Introduction to Crystallography, 결정학개론 (445.206)

- **Objective**

  Learn the basics of crystal structures based on crystallographic symmetry and understand correlations between the crystal structure and physical properties, lattice transformations, and the principle of X-ray diffraction.

- Lecturer; Chan Park (박 찬) (880-9324, 33-219, pchan@snu.ac.kr)
- Lecture; Mon & Tue, 1100 ~ 1215
- Lecture Room; 33-225 (or ZOOM)
- Teaching Assistant; **Dohyun Aeom (880-1482, 30-208, djaehgus1003@snu.ac.kr)**
- Office Hour; Mon & Wed, 0900 ~ 1030, 1400 ~ 1500
- Lecture notes can be downloaded from ETL before the lecture.

Grading & Evaluation

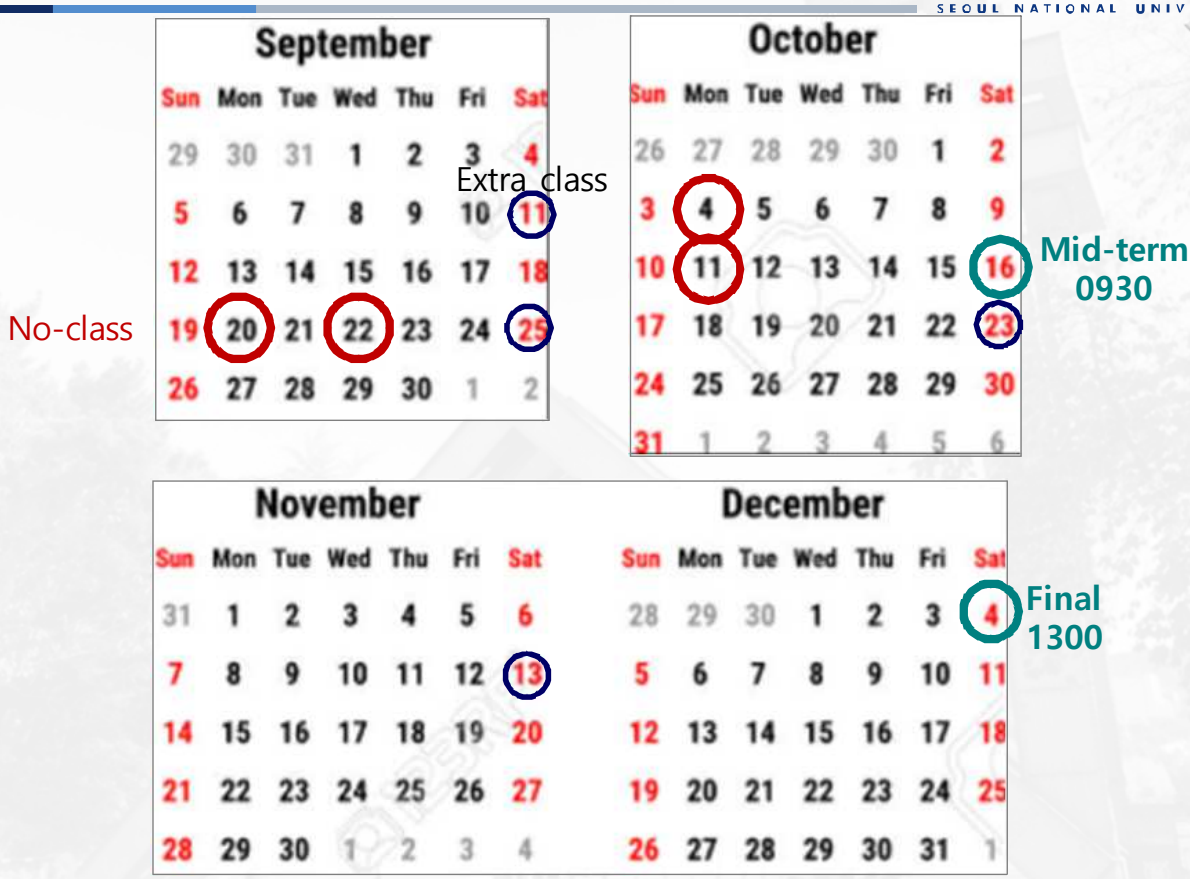
- Attendance* (10%)
- Class Attitude (5%)
- Homeworks/Quiz (25%)
- Midterm (30%) – 120min, **October 16 (Sat) 1000 ~ 1200**
- Final (30%) – 120min, **December 4 (Sat) 1300 ~ 1500**

