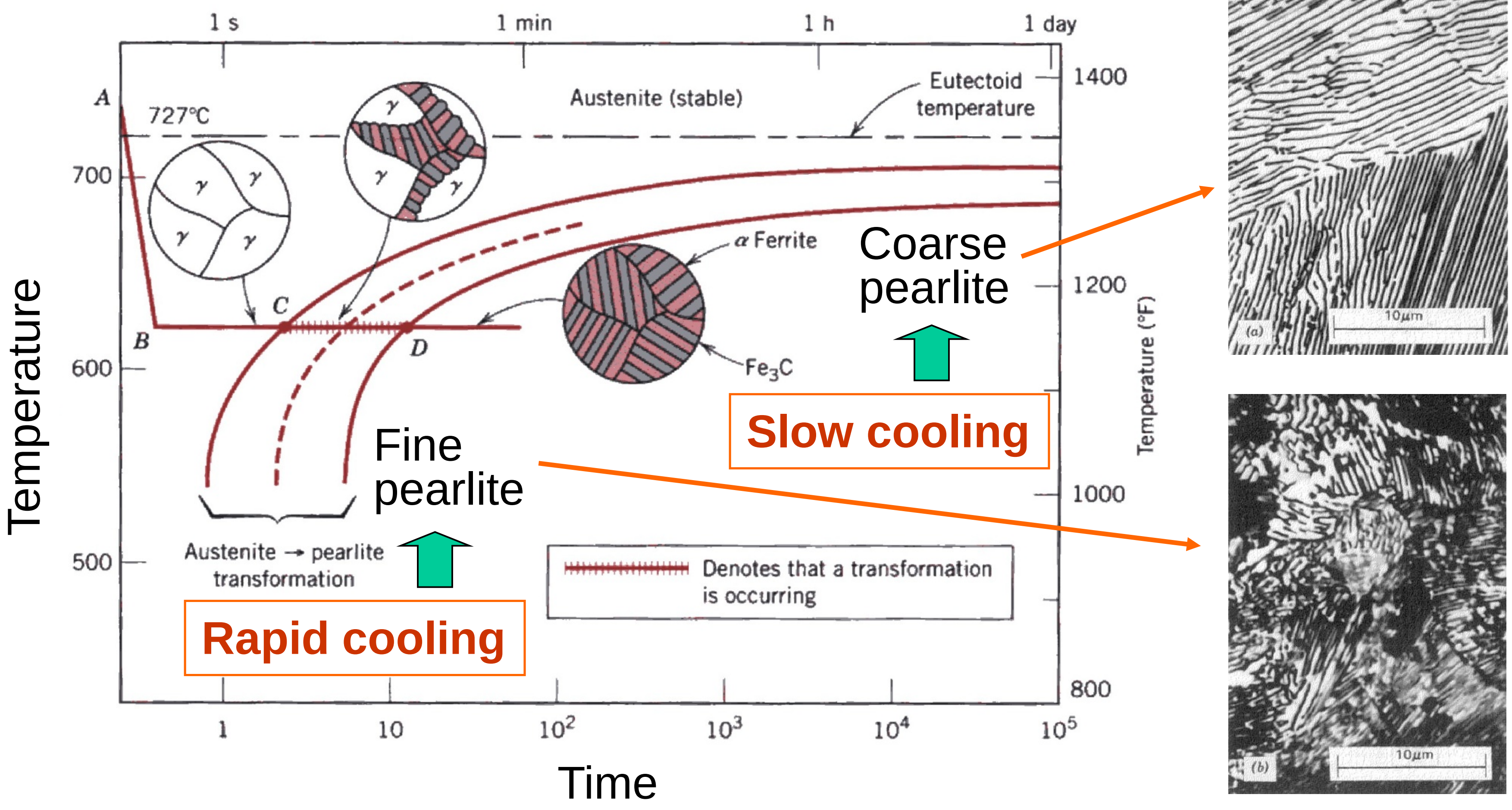
Diffusion-Controlled Phase Transformation
time dependency

Non-Equilibrium Phases

Need of Controlling
not only *Temperature* & *Composition*
but *Process conditions* (Cooling Rate)

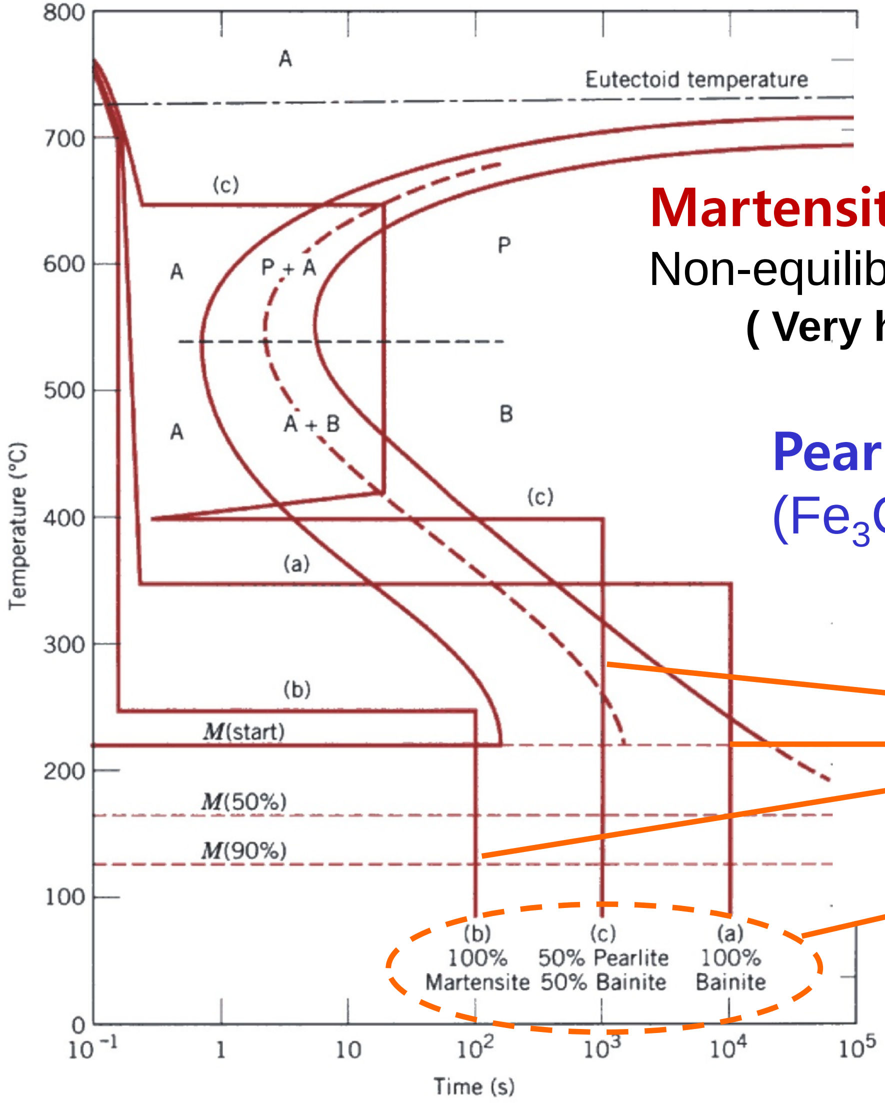
Isothermal Transformation Diagram of a Eutectoid Iron-Carbon Alloy

γ Austenite ➡ **α Ferrite + Fe_3C graphite**



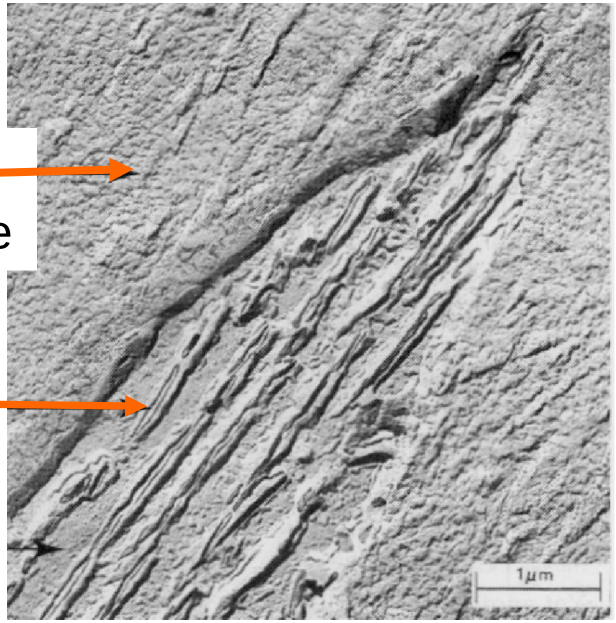
➡ ***Phase Transformation* 제어을 통한 *microstructure*의 조절 가능**

Control of Phases by Heat Treatment



Martensite ;
Non-equilibrium phase
(Very hard)

Pearlite
(Fe_3C+ferrite)



Heat Treatment 공정조절

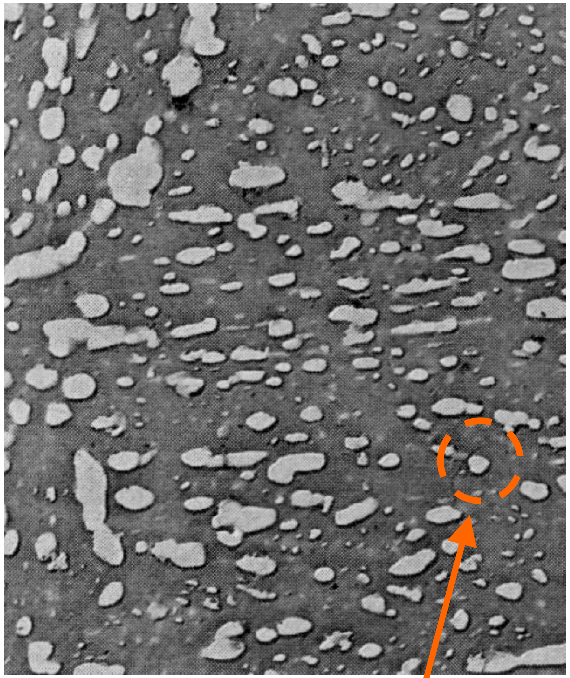
Phase & Microstructure

Properties of Material

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

공정조절

Proper heat treatment (tempering)



