1. (a) (10 points) Quantum Numbers

- **Principal quantum number, *n***
  - Energy level-shell
  - Related to the size of an electron's orbital
- **Subsidiary quantum number, *l***
  - Designates the subshell
  - Related to the shape of an electron's orbital
- **Magnetic quantum number, m_l**
  - When a magnetic field is applied, these subshell states split.
  - Related to electron obitals
- **The fourth quantum number, m_s**
  - Related to the spin moment

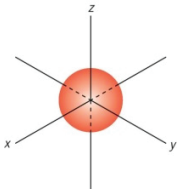


Fig. 2.4 Spherical shape of an s electron orbital.

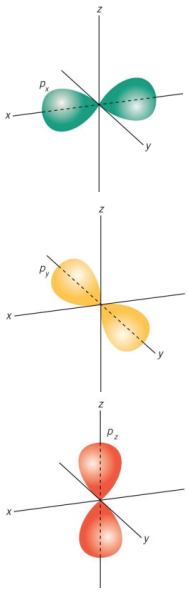


Fig. 2.5 Orientations and shapes of px, py, and pz electron orbitals.

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

1. (b)-(d)

1. (b) (3 points) Pauli's exclusion principle

- Each electron state can hold no more than two electrons that must have opposite spins.

1. (c) (3 points) The meaning of valence electrons

- Electrons occupying the outermost shell and participating in the bonding between atoms to form atomic and molecular aggregates.

1. (d) (4 points) Electron configuration of Argon (atomic number = 18)

- Electron configuration of Argon: $1s^2 2s^2 2p^6 3s^2 3p^6$
- Argon is a stable atom since the outermost shell (3p) is completely filled with electrons (6 electrons).

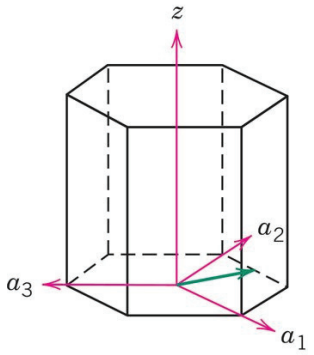
2. (a) (5 points)

- **Miller-Bravais coordinate system (four axes)**
  1. Tail point: $(x_1, y_1, z_1) = (0,0,0)$ and head point: $(x_2, y_2, z_2) = (a/2, a, 0)$
  2. $(a_1, a_2, z) = (a/2, a, 0)$
  3. Adjust to smallest integer values: (1,2,0)
  4. Enclose in square brackets, no commas, for three-axis coordinates: [UVW] = [120]
  5. Convert to four-axis Miller-Bravais lattice coordinates using equations below:

$$u = \frac{1}{3}(2U - V) = 0$$
$$v = \frac{1}{3}(2V - U) = 1$$
$$t = -(u + v) = -1$$
$$w = W = 0$$

  6. Adjust to smallest integer values and enclose in brackets:

$\therefore$ [uvtw]=[$01\bar{1}0$]



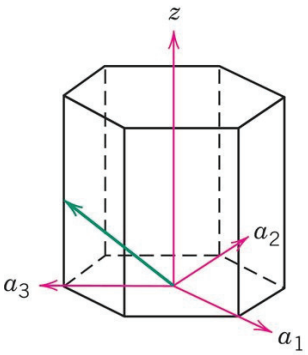
2. (b) (5 points)

- **Miller-Bravais coordinate system (four axes)**
  1. Tail point: $(x_1, y_1, z_1) = (0,0,0)$ and head point: $(x_2, y_2, z_2) = (-a, -a, c/2)$
  2. $(a_1, a_2, z) = (-2a, -2a, c)$
  3. Adjust to smallest integer values: (–2, –2, 1)
  4. Enclose in square brackets, no commas, for three-axis coordinates: [UVW] = [$\bar{2}\bar{2}1$]
  5. Convert to four-axis Miller-Bravais lattice coordinates using equations below:

$$u = \frac{1}{3}(2U - V) = -\frac{2}{3}$$
$$v = \frac{1}{3}(2V - U) = -\frac{2}{3}$$
$$t = -(u + v) = \frac{4}{3}$$
$$w = W = 1$$

  6. Adjust to smallest integer values and enclose in brackets:

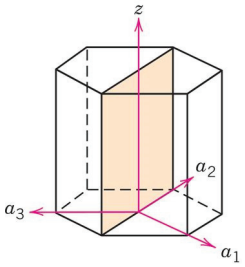
$\therefore$ [uvtw]=[$\bar{2}\bar{2}43$]



2. (c) and (d)