- Homeworks – from Ott, Hammond, Krawitz, Cullity, etc.
- A (< 30%), B (< 40%), C & below (> 30%) 재수강 95% 인정

*
- Zoom 참여자 이름 ; 본인이름_학번의 뒷자리수
- 11시와 12시 10분 참여자 명단에 포함되면 출석 인정
- 움직이면서 zoom 참여하면 결석
- VIDEO ON 필수 (PC에 camera 없으면 휴대폰으로 추가 접속 필요)

Supplementary Lectures

- No lectures in regular lecture time on
  - ✓ 9/20, 9/22, 10/4, 10/11 (4 X 75 = 300 min)
- Supplementary lecture – 720 min (dates TBD)
  - ✓ **9/11(Sat) - 120 min, 0930 ~ 1130**
  - ✓ **9/25(Sat) - 120 min, 0930 ~ 1130**
  - ✓ **10/16(Sat) - 120 min, 0930 ~ 1130 mid-term exam**
  - ✓ **10/23(Sat) - 120 min, 0930 ~ 1130**
  - ✓ **11/13(Sat) - 120 min, 0930 ~ 1130**
  - ✓ **12/04(Sat) - 120 min, 1300 ~ 1500 final exam**
- 12/06, 12/08, 12/13 – no class (225 min)(Last day of the semester 12/14)
- 720 – 300 – 225 = 195 hours (3.25 hours) (75 min X 2.6)
- 12/01 – last class



Grouping of students

- Make a team of 3 students → will be done by the professor by Sep. 11 and will let you know by ETL.

- Team members can study together, can try to work the problems together.
- Team members can have identical solutions for the problem homeworks.
- This is not a must-do. Those who want to work alone can do that after he/she discusses this with the professor **before Sep. 8**. Otherwise, you have to work together.

Textbooks

Main

- W.B. Ott, Crystallography, 3rd Ed., Springer
  - ✓ Chapter 1, 2, 3, 4, 5 (5.5, 5.7, 5.8), 6, 7, 8, 9 (9.2.2, 9.2.3, 9.2.4, 9.7), 10, 12, 13
- C. Hammond, The Basics of Crystallography and Diffraction, 4th Ed., Oxford Science Publications
  - ✓ Chapter 1 (1.9, 1.10, 1.11), 2 (2.6, 2.7, 2.8, 2.9), 3 (3.4), 4 (4.8, 4.9), 5 (5.7, 5.8, 5.9, 5.10), 6, 7 (7.5), 8, 9 (9.3, 9.4, 9.5, 9.6, 9.7, 9.8), 12, Appendix 5

Supplementary

- V.K. Pecharsky & P.Y. Zavalij, Fundamentals of powder diffraction and structural characterization of materials, 2nd Ed., Springer, 2009
  - ✓ Chapter 1, 2, 3, 4, 7, 8, 9
- D. Sherwood & J. Cooper, Crystals, X-rays, and Proteins, 2011
  - ✓ Chapter 1, 3, 4, 5, 6, (7, 8, 9)
- B.D. Cullity, Elements of X-ray Diffraction, 3rd Ed., Prentice Hall, 2001
  - ✓ Chapter 1, 2, 3, 4, A1
- A.D. Krawitz, Intro. to Diffraction in Mater. Sci. & Eng., Wiley Inter-Science, 2001
  - ✓ Chapter 1, 2, 5