Martensite

Tip of needle shape grain

→ Nucleation site of fracture

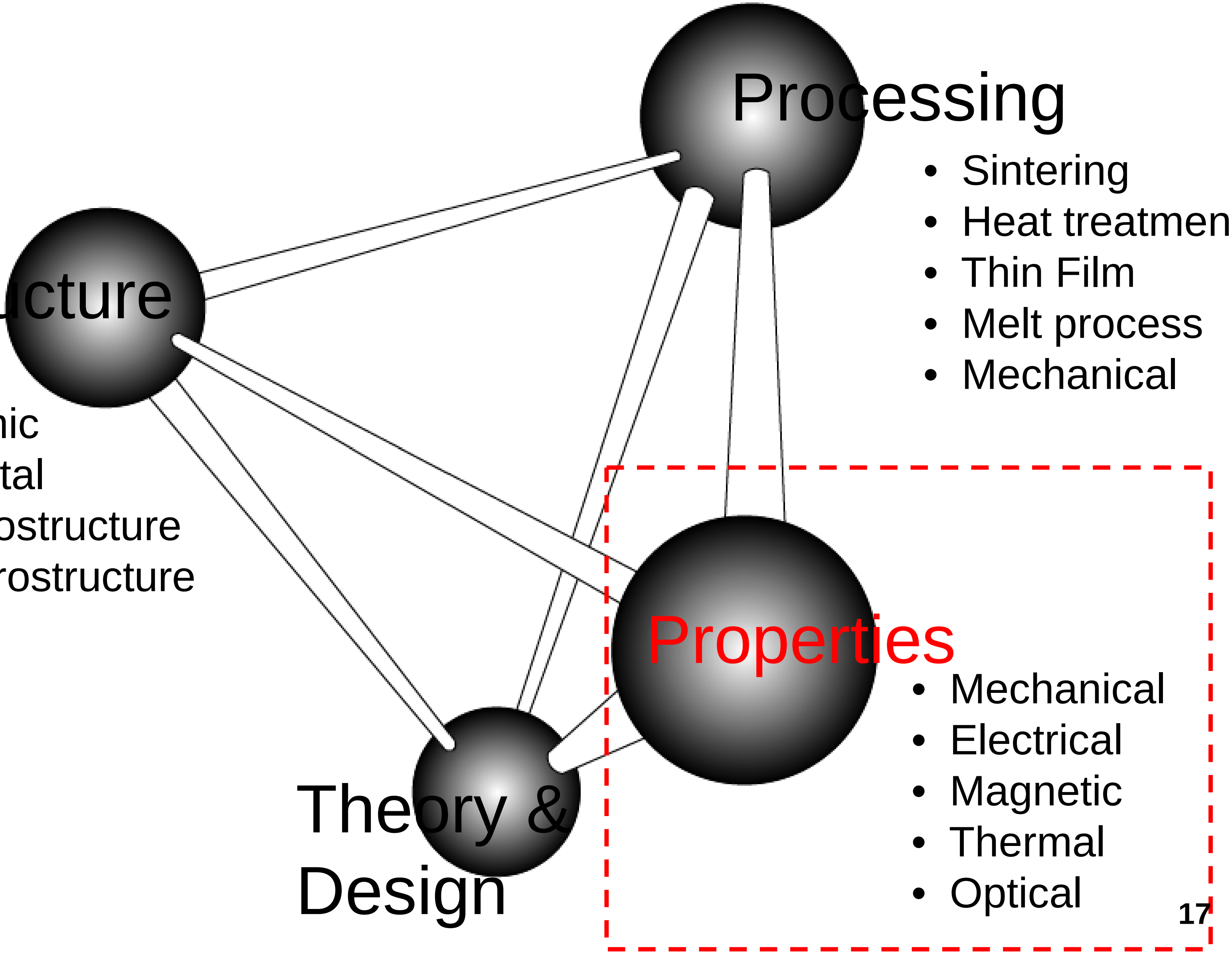
→ Brittle

Tempered martensite

→ Very small & spherical shape grain

→ Good strength, ductility, toughness

Materials Science and Engineering



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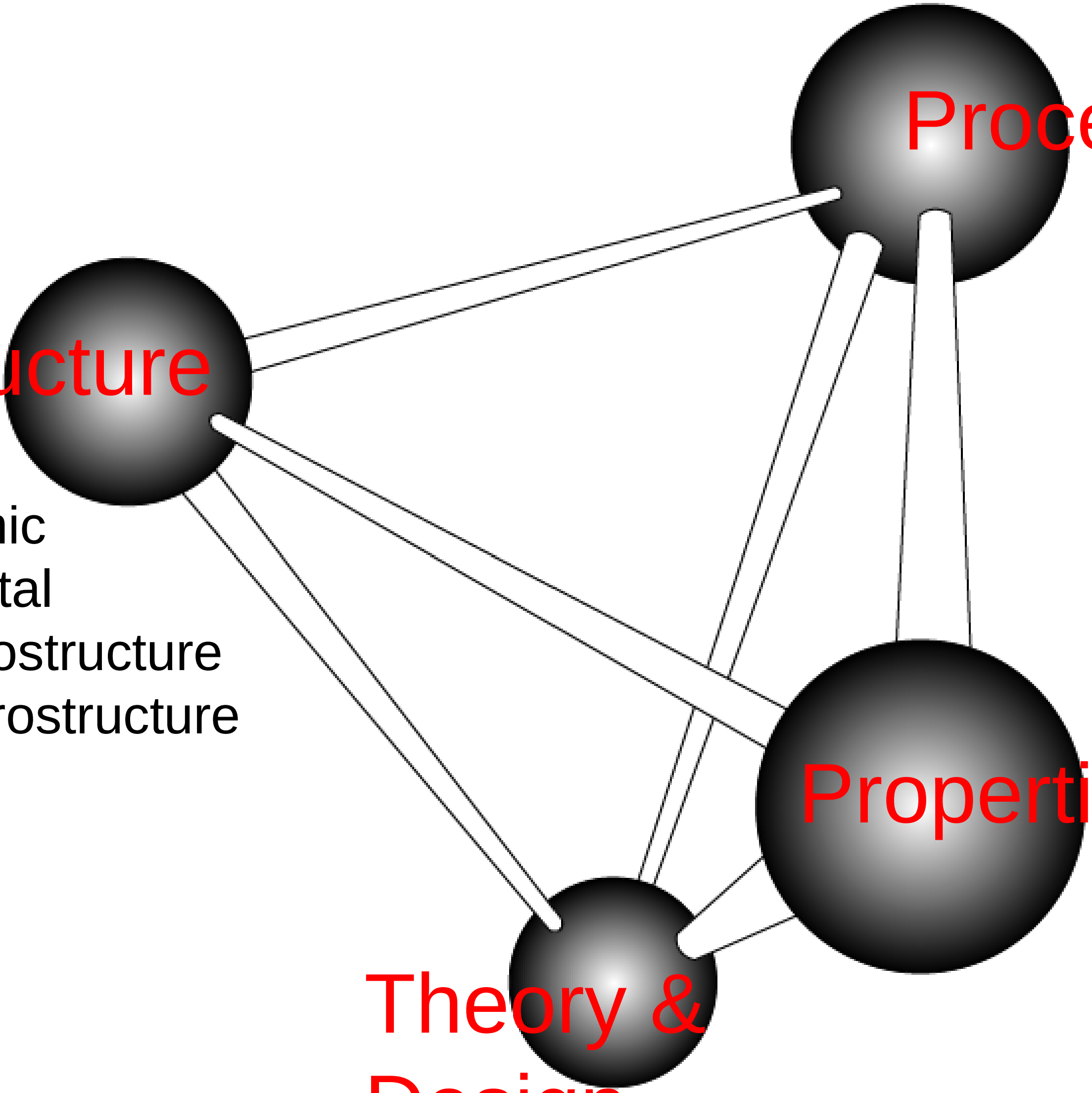
Theory & Design

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,…

Contents for previous class

Materials Science and Engineering



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Theory & Design

Materials Design-for-Properties : "Alloyed Pleasure"

신입생세미나 – 창의와 도전 – "미래를 여는 연금술사"

차시별 강의 계획

회차	수업 일시 (강의 장소)	주제 또는 수업 내용	수강생 활동 및 활용자료
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7차	10월27일(화) 17:00~18:30 30동 218-1호	**제조 시편의 미세구조 분석 II**	전자현미경 관찰 실험
8차	11월03일(화) 17:00~18:30 30동 218-1호	**제조시편 기초 물성 분석**	X-선 회절분석, 경도 등 실험
9차	11월10일(화) 17:00~18:30 30동 218-1호	**제조시편 타겟 물성 분석**	타겟 물성 평가 실험 (강도, 연신 등)
10차	11월24일(화) 17:00~18:30 30동 218-1호	**최종연구결과 발표 및 토의**	개발 합금의 미래첨단기술 적용 아이디어 제안 포함

▣ 5주차-9주차 실험의 경우, 각 팀의 동선이 충돌되지 않도록 순환 실험진행 예정

Schedule

week 1 *Introduction & Atomic Structure and Interatomic Bonding* (Chap.1 & Chap. 2)
week 2 *Fundamentals of Crystallography* (Chap. 3)
week 3 *The Structure of Crystalline Solids* (Chap. 4)
week 4 *Polymer Structures* (Chap. 5)
week 5 *Imperfections in Solids* (Chap. 6)
week 6 *Diffusion* (Chap. 7) & *Mid-term (Face-to-face examination)*
week 7 *Mechanical Properties of Metals* (Chap. 8)
week 8 *Dislocations and Strengthening Mechanisms* (Chap. 9)
week 9 *Failure* (Chap. 10)
week 10 *Phase Diagrams* (Chap. 11)
week 11 *Phase Transformations* (Chap. 12)
week 12 *Properties and Application of Metals & Ceramics* (Chap. 13 & Chap. 14)
week 13 *Properties and Application of Polymers* (Chap. 15)
week 14 *Composite Materials* (Chap. 16)
week 15 *Fabrication and Processing of Eng. Mater*. (Chap. 17) *&*
Final Exam (Face-to-face examination)

CHAPTER 2:
Atomic structure and Interatomic bonding

; 많은 경우 결합의 종류로 재료의 특성 설명

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**

I. Atomic Structure (Freshman Chem.)

- atom – electrons – 9.11 x 10^{-31} kg
  protons
  neutrons } nucleus, 1.67 x 10^{-27} kg

  electrons & protons are electrically charged: 1.60 x 10^{-19} C (기본전하)

- atomic number = # of protons in nucleus of atom (Z)
  = # of electrons of neutral species (N)

- atomic mass unit (A≈Z+N) = amu = 1/12 mass of ^{12}C

  Atomic wt = **weight** of 6.023 x 10^{23} molecules or atoms

  1 amu/atom = 1 g/mol

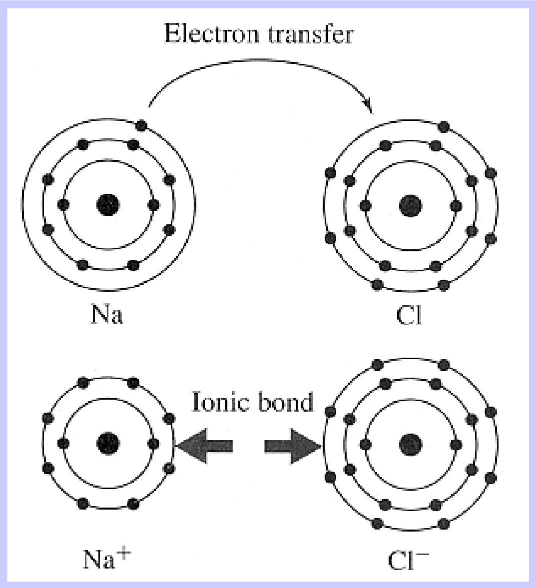
  C 12.011 A H 1.008 A
  Fe 55.85 amu/atom = **55.85 g/mol** etc.

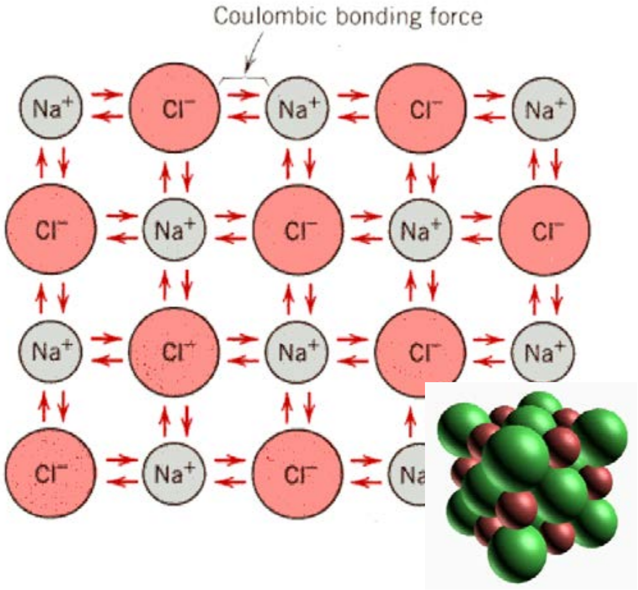
- isotope same Z, but different N: two or more different A

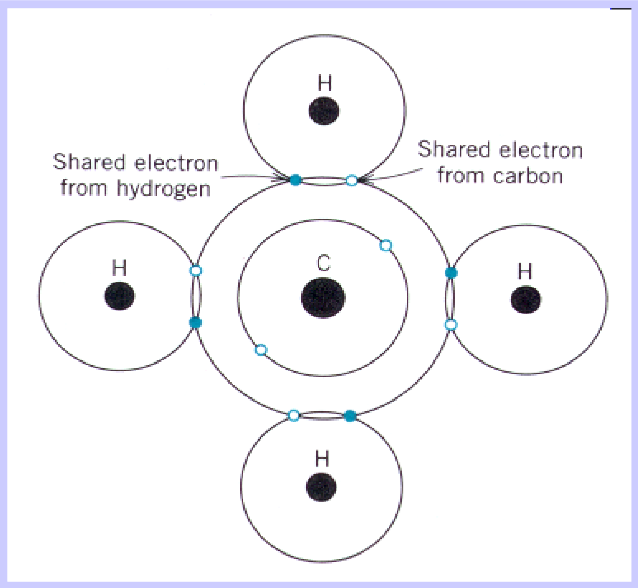
Fundamental Concepts

II. Atomic Bonding

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







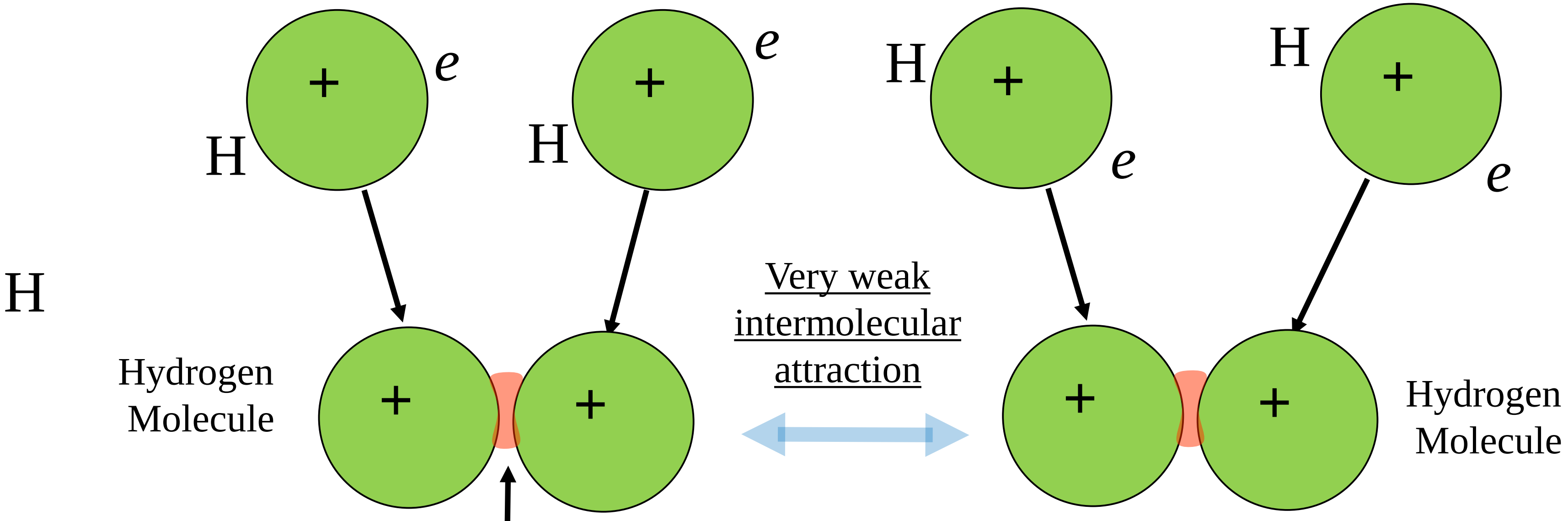
- *<u>atomic structures</u>* & *<u>electronic configurations</u>* are important ingredients to understanding **bonding**.