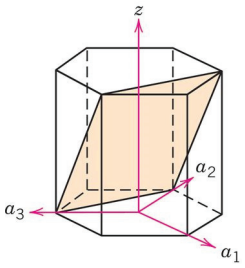
- **(5 points) Crystallographic Planes (HCP)**

		a_1	a_2	a_3	c
1.	Intercepts	1	∞	-1	∞
2.	Reciprocals	1	1/∞	-1	1/∞
3.	Reduction	1	0	-1	0
4.	Miller Indices	$(10\bar{1}0)$			



- **(5 points) Crystallographic Planes (HCP)**

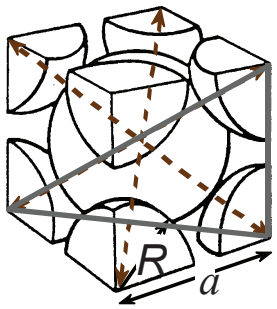
		a_1	a_2	a_3	c
1.	Intercepts	−1/2	1	1	1/2
2.	Reciprocals	−2	1	1	2
3.	Reduction	−2	1	1	2
4.	Miller Indices	$(\bar{2}112)$			



3. (a) For BCC

- **(2 points) The number of atoms per unit cell, *N***
  - For BCC crystals, $N_i = 1$, $N_f = 0$, and $N_c = 8$, therefore $N = N_i + \frac{N_f}{2} + \frac{N_c}{8} = 2$.
- **(2 points) The coordination number is 8.**
- **(2 points) APF for a body-centered cubic structure**
  - Close-packed directions: length = $4R = \sqrt{3}a$
  - APF = $\dfrac{\text{Volume of atoms in a unit cell}}{\text{Total unit cell volume}}$

$$= \frac{N \times (4/3)\pi R^3}{a^3} = \frac{2 \times (4/3)\pi(\sqrt{3}a/4)^3}{a^3} = \frac{\sqrt{3}\pi}{8}$$



- **(2 points) Theoretical Density for Metals, ρ**

$$\text{Density} = \frac{\text{Mass of atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{n\,A}{V_C\,N_A} = \frac{2\,A}{(4R/\sqrt{3})^3\,N_A} = \frac{3\sqrt{3}\,A}{32R^3\,N_A}$$

where A = atomic weight

N_A = Avogadro's number = 6.022×10^{23} atoms/mol

3. (b) For FCC

- **(2 points) The number of atoms per unit cell, *N***
  - For BCC crystals, $N_i = 0$, $N_f = 6$, and $N_c = 8$, therefore $N = N_i + \frac{N_f}{2} + \frac{N_c}{8} = 4$.
- **(2 points) The coordination number is 12.**
- **(2 points) APF for a face-centered cubic structure**
  - Close-packed directions: length = $4R = \sqrt{2}a$
  - APF = $\dfrac{\text{Volume of atoms in a unit cell}}{\text{Total unit cell volume}}$

$$= \frac{N \times (4/3)\pi R^3}{a^3} = \frac{4 \times (4/3)\pi(\sqrt{2}a/4)^3}{a^3} = \frac{\sqrt{2}\pi}{6}$$

- **(2 points) Theoretical Density for Metals, ρ**

$$\text{Density} = \frac{\text{Mass of atoms in unit cell}}{\text{Total volume of unit cell}} = \frac{n\,A}{V_C\,N_A} = \frac{4\,A}{(4R/\sqrt{3})^3\,N_A} = \frac{3\sqrt{3}\,A}{16R^3\,N_A}$$

where A = atomic weight

N_A = Avogadro's number = 6.022×10^{23} atoms/mol

4. (a) Thermoplastic and Thermosetting Polymers

- **Polymers may be classified as follows, according to the mechanical response at elevated temperatures:**
  - Thermoplastics
  - Thermosets

a) (6 points) Thermoplastics:

- Thermoplastic polymers soften when heated and harden when cooled. Simultaneous application of heat and pressure is required to fabricate these materials.
- On the molecular level, when the temperature is raised, secondary bonding forces are diminished so that the relative movement of adjacent chains is facilitated when a stress is applied.
- Most linear polymers and those having branched structures with flexible chains are thermoplastics.
- Thermoplastics are very soft and ductile.
- The commercial available thermoplasts are
  - Polyvinyl Chloride (PVC) and Polystyrene
  - Polymethyl methacrylate
  - Polystyrene