You need these chapters

- Ott - chap 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13
- Hammond – chap 1, 2, 3, 4, 5, 6, 7, 8, 9, 12
- Sherwood & Cooper – chap 3, 4, 5, 6, 8.7, 8.8
  - ✓ Page 58~104, 122~152, 269~277
- Cullity – chap 1, 2, 3, 4, A1
  - ✓ page 1~19, 31~40, 70~86, 89~103, 123~137
- Krawitz – chap 1, 2, 5
  - ✓ page 1~27, 40~71, 119~143

Course contents

- Crystal, crystallography
- Lattice, translation, unit cell, plane, miller indices, interplanar spacing
- Reciprocal lattice
- Stereographic projection
- Symmetry, symmery operation, 14 Bravais Lattices, 7 Crystal Systems, 32 point groups, 17 plane groups, 230 space groups
- Anisotropy (tensor), Neumann's Principle, properties (thermal conductivity, electrical conductivity, dielectrics, magnetism, piezoelectricity, elasticity, pyroelectricity)
- Diffraction physics
- X-ray diffraction, Laue conditions, Bragg equation, Ewald sphere, Structure factor
- Phase identification using XRD

HW1

Submit Statement
"who am I?" (a hardcopy or a pdf file), by Sep. 11

- A photo (without excessive photoshop)
- Brief introduction of yourself
- Why did you choose MSE?
- What do you plan to do after university?
- What do you want to be?
- Whatever you like to tell me
- < 2 pages

HW2

- A crystal model of isometric cube
- **Due – 13, September 2015**
- Should be portable, Should not be too small
- You can choose any material, but it has to be strong enough to carry around
- You need to show me the model before the class on September 13.

You can get help here
https://www.iucr.org/__data/assets/pdf_file/0009/3123/Class.pdf

To-dos

- Get the books
- HW 1, HW 2

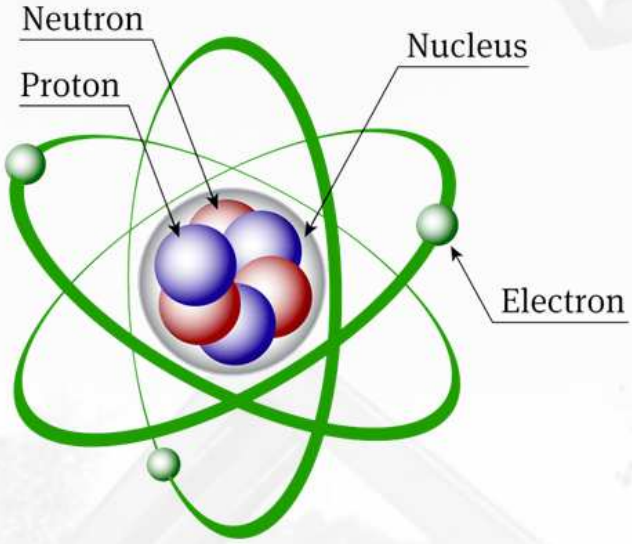
Introduction to Crystallography, 결정학개론 (445.206)

- **Crystal**
  - ✓ An anisotropic, homogeneous body consisting of a **3-dimensional periodic ordering** of atoms, ions, or molecules
  - ✓ In addition to their microscopic structure, large crystals are usually identifiable by their macroscopic geometrical shape, consisting of flat faces with specific, characteristic orientations
  - ✓ Solids which possess **long-range, 3-dimensional molecular order**

- **Crystallography** – concerned with the laws governing the **crystalline state** of solid materials with the arrangement of atoms (molecules, ions) in crystals and with their physical and chemical properties, their synthesis and their growth. (Ott)
  - ✓ 결정 구조와 이 구조에 기인하는 화학적, 물리적 성질을 연구하는 학문