Fundamental Concepts

- Two fundamental types of bonding:

- **primary bonds**: strong atom-to-atom attractions produced by changes in electron position of the ***valence*** e^- . *Example : covalent atom between two hydrogen atoms*

- **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*

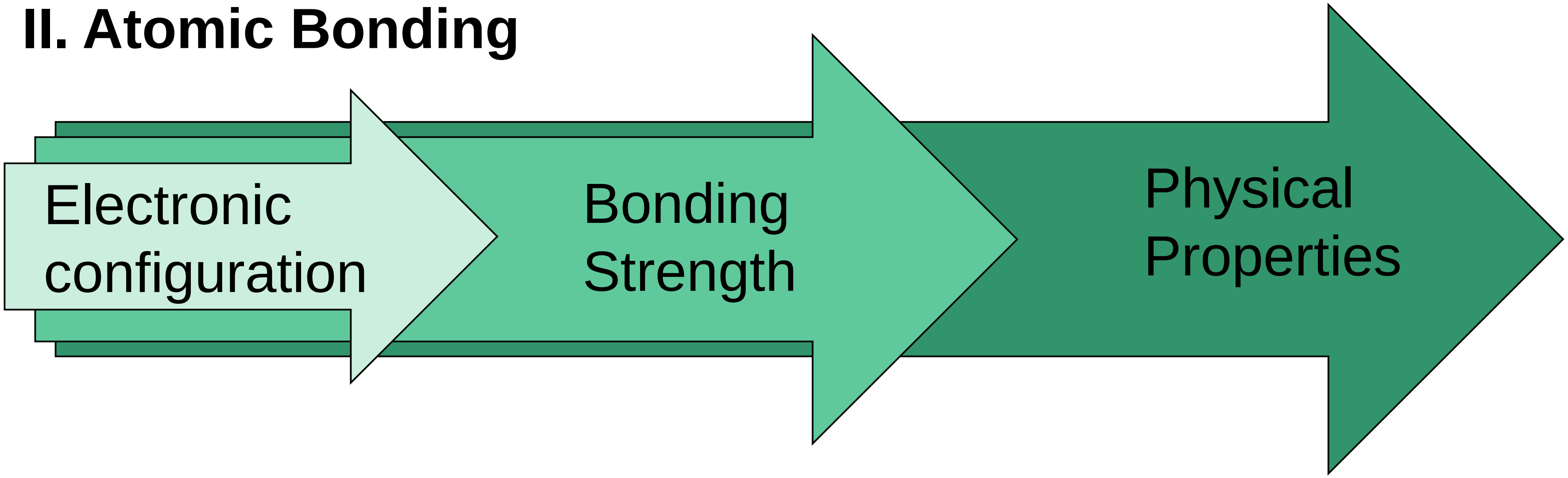


Very weak intermolecular attraction

Highest Probability density of two electrons between atoms forms very strong intramolecular covalent bond

Fundamental Concepts

II. Atomic Bonding



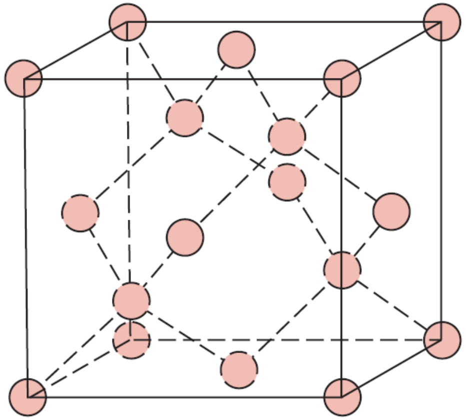
Electronic configuration

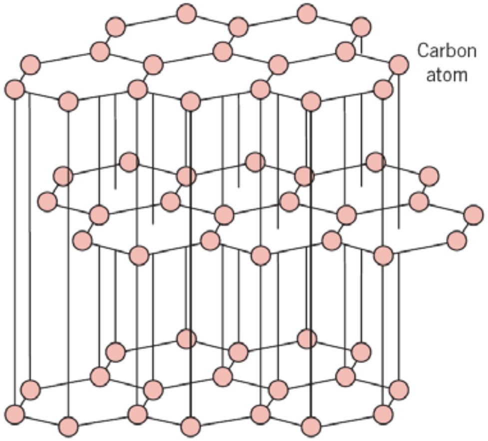
Bonding Strength

Physical Properties

☐ Example: carbon exists as ***graphite*** (soft with greasy feeling) or ***diamond*** (hardest known material)

diamond

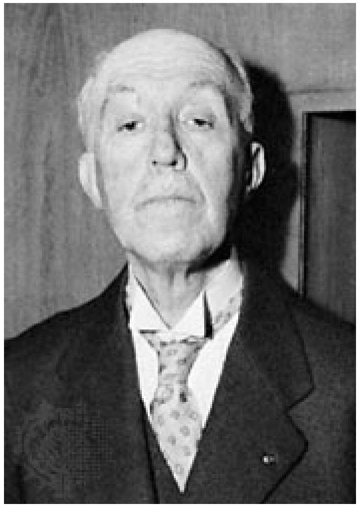




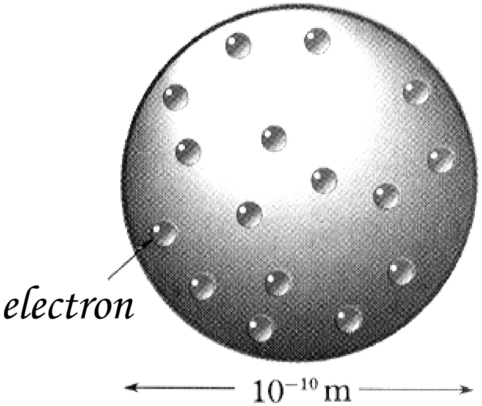
graphite

Early atomic model

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



Louis-Victor Broglie 1958

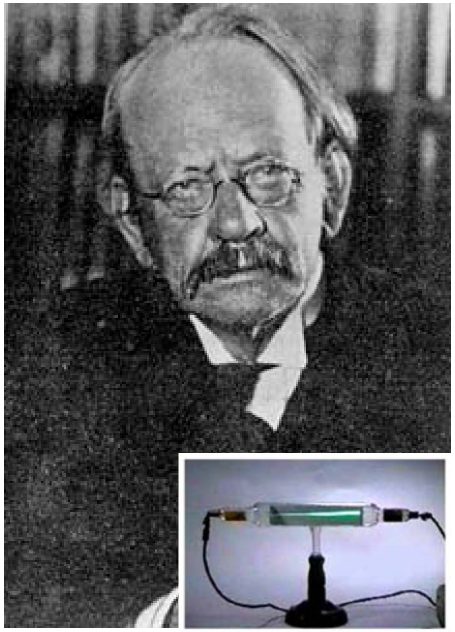


Photoelectric effect – particle
Diffraction – wave like

Sir George Paget Thomson

(1895-1975),
Nobel Prize in 1937

Thomson, Sir Joseph John

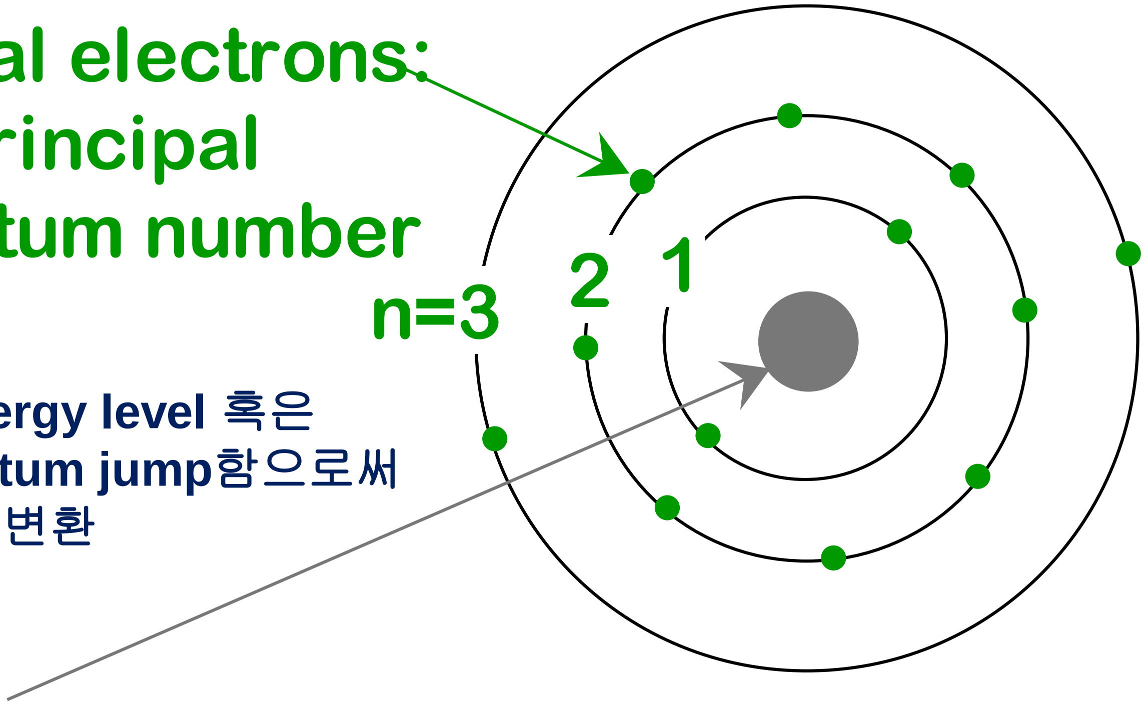


(1856-1940),
Nobel Prize in 1897

III. Bohr Atomic model: 양자역학의 초기개념

전자는 정해진 궤도를 가지고 원자주위를 돌고 있다고 가정

(원자내 전자의 위치_'전자궤도'와 에너지_'양자화된 에너지 수준'을 설명)



orbital electrons:
n = principal
quantum number

각 orbital (energy level 혹은 state)를 quantum jump함으로써 전자의 에너지 변환

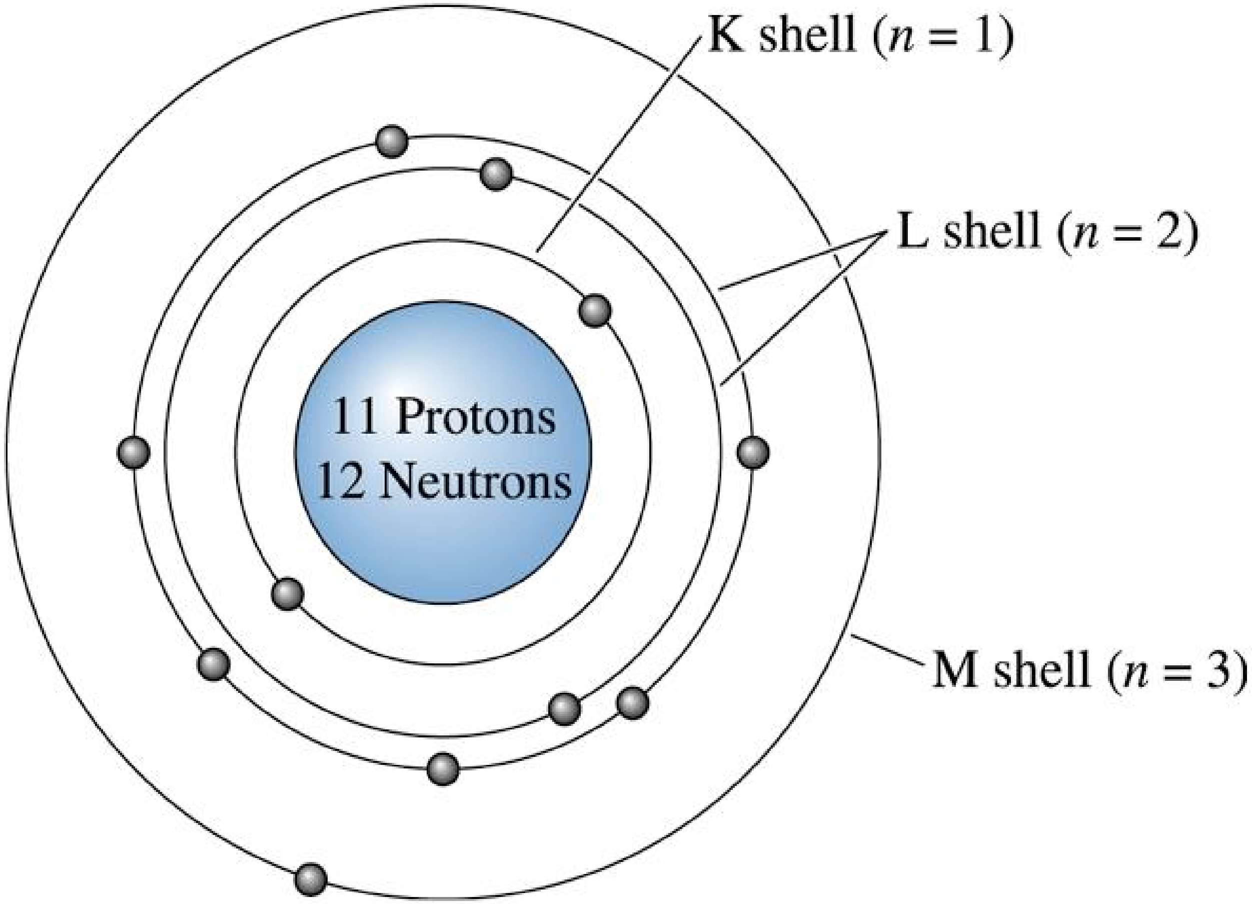
Nucleus ; Z = # protons

= 1 for hydrogen to 94 for plutonium

N = # neutrons

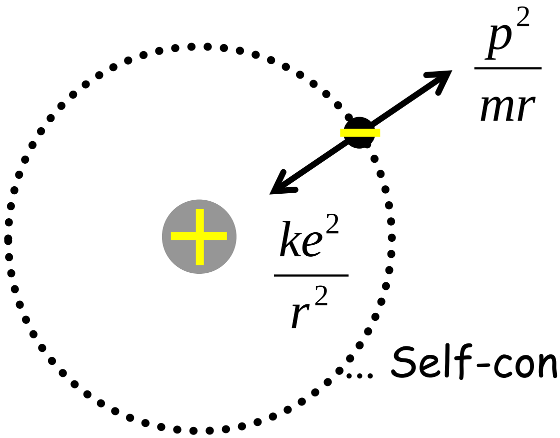
Atomic mass A ~ Z + N

Atomic structure of sodium (Na)



