The Crystal Structure of Materials

Presented by Prof. Soung Soo Yi

2011-2

Syllabus Fall Semester 2011

- General Information

Course Title	Materials Crystallography		Course No.	43045	
Course	Major	Unit/Hours	3/3	Dept.	Electronic Materials Engineering

- Instructor's Information

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- Course Information

Prerequisite	Fundamental Physics	Restricted Dept.	
Registering Dept.	Electronic Materials Engineering	Course Type	Lecture and discucssion
Required Equipment	Beam Projector	Instructional Materials	Lecture Notes
Language	English	S/W	MS-office, 한글 word
Team Teaching		Others	

Course Goal & Description

Course Goals	Understanding the physical concepts related to the structure of materials and crystallography.
Course Description	We will discuss the kind and characteristic properties of crystalline lattices and learn the principle analyzing the crystalline phase and lattice structure of solid state materials by using X-ray diffraction patterns. Also, this course will cover the directional bonding, atoms packing, lattice, symmetry, unit cell, diffraction of wave and Fourier transform.

Grading Policy

Attendance	Assignment	Midterm	Final	Participation	Others	Total
10	10	30	40	10		100

Textbook & References

No.	Text	Authors	Publisher	Date of Issue	Remarks
1	The crystal structure of materials	Lee, Jeong Yong	Chung Moon Gak	2008.02	
2	Introduction to solid state physics	C. Kittle	Wiley	2005.02	

- # Course Calendar

Week	Content	Required Equipment	Assignments	Remarks
1	Introduction of the course Ch. 1 Atomic Bonds			
2	1-1 Electrons in Atoms			
3	1-2 Chemical Bonds in Atoms		HW #1 Exercise of Ch.1	Discussion for Ch.1
4	Ch.2 Packing Atoms 2-1 Directional binding of atoms			
5	2-2 Directional binding of same size atoms 2-3 Directional binding of different size atoms			
6	2-4 Crystal structure of Oxide Amorphous		HW #2 Exercise of Ch.2	Discussion for Ch.2
7	Ch.3 Lattice and Symmetry in Crystal 3-1 Lattice and unit cell, 3-2 Symmetry			
8	Midterm Exam.			
9	3-3 Crystal systems, 3-4 Lattice in crystal			
10	3-5 Lattice plane and irection 3-6 Reciprocal vector		HW #3 Exercise of Ch.3	Discussion for Ch.3
11	Ch.5 Crystal structure 5-1 The crystal structure of metals			
12	5-2 The crystal structure of chemical compounds			
13	Ch.7 Wave and diffraction in solid 7-1 Wave and Fourier transform		HW #4 Exercise of Ch.5	Discussion for Ch.5
14	7-2 X-ray Diffraction in crystal			
15	Review and Final Exam		HW #5 Exercise of Ch.7	Discussion for Ch.7

Chap. 1 Atomic Bonds

1-1 Electrons in atoms

1-1-1 The characteristics of electrons

- It is necessary to understand the properties of electrons before we study the structure of solids, atom's packing and binding of atoms.
- To understand the behavior of electrons, we need to study the quantum mechanical characteristics of electrons.

Quantum mechanical characteristics of electrons

1. Quantization of electron energy.
2. Electrons comply with the Pauli exclusion principle.
3. Heisenberg’s uncertainty principle.
4. Schrodinger’s wave equation.

Quantization of electron energy.

- For the atom that has proton's number 'Z' , nucleus charge '+Ze', the electron 'e' is under the attraction of nucleon by the coulomb force.

$$F_{\text{Coul}} = \frac{(+Ze)(-e)}{4\pi\varepsilon_o r^2} \quad (1\text{-}1)$$

Where $\varepsilon_0 = 8.85\times10^{-12}$ F/m : dielectric permeability of vaccum

$$F_{\text{centr}} = -\frac{m_e\upsilon^2}{r} \quad (1\text{-}2)$$

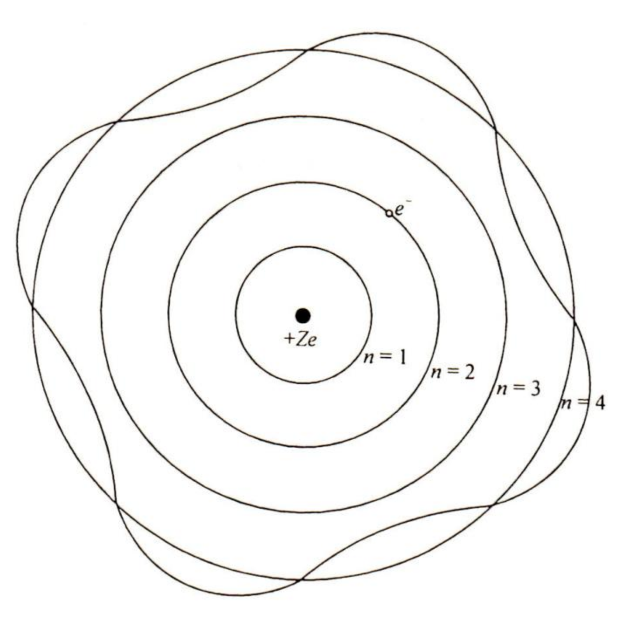

Fig. 1-1 Bohr's atomic model.
Electron moves on the circular orbital and the length of circumference of the circle is equal to the integer multiple of wavelength of electron wave

$$-\frac{Ze^2}{4\pi\varepsilon_o r^2} = -\frac{m_e \upsilon^2}{r},$$

$$r = \frac{Ze^2}{4\pi\varepsilon_o m_e \upsilon^2} \quad (1\text{-}3)$$

υ는 전자의 궤도 속도이고 m_e는 전자 질량 (9.11×10^{-31} kg)이다.