- Perfect crystal vs. Crystals with defects

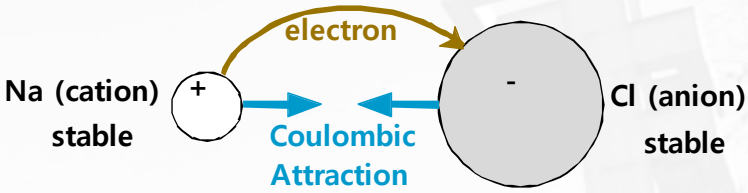
Atom and Atomic Bonds



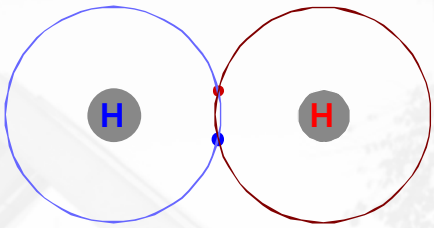
- Atomic number = # of protons in nucleus of atom
  = # of electrons in neutral species
- Atomic weight = weight of 6.022 x 1023 atoms
  ex) Carbon 12.011 g/mol

Bonding

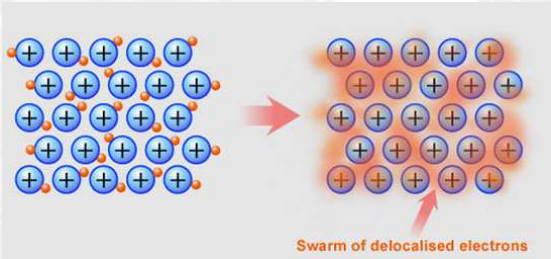
Ionic



Covalent

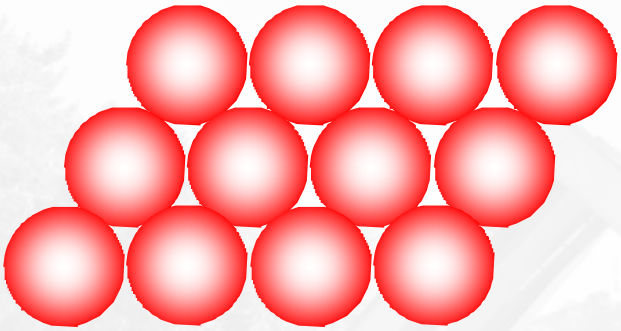


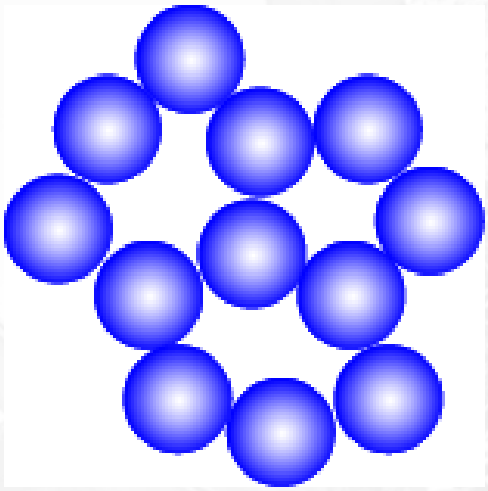
Metallic



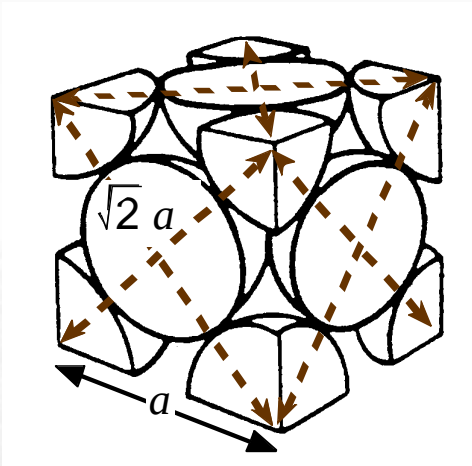
Source: Metallic Bonding, ABC Science

How to Stack in 2D and 3D





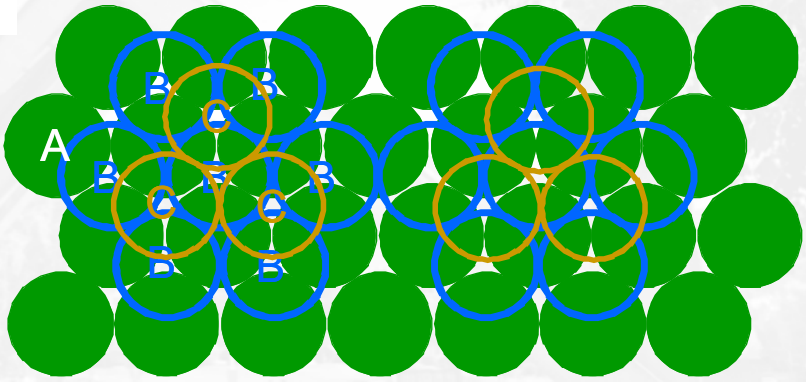
Stacking - FCC



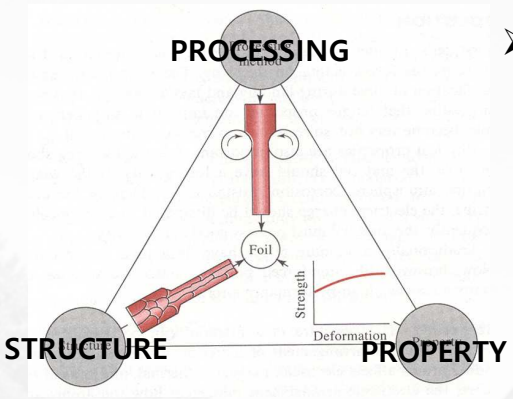