Limitations in Bohr’s model

… Classic mechanical theory was employed …

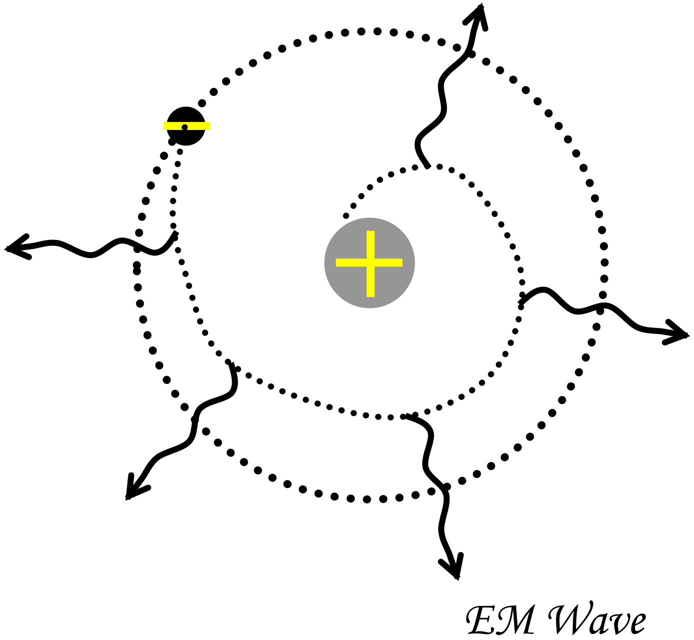


… What if there are more than two electrons ? …

… Quantum condition fails …

… Self-contradiction in terms of Heisenberg uncertainty principle …

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

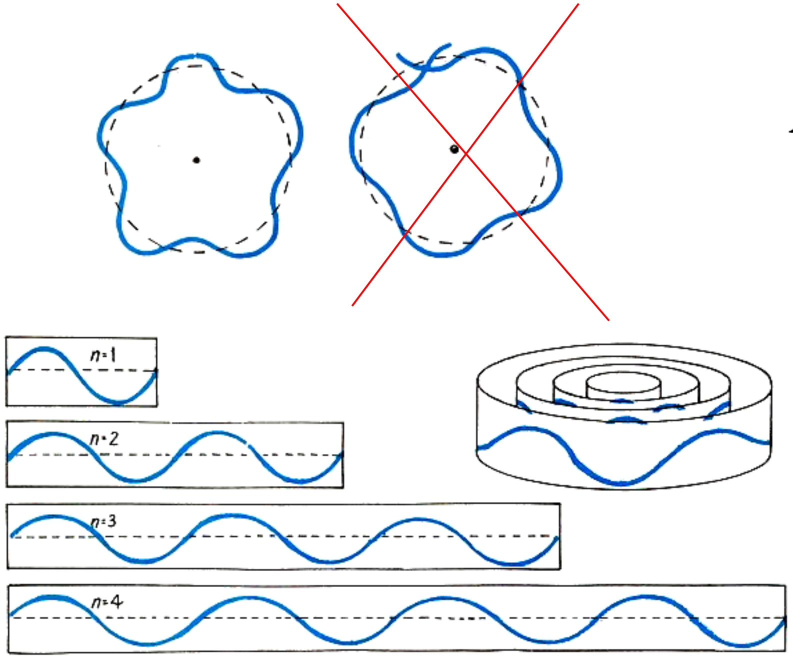


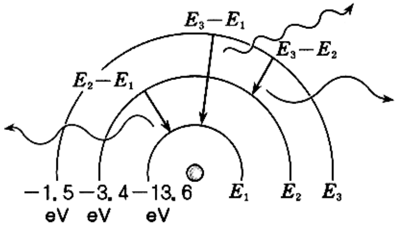
- ✓ Circumferential motion of charged particles should emit EM wave
- ✓ Discontinuous emission spectra cannot be understood

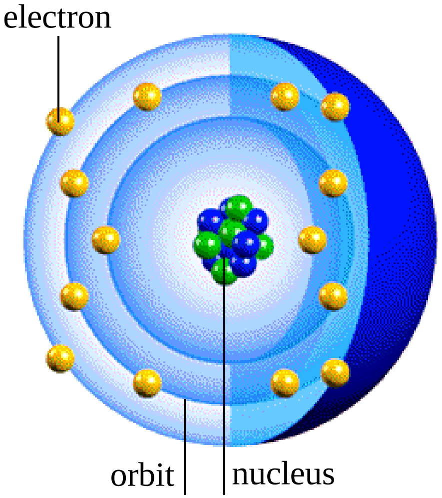
IV. Bohr’s model + Wave-mechanical model

To resolve the discontinuous emission spectra…

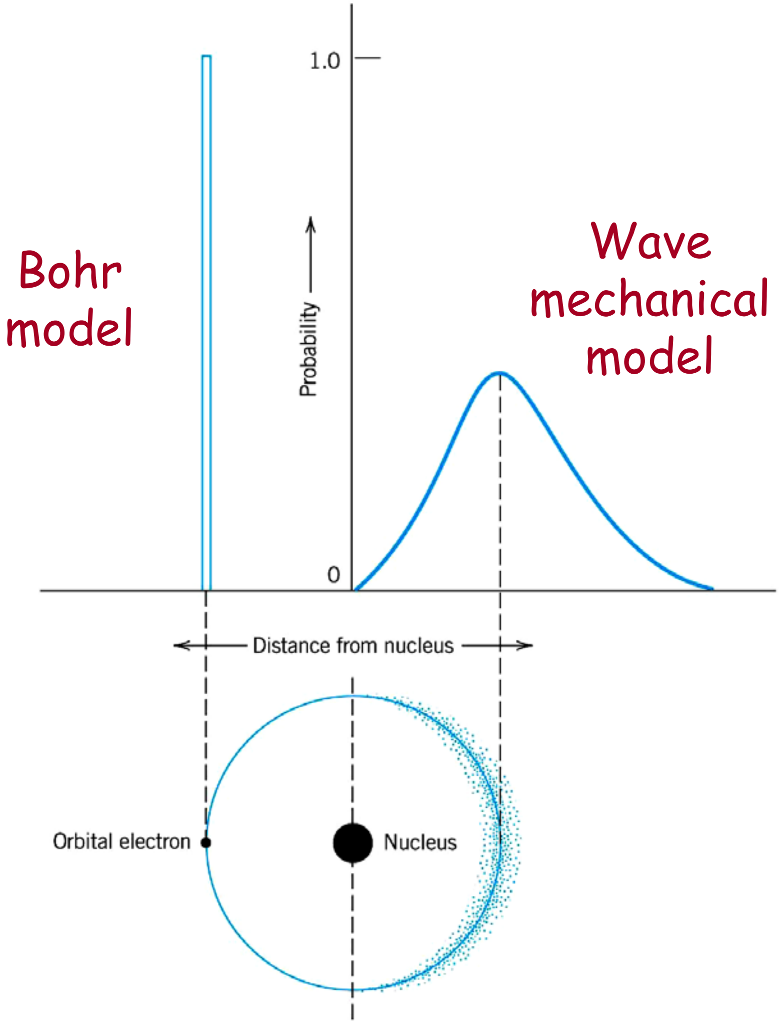
… Therefore, in discussing the motion of an electron of known energy or momentum about a nucleus, it is necessary to speak only in terms of <u>the probability of finding that electron at any particular position</u> …
(파동역학모델: 전자는 파동성과 입자성을 동시에 갖는다 가정,
전자 = 입자 → 전자의 위치 확률분포 혹은 전자구름)

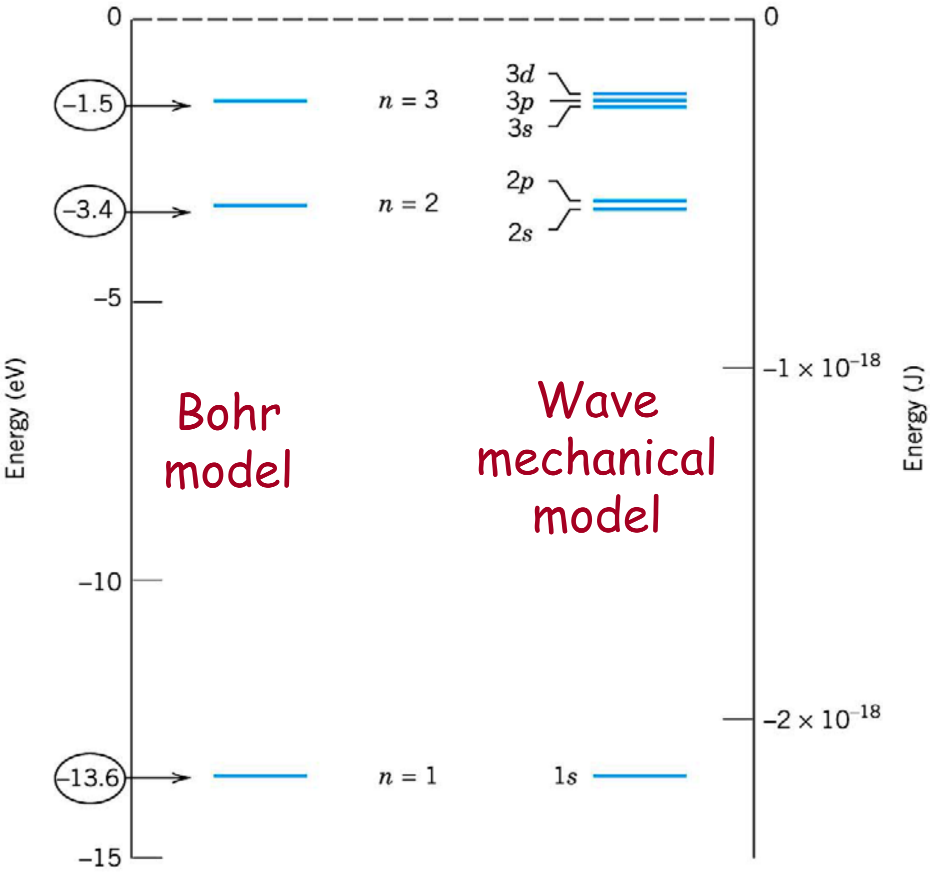






Bohr vs. wave mechanical model



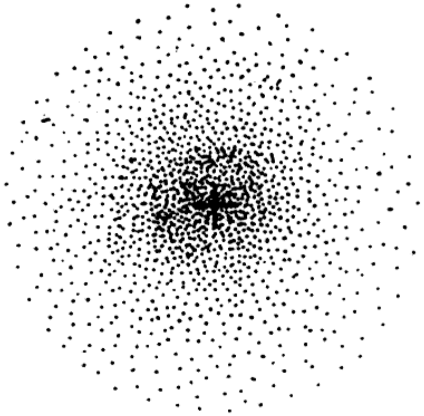


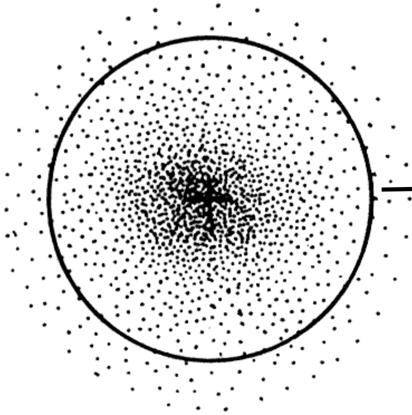
Electron position is described by
a probability distribution
or electron cloud

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 ...

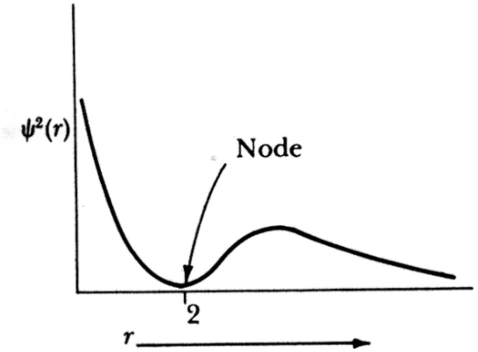


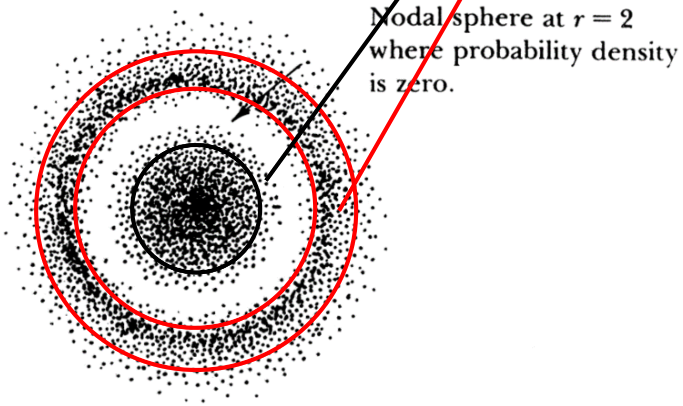


" orbital "

, which cannot be defined by a discrete line but a region of a volume due to Heisenberg uncertainty principle

Then, what if there are two available rooms for an electron ...