When we consider the electrons motion as a wave, the wavelength of the electron wave is

$$\lambda = \frac{h}{p} \quad (1\text{-}4)$$

h 는 플랑크 상수(h = 6.63×10^{-34} J·s)이고, p 는 운동량이다.

According to the de Broglie relationship,

$$2\pi r = n\lambda$$

$$\lambda = \frac{2\pi r}{n} \quad (1\text{-}5)$$

From the relationship between momentum and wavelength of electron

$$p = m_e \upsilon = \frac{h}{\lambda} \qquad (1\text{-}6)$$

And if you substitute the wavelength of eq. (1-5) to the eq. (1-6), then we can find the velocity of electron

$$\upsilon = \left(\frac{h}{m_e}\right)\left(\frac{n}{2\pi r}\right) \qquad (1\text{-}7)$$

And if you substitute this to the eq. (1-3), then we can find the radii of orbitals.

$$r = r_n = \frac{h^2 \varepsilon_0}{\pi e^2 m_e} \frac{n^2}{Z} \qquad (1\text{-}8)$$

The radii of orbitals are quantized.

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If we calculate the quantized radii of quantized orbitals by substituting the constants in the above equation.

$$r_1 = 0.0529 \text{ nm}$$

$$r_2 = 0.2116 \text{ nm}$$

$$r_3 = 0.4761 \text{ nm}$$

$$r_4 = 0.8464 \text{ nm}$$

The quantized energy of the electron

And then we can derive the quantized energy of the electrons.

The kinetic energy of the electron is given by

$$E_k = \frac{1}{2} m_e \upsilon^2 \tag{1-9}$$

And the coulomb potential is given by

$$E_p = -\frac{Ze^2}{4\pi\varepsilon_o r} \tag{1-10}$$

Then, the total energy will be

$$\begin{aligned} E &= E_k + E_p \\ &= \frac{1}{2} m_e \upsilon^2 + \left(-\frac{Ze^2}{4\pi\varepsilon_o r} \right) \end{aligned} \tag{1-11}$$

After we multiply –r/2 on both sides of the eq. (1-3), the eq. (1-11) will be

$$E = \frac{Ze^2}{8\pi\varepsilon_o r} + \left(-\frac{Ze^2}{4\pi\varepsilon_o r}\right) = -\frac{Ze^2}{8\pi\varepsilon_o r} \quad (1\text{-}12)$$

If we substitute the eq. of orbital radii, then we can get the equation for the quantized energies.

$$E = E_n = -\frac{e^4 m_e}{8h^2\varepsilon_o^2}\frac{Z^2}{n^2} = -13.6\frac{Z^2}{n^2}\ \text{eV} \quad (1\text{-}13)$$

Wher the'-" sign means that the electron is restricted by nucleon and n is the principle quantum number, n=1, 2, 3,……

. For Hydrogen atom, Z=1, then the energy of the electron will be

$$E_n = -\frac{13.6}{n^2} \text{ eV} \qquad (1\text{-}14)$$

. For n=1, 2, 3 and 4

$$E_1 = -13.6 \text{ eV}$$
$$E_2 = -3.40 \text{ eV}$$
$$E_3 = -1.50 \text{ eV}$$
$$E_4 = -0.80 \text{ eV}$$

. For n=1 K-shell
n=2 L-shell
n=3 M-shell
n=4 N-shell
n=5 O-shell

- To change the energy level of electron, the electron should absorb or emit the energy difference between energy levels

$$\Delta E = h\nu \tag{1-15}$$

$\Delta E < 0$ For the emission of radiation energy

$\Delta E > 0$ For the absorption of radiation energy

- The energy difference between the energy levels n=1 and n=2, that is, the energy difference between K-shell and L-shell

$$\begin{aligned}\Delta E &= -13.6\, Z^2\left(\frac{1}{1^2} - \frac{1}{2^2}\right) \text{ eV} \\ &= -13.6\,\frac{3}{4}\, Z^2 \text{ eV}\end{aligned} \tag{1-16}$$

2. Pauli exclusion principle

On the one energy state, only one electron can exist.

→ on the one energy level, only two electrons that have opposite spins can exist.

