Mid-Term Exam

2018. 04. 26. 15:00~17:00, Closed Book
Instructor: Seungtae CHOI

1. (10 points) Please answer to the following questions about electrons in atoms.

(a) List up and explain four quantum numbers characterizing electron states in an atom.

(1) Principal quantum number, n
- ✓ Energy level-shell
- ✓ Related to the size of an electron's orbital

(2) Subsidiary quantum number, l
- ✓ Designates the subshell
- ✓ Related to the shape of an electron's orbital

(3) Magnetic quantum number, ml
- ✓ When a magnetic field is applied, these subshell states split.
- ✓ Related to electron obitals

(4) The fourth quantum number, ms
- ✓ Related to the spin moment

(5)

Quantum Number	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	(-l to +l)
m_s = spin	½, -½	

(b) Explain three types of primary interatomic bonds.

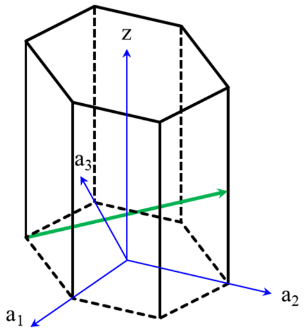
(1) Ionic bonding
- ✓ Ionic bonding is always found in compounds composed of both metallic elements (+ ions) and nonmetallic elements (- ions).
- ✓ Ionic bonding requires electron transfer and thus large difference in electronegativity.
- ✓ Ionic bonding is nondirectional.

(2) Covalent bonding
- ✓ Similar electronegativity → share electrons
- ✓ Bonds determined by valence – s & p orbitals dominate bonding
- ✓ Covalent bonding is directional.

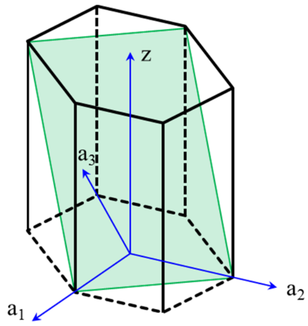
(3) Metallic Bonding
- ✓ The valence electrons form a "sea of electrons" or "electron cloud" that can freely move around the metal ion cores, which makes metals electrically conductive.
- ✓ These free electrons act as a "glue" to hold the ion cores together.
- ✓ The metallic bond is nondirectional.

2. (10 points) Determine indices for the direction and plane shown in the following hexagonal unit cells.

(a)



(b)



1. Tail point: (0,-a,0) and head point: (0, a, c/2)
2. (a_1, a_2, z) = (0, 2a, c/2)
3. Adjust to smallest integer values: (0, 4, 1)
4. Enclose in square brackets: [UVW] = [041]
5. Convert to four-axis Miller-Bravais system:
   u = (2U-V)/3 = -4/3, v = (2V-U)/3 = 8/3
   t = -(u+v) = -4/3, w = W = 1
6. Adjust to smallest integer values
   ∴ [uvtw]=[$\bar{4}8\bar{4}3$]

	a_1	a_2	a_3	c
1. Intercepts	1	1	-1/2	1/2
2. Reciprocals	1/1	1/1	-2/1	2/1
3. Reduction	1	1	-2	2
4. Miller Index	($11\bar{2}2$)			

3. (10 points) Regarding dislocations-linear defects in crystalline solids, please explain the following terminologies.

   (a) Burgers vector, (b) Dislocation line, (c) Edge dislocation, (d) Screw dislocation

Dislocations are one-dimensional defects around which atoms are misaligned.

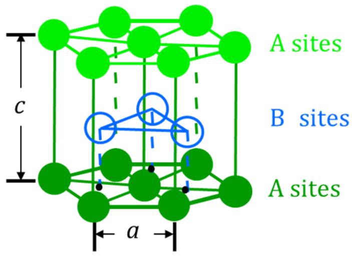
(a) Burgers vector, named after Dutch physicist Jan Burgers, is a vector, often denoted as **b**, that represents the magnitude and direction of the lattice distortion resulting from a dislocation in a crystal lattice.

(b) Dislocation
- ✓ A dislocation line represents a curve connecting dislocation core (line defect) in crystal structures.
- ✓ A dislocation line cannot end within a crystal.

(c) Edge dislocation:
- ✓ Extra half-plane of atoms inserted in a crystal structure.
- ✓ Burgers vector is perpendicular to dislocation line.

(d) Screw dislocation:
- ✓ Spiral planar ramp resulting from shear deformation.
- ✓ Burgers vector is parallel to dislocation line.

4. (10 points) For hexagonal close-packed (HCP) crystal structures, determine the following values and show the procedure. Please use $c/a = 1.633$.
   (a) The number of atoms per unit cell, N
   (b) Coordination number
   (c) Atomic packing factor (APF)



   (a) The number of atoms per unit cell, N
   ✓ $N = N_i + N_f/2 + N_c/6 = 3 + 2/2 + 12/6 = 6$

   (b) Coordination number
   ✓ The coordination number of HCP crystals is 12.

   (c) Atomic packing factor (APF)
   ✓ $APF = N\times(4/3)\pi R^3 / ((3\sqrt{3}/2)a^2c)$
   $= 16\ \pi R^3 / (1.633 \times 3\sqrt{3})a^3$
   $= 2\pi / (1.633 \times 3\sqrt{3})$
   $= 0.74.$

5. (60 points) Regarding the following questions, please make a circle on T if you think the statement is true, or make a circle on F if you think the statement is not true. It should be noted that minus points will be given to incorrect answers, and thus, if you are not sure about the correct answer, you would better not choose any one of T or F.