V. 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".

Quantum #	Designation
n = principal (energy level-shell)	*K*, *L*, *M*, *N*, *O* (1, 2, 3, etc.)
ℓ = subsidiary (orbitals)	*s*, *p*, *d*, *f* (0, 1, 2, 3,…, n-1)
m_l = magnetic	1, 3, 5, 7 ($-\ell$ to $+\ell$)
m_s = spin	½, -½

V-a. 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, ---, ±l
  - Determines the orientation of the orbital
- m_s spin quantum number ½, -½

V-b. 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 …

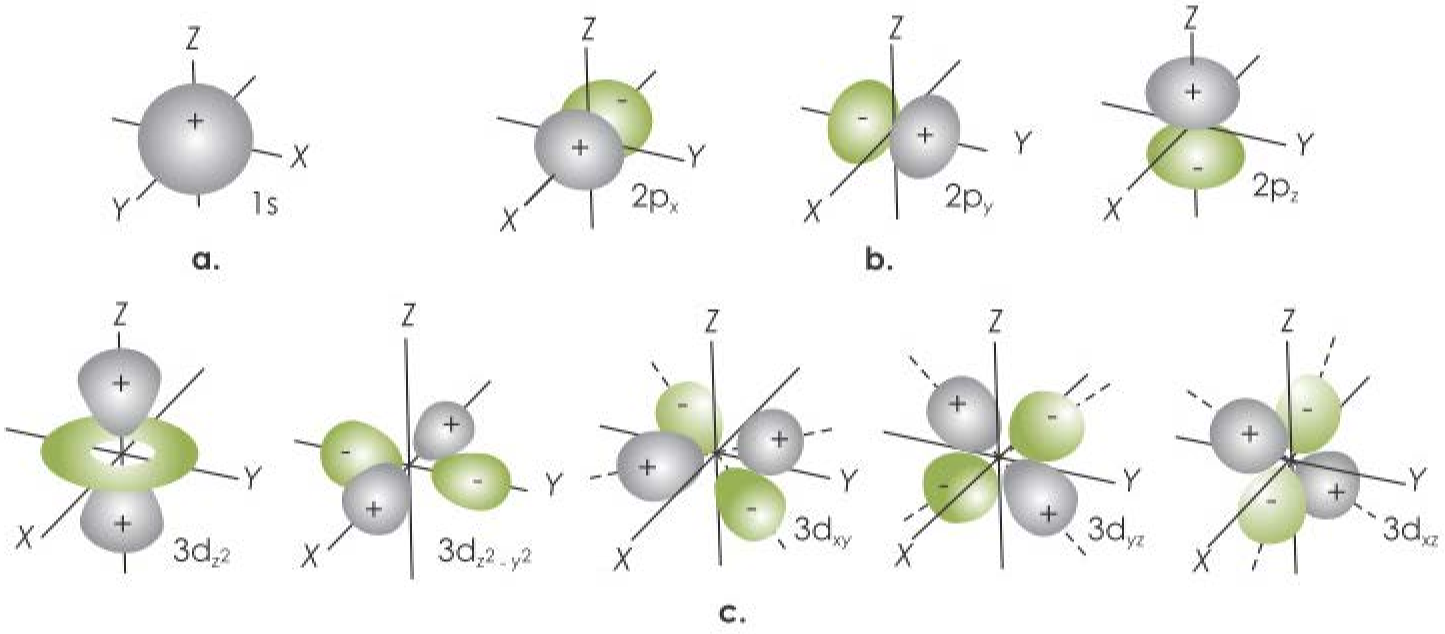
  → Each orbital will hold up to two electrons There can never be more than one electron in the same quantum state
- Only one electron can be in a particular quantum state at a given time
- Each electron state cannot hold more than two electrons with opposite spins

V-a. Meaning of quantum numbers

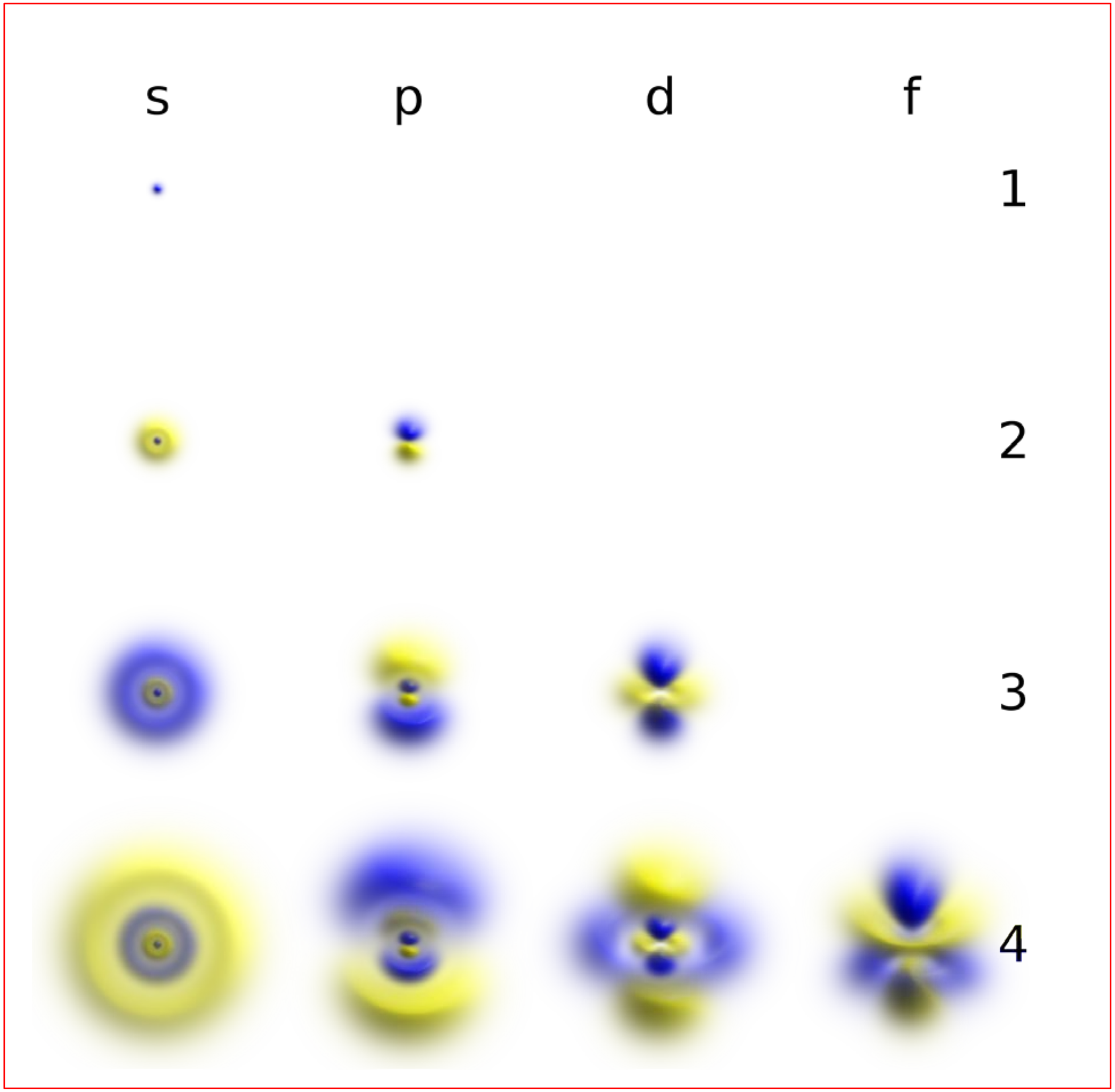
(1) ***n*** determines the size

(2) ***l*** determines the shape

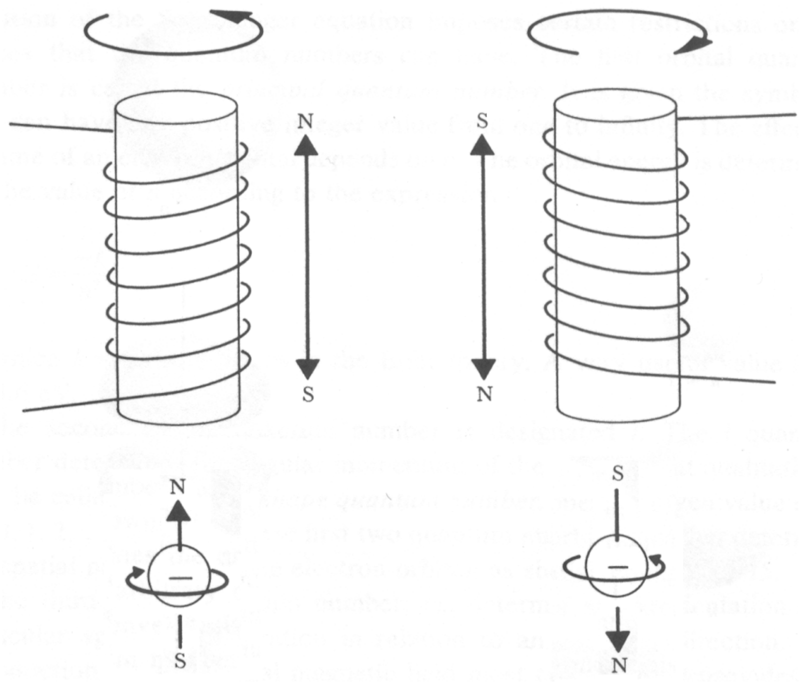
(3) m_l determines the orientation



3-dimensional view of electron orbitals



V-a. Meaning of quantum numbers



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

Therefore, complete description of an electron requires **4 quantum numbers**

V-b. Pauli exclusion principle

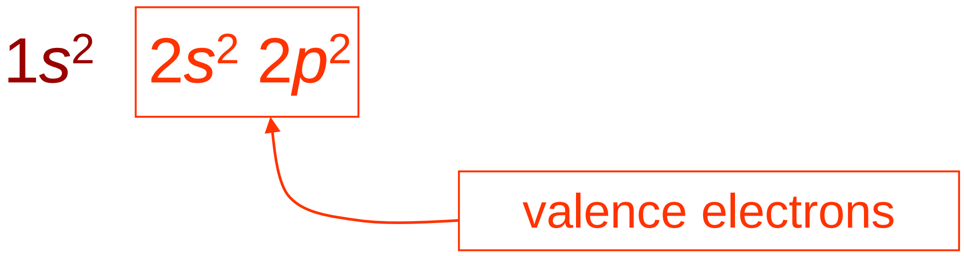
... No two interacting entities can have the same set of the quantum # ...

→ Each orbital will hold up to two electrons

VI. 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)



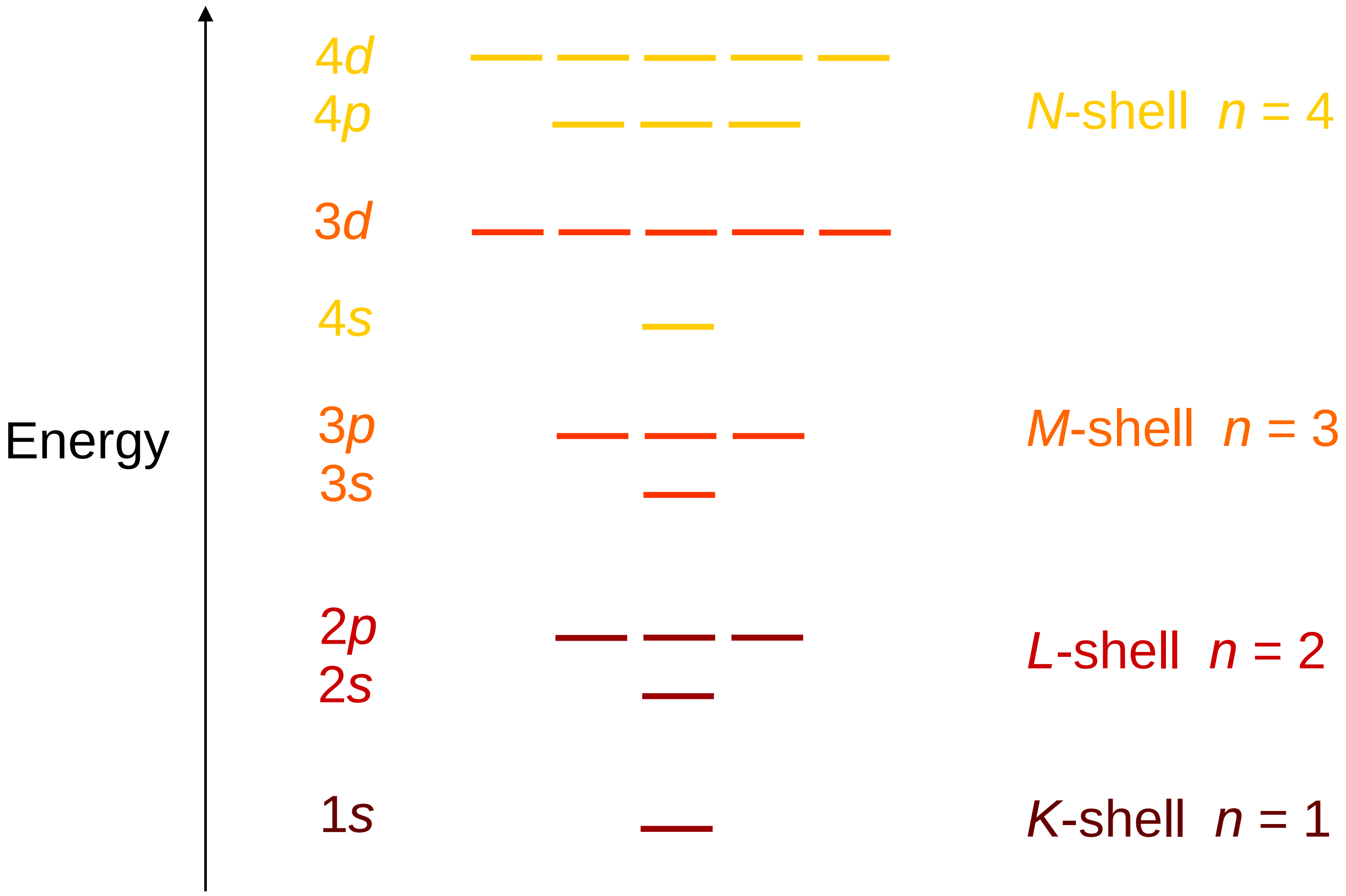
$1s^2 \; \boxed{2s^2 \, 2p^2}$

valence electrons

Electron Energy States

Electrons...