3. Uncertainty principle

$$\Delta p_x \cdot \Delta x \geq \frac{h}{2\pi} = \hbar \qquad (1\text{-}17)$$

Δp_x The uncertainty of linear momentum

Δx The uncertainty of position

The uncertainty principle for ΔE and Δt

$$\Delta E \cdot \Delta t \geq \frac{h}{2\pi} = \hbar \qquad (1\text{-}18)$$

4. Schrodinger equation

- To describe the motion and state of electron, the Schrodinger equation, the differential equation, should be solved.
- The quantized energy levels and energy states can be explained by standing wave.

$$y = A \sin \frac{2\pi}{\lambda} x \tag{1-19}$$

Where A is the amplitude and 2πx/λ is the wave phase, λ is wavelength.

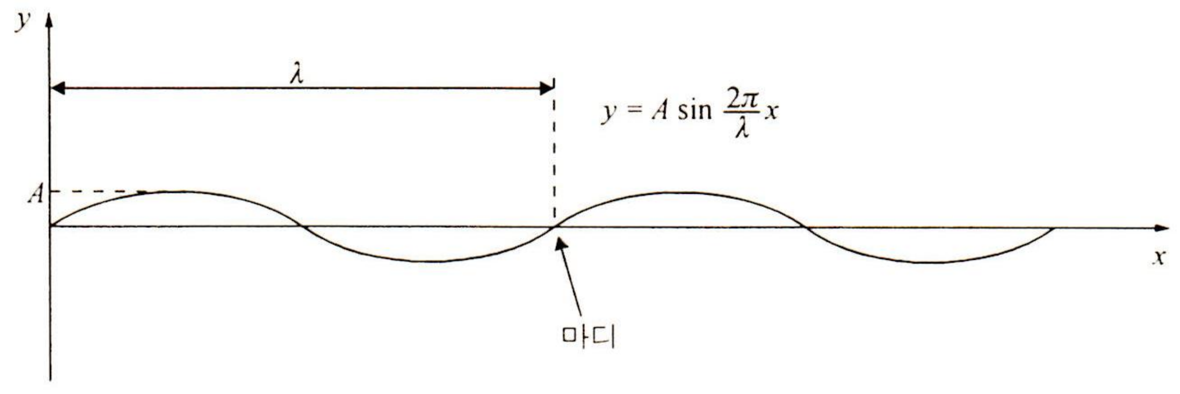

Fig. 1-2 Standing wave of string

The traveling wave with the velocity ‘v’

$$y = A \sin \frac{2\pi}{\lambda}(x \pm \upsilon t) \qquad (1\text{-}20)$$

From the standing wave

$$y = A \sin \frac{2\pi}{\lambda} x \qquad (1\text{-}21)$$

If we differentiate the eq.(1-21) with ‘x’

$$\frac{\partial y}{\partial x} = \frac{2\pi}{\lambda} A \cos \frac{2\pi}{\lambda} x \qquad (1\text{-}22)$$

And we differentiate the eq.(1-22) with ‘x’ one more

$$\frac{\partial^2 y}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} A \sin \frac{2\pi}{\lambda} x \qquad (1\text{-}23)$$

- Then the equation will be

$$\frac{\partial^2 y}{\partial x^2} + \left(\frac{2\pi}{\lambda}\right)^2 y = 0 \qquad (1\text{-}24)$$

And the de Broglie wavelength

$$\lambda = \frac{h}{p} \qquad (1\text{-}4)$$

If we substitute this to eq. (1-24)

$$\frac{\partial^2 y}{\partial x^2} + \frac{4\pi^2 p^2}{h^2} y = 0 \qquad (1\text{-}25)$$

And we use the linear momentum $p = m_e \upsilon$

$$\frac{\partial^2 y}{\partial x^2} + \frac{4\pi^2 m_e{}^2 \upsilon^2}{h^2} y = 0 \qquad (1\text{-}26)$$

And the total energy E=Ek+Ep, then we substitute these eqs to eq. (1-26) .

$$\frac{\partial^2 y}{\partial x^2} + \frac{8\pi^2 m_e}{h^2}(E - E_p)y = 0 \qquad (1\text{-}27)$$

Then, the schrodinger wave equation using ψ instead of y will be

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m_e}{h^2}(E - E_p)\psi = 0 \qquad (1\text{-}28)$$

Then, if we extend this to 3-dimension and using the 'Laplacian operator'

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad (1\text{-}29)$$

Then, the schrodinger wave equation in 3-dimension will be

$$\nabla^2 \psi + \frac{8\pi^2 m_e}{h^2}(E - E_p)\psi = 0 \qquad (1\text{-}30)$$

And if we rewrite time-independent the schrodinger wave equation

$$\left(-\frac{h^2 \nabla^2}{8\pi^2 m_e} + E_p\right)\psi = E\psi \qquad (1\text{-}31)$$

And $$H\psi = E\psi \qquad (1\text{-}32)$$

Where H is the Hamiltonian operator

$$H = -\frac{h^2}{8\pi^2 m_e}\nabla^2 + E_p \qquad (1\text{-}33)$$

When we solve the schrodinger eq. using the boundary condition, the solution of the equation is ‘eigenfunction’ or ‘eigenstate’. And each eigenstate has ‘eigenvalue’.

$$E_n = -\frac{e^4 m_e}{8h^2 \varepsilon_o^2}\frac{Z^2}{n^2}$$
$$= -13.6\frac{Z^2}{n^2}\ \text{eV} \qquad (1\text{-}13)$$