A sites

B sites

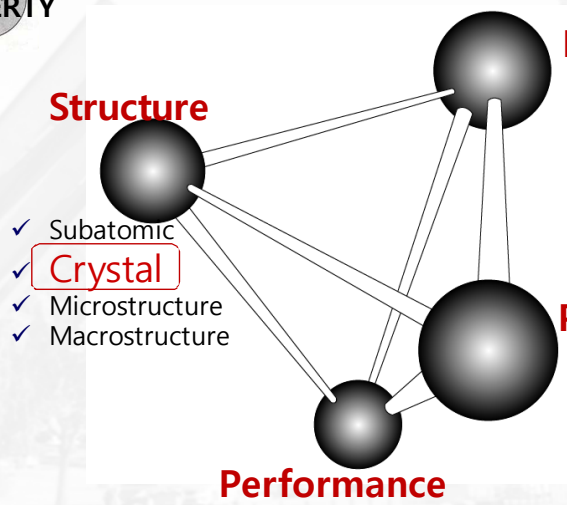
C sites



Materials Science & Engineering



➢ Relation between
STRUCTURE, PROPERTY & PROCESSING



Structure
- ✓ Subatomic
- ✓ Crystal
- ✓ Microstructure
- ✓ Macrostructure

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

Properties
- ✓ Mechanical
- ✓ Electrical
- ✓ Magnetic
- ✓ Thermal
- ✓ Optical
- ✓ Deteriorative

Performance

화상강연 관련 정보

- ➢ ZOOM 참가자 이름을 "이름_학번 (학번의 뒷 숫자5개)" 으로 만들어 주세요. 참여자 이름이 정확하게 표시되지 않으면 출석 확인이 어려울 수 있습니다. 참여자 신분 확인이 어려우면 참여할 수 없습니다.
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- ➢ 11시~12시 10분 사이에는 접속이 되어 있어야 출석 인정합니다.
- ➢ 소리가 들리지 않거나, 음량을 올려도 소리가 작게 들리는 학생들은 채팅으로 알려주세요.