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



4*d*

4*p*

N-shell $n = 4$

3*d*

4*s*

Energy

3*p*

M-shell $n = 3$

3*s*

2*p*

L-shell $n = 2$

2*s*

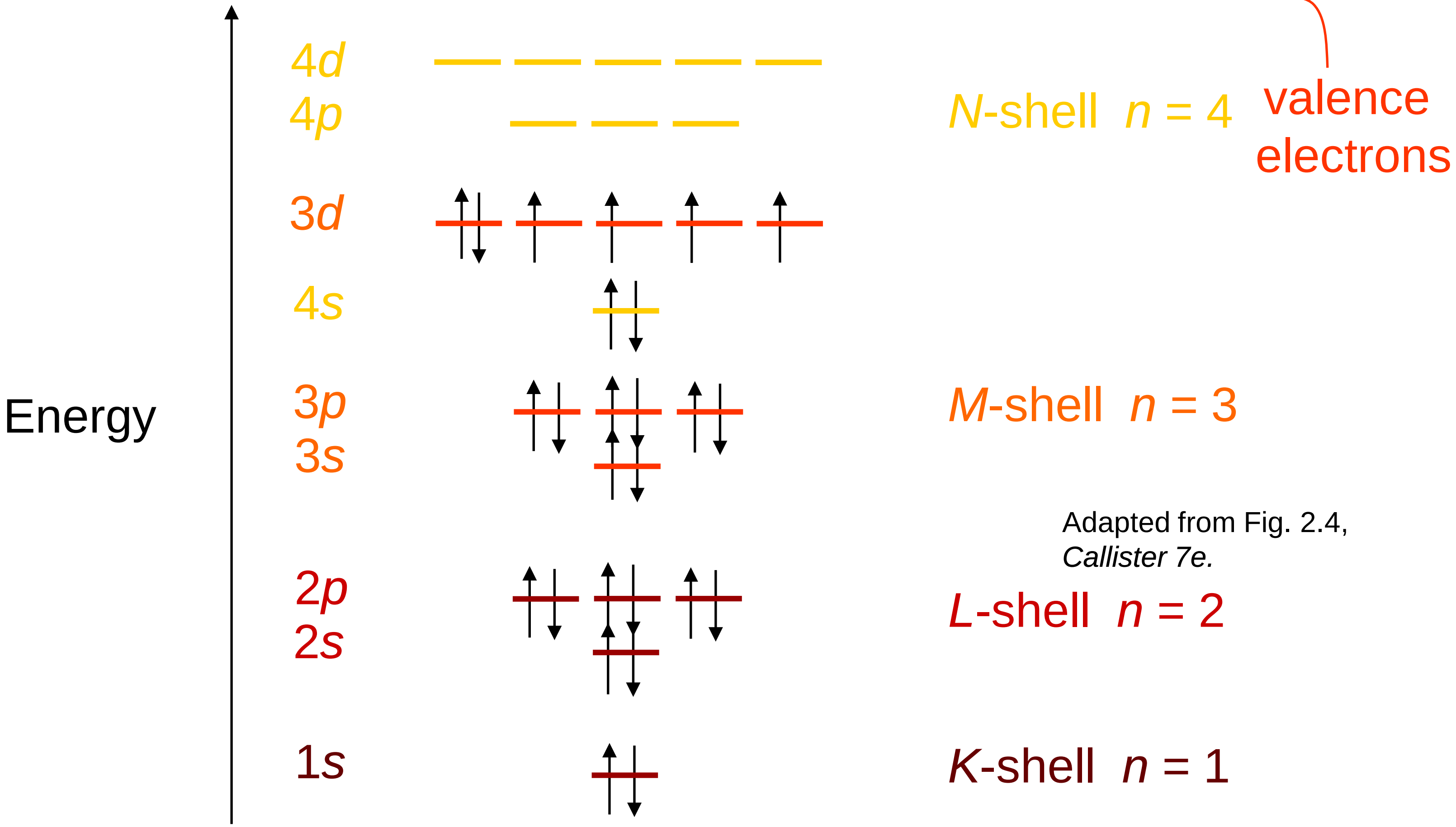
1*s*

K-shell $n = 1$

Adapted from Fig. 2.4, *Callister 7e.*

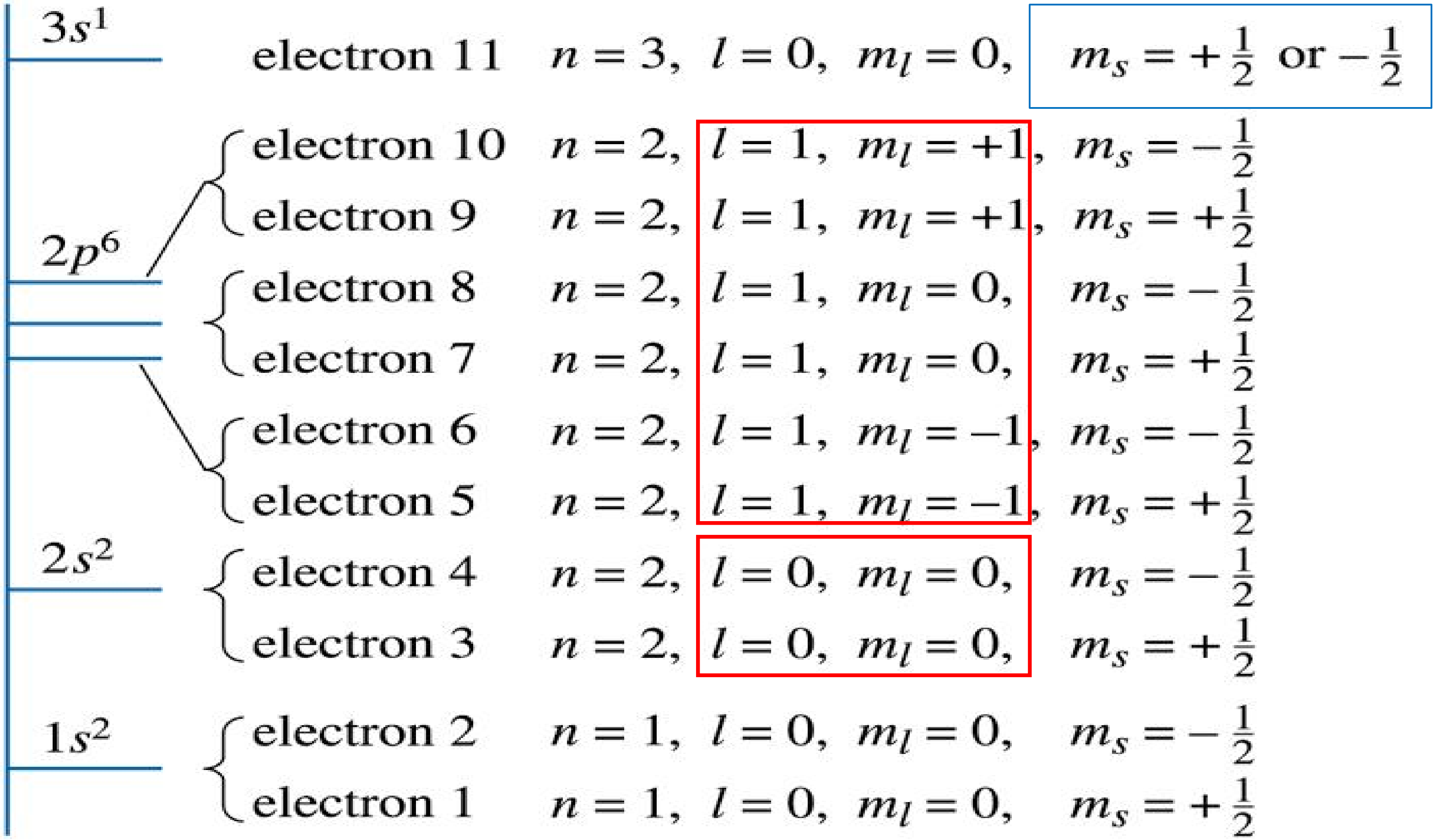
Electronic Configurations

ex: Fe - atomic # = 26 $1s^2 \; 2s^2 \, 2p^6 \; 3s^2 \, 3p^6 \; \boxed{3d^6 \;\; 4s^2}$



Adapted from Fig. 2.4, *Callister 7e.*

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



$3s^1$

electron 11 $n = 3,\ l = 0,\ m_l = 0,\ m_s = +\frac{1}{2}$ or $-\frac{1}{2}$

$2p^6$

electron 10 $n = 2,\ l = 1,\ m_l = +1,\ m_s = -\frac{1}{2}$

electron 9 $n = 2,\ l = 1,\ m_l = +1,\ m_s = +\frac{1}{2}$

electron 8 $n = 2,\ l = 1,\ m_l = 0,\ m_s = -\frac{1}{2}$

electron 7 $n = 2,\ l = 1,\ m_l = 0,\ m_s = +\frac{1}{2}$

electron 6 $n = 2,\ l = 1,\ m_l = -1,\ m_s = -\frac{1}{2}$

electron 5 $n = 2,\ l = 1,\ m_l = -1,\ m_s = +\frac{1}{2}$

$2s^2$

electron 4 $n = 2,\ l = 0,\ m_l = 0,\ m_s = -\frac{1}{2}$

electron 3 $n = 2,\ l = 0,\ m_l = 0,\ m_s = +\frac{1}{2}$

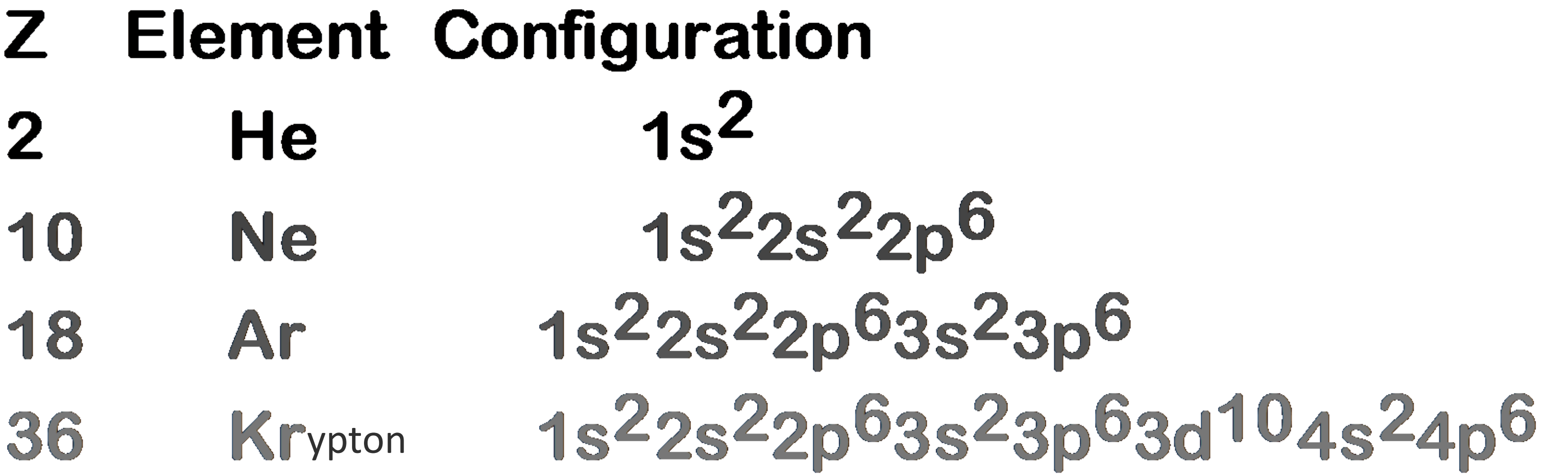
$1s^2$

electron 2 $n = 1,\ l = 0,\ m_l = 0,\ m_s = -\frac{1}{2}$

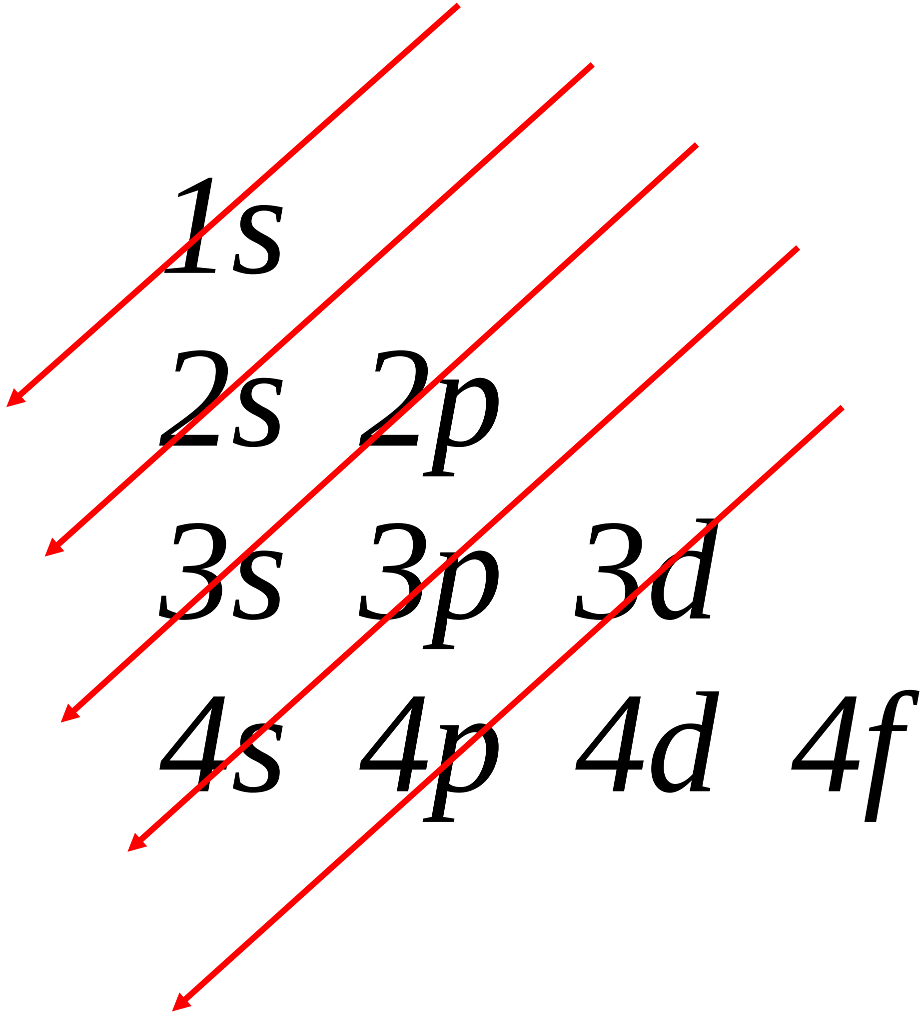
electron 1 $n = 1,\ l = 0,\ m_l = 0,\ m_s = +\frac{1}{2}$

Stable Electron Configurations

- Stable electron configurations...
  - – have complete s and p subshells
  - – tend to be *non-reactive* (불활성).