1) CH_4 (Methane), H_2O (Water), HF (Hydrofluoric Acid), GaAs (Gallium Arsenide), and LiF (Lithium Fluoride) are typical examples of covalent bonding.	T	**F**
Note: LiF (Lithium Fluoride) is a typical example of ionic bonding.		
2) Magnesium atoms (atomic number = 12 and electronic configuration = $1s^2 2s^2 2p^6 3s^2$) have two valence electrons.	**T**	F
3) Graphite (parallel layers of interconnecting hexagons) has sp^2 hybridized bonds in layers and weak van der Waals bonding between layers.	**T**	F
4) In metals, the valence electrons form a "sea of electrons" that can freely move around the metal ion cores, which makes metals electrically conductive.	**T**	F
5) According to Pauli exclusion principle, each electron state can hold no more than two electrons that must have opposite spins.	**T**	F
6) In orthorhombic structures, three edge lengths a, b, and c, and three interaxial angles, α, β, and γ have the following relations: $a=b\neq c$ and $\alpha=\beta=\gamma$.	T	**F**
Note: In orthorhombic structures, $a\neq b\neq c$ and $\alpha=\beta=\gamma$.		
7) In faced-centered cubic crystals, one atom is located at the point coordinate (1½½).	**T**	F

8) [100] and [110] directions in simple cubic crystals have the same elastic stiffness.	T	F
Note: [100] and [110] directions in simple cubic crystals have different elastic stiffnesses.		
9) In Miller index system, <hkl> and {hkl} represent a family of crystallographic directions and planes, respectively.	T	F
10) A plane intersecting three points P_1 (0,0,0), P_2 (½a,0,a), and P_3 (½a,a,a) in a simple cubic crystal (a = lattice constant) is (211) crystallographic plane.	T	F
Note: A plane intersecting three points P_1 (0,0,0), P_2 (½a,0,a), and P_3 (½a,a,a) in a simple cubic crystal (a = lattice constant) is (201) crystallographic plane.		
11) The number of atoms per unit cell, *N*, of the body-centered cubic (BCC) crystals is 4.	T	F
Note: The number of atoms per unit cell, *N*, of BCC crystals is 2.		
12) The coordination number (the number of nearest neighbor or touching atoms) of the face-centered cubic (FCC) crystals is 8.	T	F
Note: The coordination number of the face-centered cubic (FCC) crystals is 12.		
13) The atomic packing factor (APF) of the face-centered cubic (FCC) crystals is lower than that of body-centered cubic (BCC) crystals.	T	F
Note: The APF of the FCC crystals is higher than that of BCC crystals.		
14) Carbon Nanotubes (CNTs) have hexagonal crystal structure rolled into a cylindrical shape with sp^2 hybridized bonds.	T	F
15) X-Ray Diffraction (XRD) method to determine crystal structures is based on Snell's law.	T	F
Note: X-Ray Diffraction (XRD) method to determine crystal structures is based on Bragg's law.		
16) The repeating unit of poly(vinyl chloride) (PVC) is $C_2H_2Cl_2$.	T	F
Note: The repeating unit of poly(vinyl chloride) (PVC) is C_2H_3Cl.		
17) Most of cross-linked polymers, network polymers and branched polymers can be classified as thermosets.	T	F
Note: Branched polymers can be classified as thermoplastics.		
18) Thermoplastic polymers such as polyvinyl chloride (PVC), polystyrene, and polyethylene (PE) soften when heated and harden when cooled.	T	F
19) Methane, ethane, and propane are typical examples of isomerism of Paraffin compounds.	T	F
Note: Isomerism represents different atomic arrangements of hydrocarbon		

compounds with the same chemical formula. Therefore, methane, ethane, and propane are not typical examples of isomerism.		
20) In copolymers, alternating copolymers have long sequences of a monomer followed by long sequences of another monomer. Note: In copolymers, block copolymers have long sequences of a monomer followed by long sequences of another monomer.	T	F
21) Substitutional solid solution can be obtained only if impurity atoms have the same crystal structure as the host atom. Note: Substitutional solid solution can also be obtained with atoms having FCC and HCP crystal structures.	T	F
22) In statistical thermodynamics, generally defect concentration exponentially increases as temperature increases.	T	F
23) The Burgers vector of an edge dislocation is parallel to the dislocation line. Note: Burgers vector of an edge dislocation is perpendicular to the dislocation line.	T	F
24) After a polycrystalline surface is properly polished and etched, dislocation lines can be observed with optical microscope. Note: Dislocation lines can be observed with SEM or TEM but not with optical microscope.	T	F
25) Grain boundaries are slightly disordered, and more chemically reactive than the grains themselves.	T	F
26) In an alloy, atoms tend to migrate from regions of high concentration to regions of low concentration.	T	F
27) Generally, diffusion coefficient exponentially decreases with increasing temperature. Note: Generally, diffusion coefficient exponentially increases with increasing temperature.	T	F
28) Two diffusion mechanisms are vacancy diffusion and substitutional diffusion. Note: Two diffusion mechanisms are vacancy diffusion and interstitial diffusion.	T	F
29) In steady-state diffusion, diffusion flux is proportional to diffusion coefficient and concentration gradient.	T	F
30) Diffusion of substitutional atoms is much higher than that of interstitial atoms. Note: Diffusion of substitutional atoms is much lower than that of interstitial atoms.	T	F