Z	Element	Configuration
2	He	$1s^2$
10	Ne	$1s^22s^22p^6$
18	Ar	$1s^22s^22p^63s^23p^6$
36	Krypton	$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$



1s

2s 2p

3s 3p 3d

4s 4p 4d 4f

$1s^1$

$1s^2$

$2s^1$

$2s^2$

$2p^1$

.

.

.

$2p^6$

$3s^1$

$3s^2$

3p

4s ⬅

3d

4p

SURVEY OF ELEMENTS

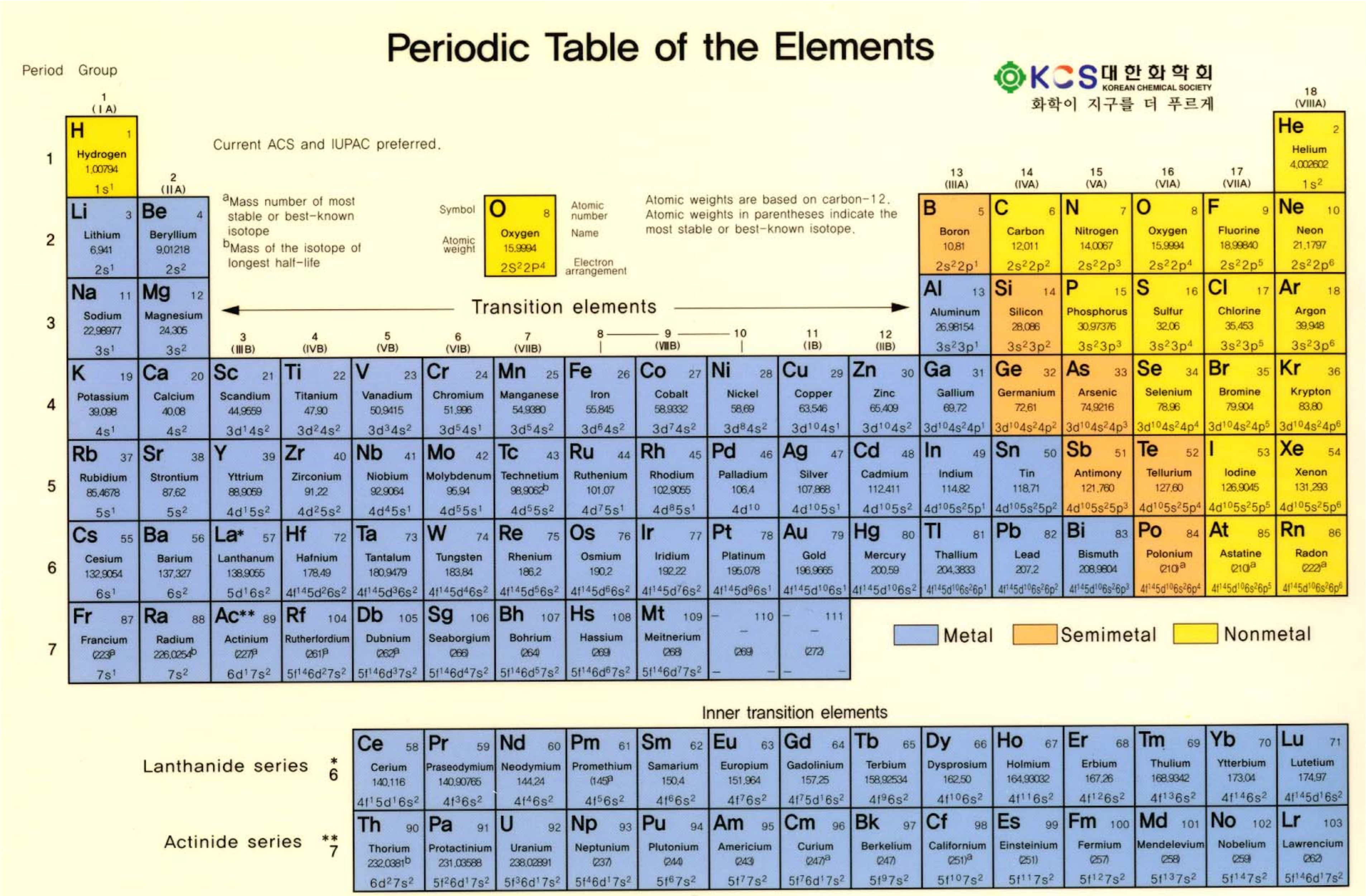
- **Most elements: Electron configuration not stable.**

Element	Atomic #	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	$1s^2 2s^2 2p^1$
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)

Adapted from Table 2.2, *Callister 7e.*

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

Chapter 2.4 모든 원소는 주기율표 상의 전자 배위에 의해 분류



Periodic Table of the Elements

KCS 대한화학회
KOREAN CHEMICAL SOCIETY
화학이 지구를 더 푸르게

Current ACS and IUPAC preferred.

[a]Mass number of most stable or best-known isotope
[b]Mass of the isotope of longest half-life

Symbol	O
Atomic number	8
Name	Oxygen
Atomic weight	15.9994
Electron arrangement	$2S^2 2P^4$

Atomic weights are based on carbon-12. Atomic weights in parentheses indicate the most stable or best-known isotope.

Transition elements

Period	Group 1 (IA)	2 (IIA)	3 (IIIB)	4 (IVB)	5 (VB)	6 (VIB)	7 (VIIB)	8	9 (VIIIB)	10	11 (IB)	12 (IIB)	13 (IIIA)	14 (IVA)	15 (VA)	16 (VIA)	17 (VIIA)	18 (VIIIA)
1	🟨 **H** 1 Hydrogen 1.00794 $1s^1$																	🟨 **He** 2 Helium 4.002602 $1s^2$
2	🟦 **Li** 3 Lithium 6.941 $2s^1$	🟦 **Be** 4 Beryllium 9.01218 $2s^2$											🟧 **B** 5 Boron 10.81 $2s^2 2p^1$	🟨 **C** 6 Carbon 12.011 $2s^2 2p^2$	🟨 **N** 7 Nitrogen 14.0067 $2s^2 2p^3$	🟨 **O** 8 Oxygen 15.9994 $2s^2 2p^4$	🟨 **F** 9 Fluorine 18.99840 $2s^2 2p^5$	🟨 **Ne** 10 Neon 21.1797 $2s^2 2p^6$
3	🟦 **Na** 11 Sodium 22.98977 $3s^1$	🟦 **Mg** 12 Magnesium 24.305 $3s^2$											🟦 **Al** 13 Aluminum 26.98154 $3s^2 3p^1$	🟧 **Si** 14 Silicon 28.086 $3s^2 3p^2$	🟨 **P** 15 Phosphorus 30.97376 $3s^2 3p^3$	🟨 **S** 16 Sulfur 32.06 $3s^2 3p^4$	🟨 **Cl** 17 Chlorine 35.453 $3s^2 3p^5$	🟨 **Ar** 18 Argon 39.948 $3s^2 3p^6$
4	🟦 **K** 19 Potassium 39.098 $4s^1$	🟦 **Ca** 20 Calcium 40.08 $4s^2$	🟦 **Sc** 21 Scandium 44.9559 $3d^1 4s^2$	🟦 **Ti** 22 Titanium 47.90 $3d^2 4s^2$	🟦 **V** 23 Vanadium 50.9415 $3d^3 4s^2$	🟦 **Cr** 24 Chromium 51.996 $3d^5 4s^1$	🟦 **Mn** 25 Manganese 54.9380 $3d^5 4s^2$	🟦 **Fe** 26 Iron 55.845 $3d^6 4s^2$	🟦 **Co** 27 Cobalt 58.9332 $3d^7 4s^2$	🟦 **Ni** 28 Nickel 58.69 $3d^8 4s^2$	🟦 **Cu** 29 Copper 63.546 $3d^{10} 4s^1$	🟦 **Zn** 30 Zinc 65.409 $3d^{10} 4s^2$	🟦 **Ga** 31 Gallium 69.72 $3d^{10} 4s^2 4p^1$	🟧 **Ge** 32 Germanium 72.61 $3d^{10} 4s^2 4p^2$	🟧 **As** 33 Arsenic 74.9216 $3d^{10} 4s^2 4p^3$	🟨 **Se** 34 Selenium 78.96 $3d^{10} 4s^2 4p^4$	🟨 **Br** 35 Bromine 79.904 $3d^{10} 4s^2 4p^5$	🟨 **Kr** 36 Krypton 83.80 $3d^{10} 4s^2 4p^6$
5	🟦 **Rb** 37 Rubidium 85.4678 $5s^1$	🟦 **Sr** 38 Strontium 87.62 $5s^2$	🟦 **Y** 39 Yttrium 88.9059 $4d^1 5s^2$	🟦 **Zr** 40 Zirconium 91.22 $4d^2 5s^2$	🟦 **Nb** 41 Niobium 92.9064 $4d^4 5s^1$	🟦 **Mo** 42 Molybdenum 95.94 $4d^5 5s^1$	🟦 **Tc** 43 Technetium 98.9062^b $4d^5 5s^2$	🟦 **Ru** 44 Ruthenium 101.07 $4d^7 5s^1$	🟦 **Rh** 45 Rhodium 102.9055 $4d^8 5s^1$	🟦 **Pd** 46 Palladium 106.4 $4d^{10}$	🟦 **Ag** 47 Silver 107.868 $4d^{10} 5s^1$	🟦 **Cd** 48 Cadmium 112.411 $4d^{10} 5s^2$	🟦 **In** 49 Indium 114.82 $4d^{10} 5s^2 5p^1$	🟦 **Sn** 50 Tin 118.71 $4d^{10} 5s^2 5p^2$	🟧 **Sb** 51 Antimony 121.760 $4d^{10} 5s^2 5p^3$	🟧 **Te** 52 Tellurium 127.60 $4d^{10} 5s^2 5p^4$	🟨 **I** 53 Iodine 126.9045 $4d^{10} 5s^2 5p^5$	🟨 **Xe** 54 Xenon 131.293 $4d^{10} 5s^2 5p^6$
6	🟦 **Cs** 55 Cesium 132.9054 $6s^1$	🟦 **Ba** 56 Barium 137.327 $6s^2$	🟦 **La*** 57 Lanthanum 138.9055 $5d^1 6s^2$	🟦 **Hf** 72 Hafnium 178.49 $4f^{14} 5d^2 6s^2$	🟦 **Ta** 73 Tantalum 180.9479 $4f^{14} 5d^3 6s^2$	🟦 **W** 74 Tungsten 183.84 $4f^{14} 5d^4 6s^2$	🟦 **Re** 75 Rhenium 186.2 $4f^{14} 5d^5 6s^2$	🟦 **Os** 76 Osmium 190.2 $4f^{14} 5d^6 6s^2$	🟦 **Ir** 77 Iridium 192.22 $4f^{14} 5d^7 6s^2$	🟦 **Pt** 78 Platinum 195.078 $4f^{14} 5d^9 6s^1$	🟦 **Au** 79 Gold 196.9665 $4f^{14} 5d^{10} 6s^1$	🟦 **Hg** 80 Mercury 200.59 $4f^{14} 5d^{10} 6s^2$	🟦 **Tl** 81 Thallium 204.3833 $4f^{14} 5d^{10} 6s^2 6p^1$	🟦 **Pb** 82 Lead 207.2 $4f^{14} 5d^{10} 6s^2 6p^2$	🟦 **Bi** 83 Bismuth 208.9804 $4f^{14} 5d^{10} 6s^2 6p^3$	🟧 **Po** 84 Polonium $(210)^a$ $4f^{14} 5d^{10} 6s^2 6p^4$	🟨 **At** 85 Astatine $(210)^a$ $4f^{14} 5d^{10} 6s^2 6p^5$	🟨 **Rn** 86 Radon $(222)^a$ $4f^{14} 5d^{10} 6s^2 6p^6$
7	🟦 **Fr** 87 Francium $(223)^a$ $7s^1$	🟦 **Ra** 88 Radium 226.0254^b $7s^2$	🟦 **Ac**** 89 Actinium $(227)^a$ $6d^1 7s^2$	🟦 **Rf** 104 Rutherfordium $(261)^a$ $5f^{14} 6d^2 7s^2$	🟦 **Db** 105 Dubnium $(262)^a$ $5f^{14} 6d^3 7s^2$	🟦 **Sg** 106 Seaborgium (266) $5f^{14} 6d^4 7s^2$	🟦 **Bh** 107 Bohrium (264) $5f^{14} 6d^5 7s^2$	🟦 **Hs** 108 Hassium (269) $5f^{14} 6d^6 7s^2$	🟦 **Mt** 109 Meitnerium (268) $5f^{14} 6d^7 7s^2$	🟦 – 110 – (269) – –	🟦 – 111 – (272) – –							

🟦 Metal 🟧 Semimetal 🟨 Nonmetal

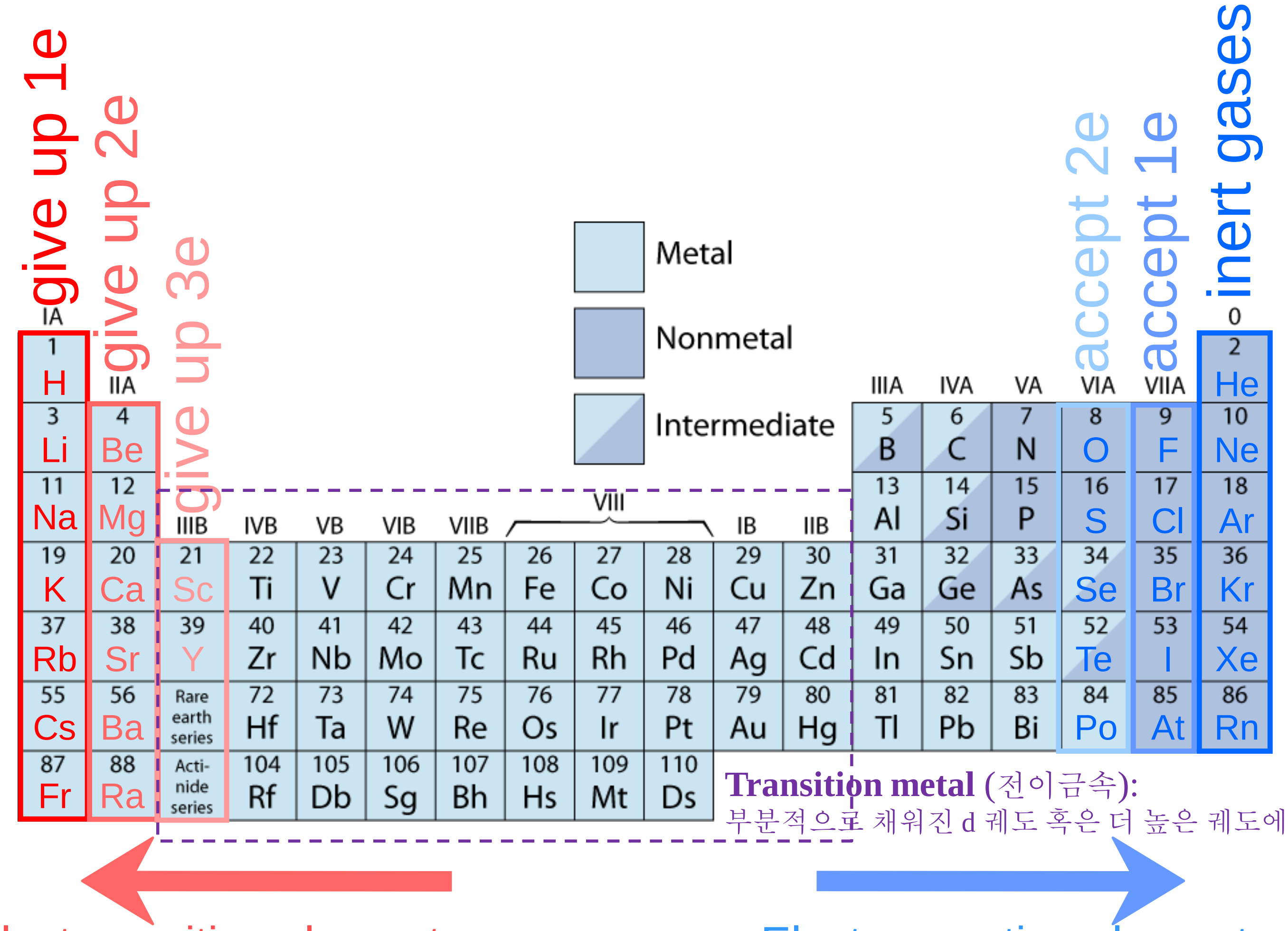
Inner transition elements

Lanthanide series *6	🟦 **Ce** 58 Cerium 140.116 $4f^1 5d^1 6s^2$	🟦 **Pr** 59 Praseodymium 140.90765 $4f^3 6s^2$	🟦 **Nd** 60 Neodymium 144.24 $4f^4 6s^2$	🟦 **Pm** 61 Promethium $(145)^a$ $4f^5 6s^2$	🟦 **Sm** 62 Samarium 150.4 $4f^6 6s^2$	🟦 **Eu** 63 Europium 151.964 $4f^7 6s^2$	🟦 **Gd** 64 Gadolinium 157.25 $4f^7 5d^1 6s^2$	🟦 **Tb** 65 Terbium 158.92534 $4f^9 6s^2$	🟦 **Dy** 66 Dysprosium 162.50 $4f^{10} 6s^2$	🟦 **Ho** 67 Holmium 164.93032 $4f^{11} 6s^2$	🟦 **Er** 68 Erbium 167.26 $4f^{12} 6s^2$	🟦 **Tm** 69 Thulium 168.9342 $4f^{13} 6s^2$	🟦 **Yb** 70 Ytterbium 173.04 $4f^{14} 6s^2$	🟦 **Lu** 71 Lutetium 174.97 $4f^{14} 5d^1 6s^2$
Actinide series **7	🟦 **Th** 90 Thorium 232.0381^b $6d^2 7s^2$	🟦 **Pa** 91 Protactinium 231.03588 $5f^2 6d^1 7s^2$	🟦 **U** 92 Uranium 238.02891 $5f^3 6d^1 7s^2$	🟦 **Np** 93 Neptunium (237) $5f^4 6d^1 7s^2$	🟦 **Pu** 94 Plutonium (244) $5f^6 7s^2$	🟦 **Am** 95 Americium (243) $5f^7 7s^2$	🟦 **Cm** 96 Curium $(247)^a$ $5f^7 6d^1 7s^2$	🟦 **Bk** 97 Berkelium (247) $5f^9 7s^2$	🟦 **Cf** 98 Californium $(251)^a$ $5f^{10} 7s^2$	🟦 **Es** 99 Einsteinium (251) $5f^{11} 7s^2$	🟦 **Fm** 100 Fermium (257) $5f^{12} 7s^2$	🟦 **Md** 101 Mendelevium (258) $5f^{13} 7s^2$	🟦 **No** 102 Nobelium (259) $5f^{14} 7s^2$	🟦 **Lr** 103 Lawrencium (262) $5f^{14} 6d^1 7s^2$

Chapter 2.4

VII. The Periodic Table

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



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
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	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								

Transition metal (전이금속):
부분적으로 채워진 d 궤도 혹은 더 높은 궤도에 1-2개 전자 포함

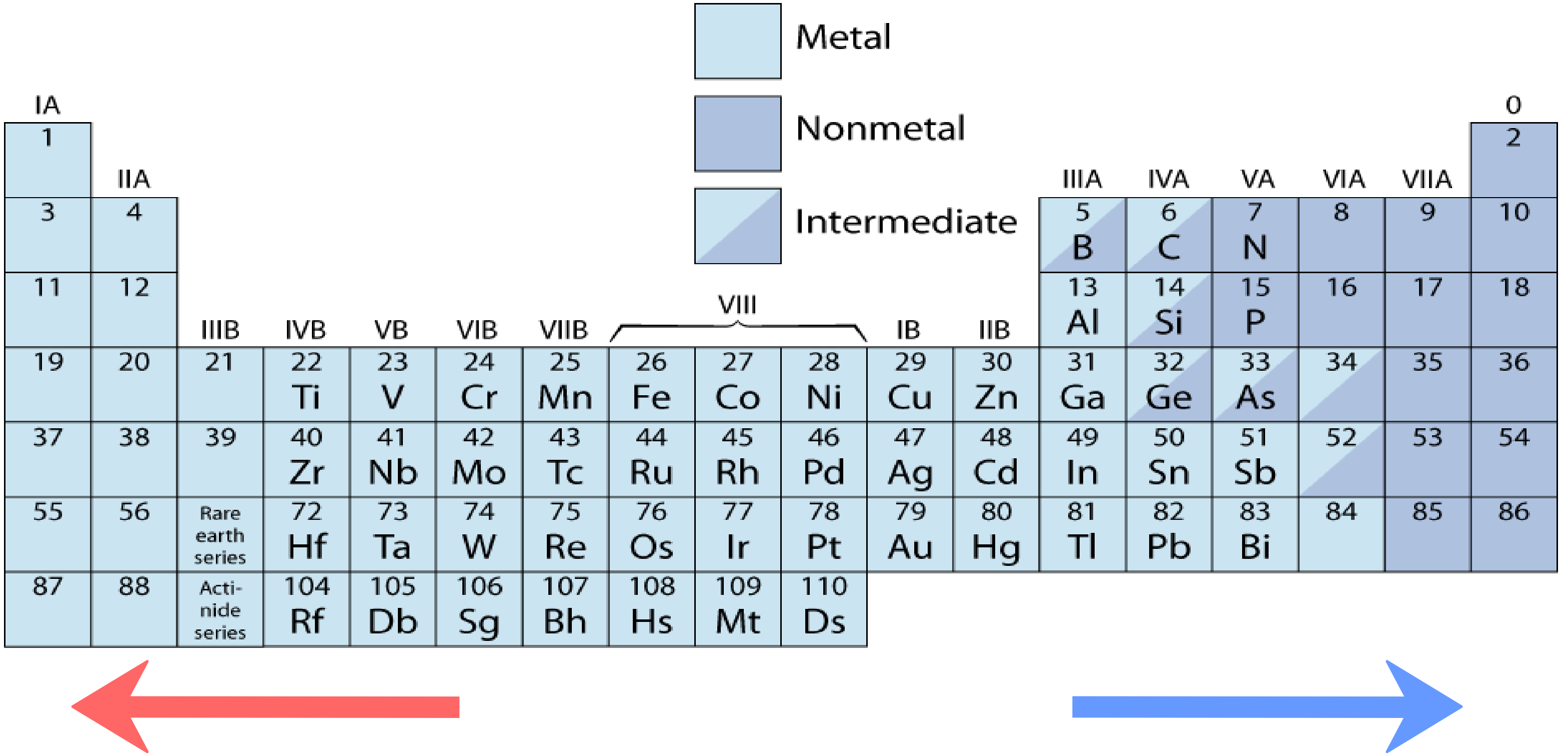
Adapted from Fig. 2.6, *Callister 7e.*

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

Electronegative elements:
Readily acquire electrons
to become **- ions.**

Electronegativity (전기음성도)

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



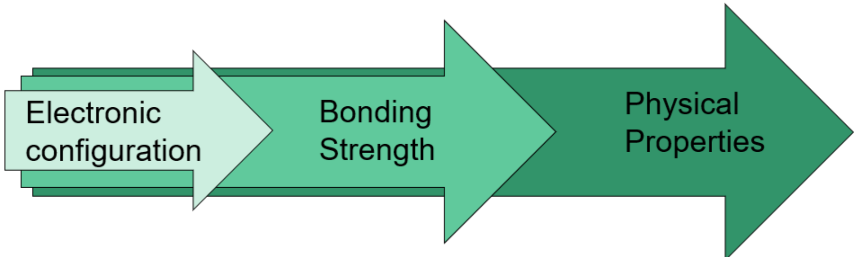
Smaller electronegativity

Larger 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



Electronic configuration

Bonding Strength

Physical Properties

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

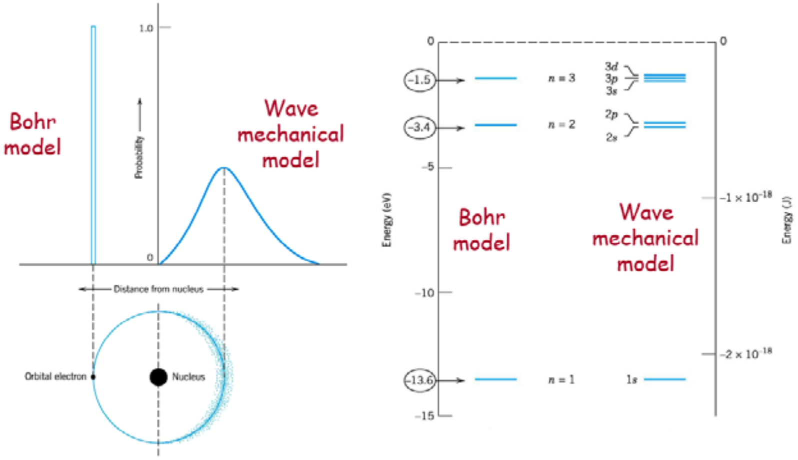
전자는 파동성과 입자성을 동시에 갖는다 가정= 전자구름

b. Quantum #s (양자수)

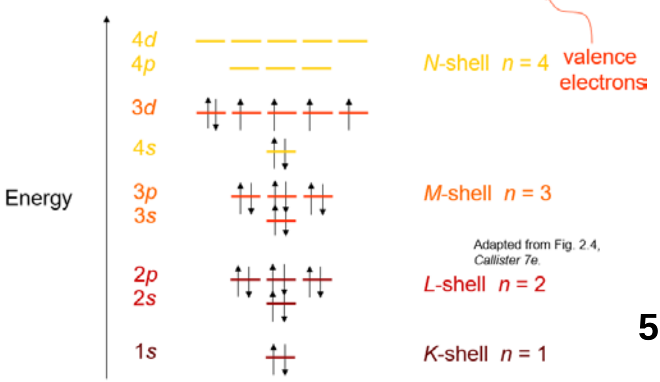
n = principal (energy level-shell)	*K, L, M, N, O* (1, 2, 3, etc.)
ℓ = subsidiary (orbitals)	*s, p, d, f* (0, 1, 2, 3,…, *n*-1)
m_l = magnetic	1, 3, 5, 7 (-*ℓ* to +*ℓ*)
m_s = spin	½, -½

c. Electron configurations (전자배위)

Bohr vs. wave mechanical model



ex: Fe - atomic # = 26 $1s^2$ $2s^2\,2p^6$ $3s^2\,3p^6$ $\boxed{3d^6\ 4s^2}$



Adapted from Fig. 2.4, Callister 7e.

2.4 **Periodic table**

모든 원소는 주기율표 상의 전자 배위에 의해 분류

: <u>특성의 규칙적인 변화 양상</u> 확인 가능