4. (a) Thermoplastic and Thermosetting Polymers

b) (6 points) Thermosets

- Thermosetting polymers become soft during their first heating and become permanently hard when cooled. They do not soften during subsequent heating. Hence, they cannot be remolded/reshaped by subsequent heating.
- In thermosets, during the initial heating, covalent cross-links are formed between adjacent molecular chain. These bonds anchor the chains together to resist the vibration and rotational chain motions at high temperatures. Cross linking is usually extensive in that 10 to 15% of the chain mer units are cross linked. Only heating to excessive temperatures will cause severance of these crosslink bonds and polymer degradation. Thermoset polymers are harder, stronger, more brittle than thermoplastics and have better dimensional stability.
- They are more usable in processes requiring high temperatures
- Most of the cross linked and network polymers, including Vulcanized rubbers, Epoxies, Phenolic, and Polyester resins, are thermosetting polymers.
- Thermosets cannot be recycled, do not melt, are usable at higher temperatures than thermoplastics, and are more chemically inert

4. (b) Copolymers

- **Copolymers:** Consist of two or more constitutional repeating units (A-B)
- **Several classes of copolymer are possible**
  - **(2 points) Statistical copolymer (Random)**: Two or more different repeating unit are distributed randomly

    ABAABABBBAABAABB
  - **(2 points) Alternating copolymer** are made of alternating sequences of the different monomers

    ABABABABABABABAB
  - **(2 points) Block copolymer**: Long sequences of a monomer are followed by long sequences of another monomer

    AAAAAAAAAABBBBBBBBB
  - **(2 points) Graft copolymer** consist of a chain made from one type of monomers with branches of another type

    AAAAAAAAAAAAAAAAAA

    B B B

    B B B

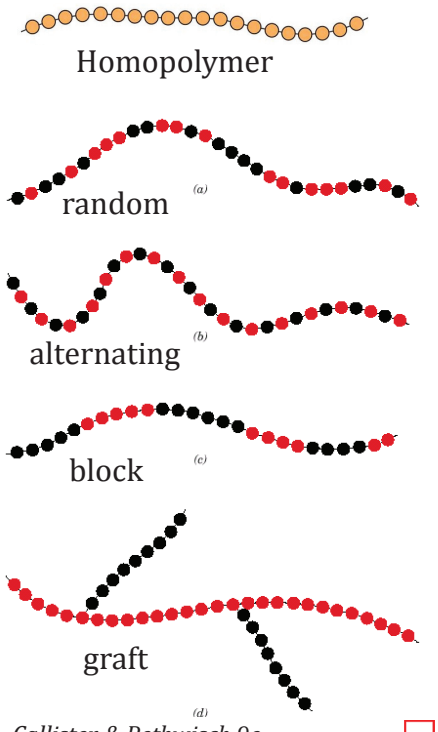


Fig. 5.9, *Callister & Rethwisch 9e.*

5. Close-Packed Crystal Structures

- **(2 points) FCC & HCP crystal structures**
  - The most efficient way of packing together equal-sized spheres and stacking close-packed atomic planes in three dimensions.
  - Coordination Number = 12, APF = 0.74
- **(3 points) FCC Stacking Sequence**
  - Close-Packed Plane: (111) plane
  - ABCABC Stacking Sequence
- **(3 points) HCP Stacking Sequence**
  - Close-Packed Plane: (0001) plane
  - ABAB Stacking Sequence

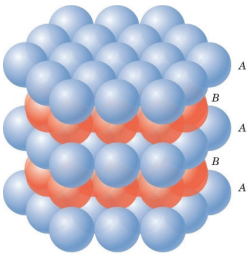
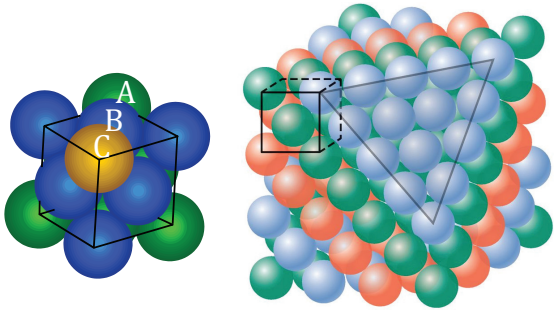
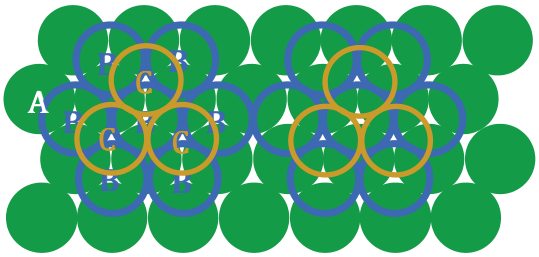


Fig. 4.24 Close-packed plane stacking sequence for the HCP structure.

- **(2 points)** Figures





A sites B sites C sites

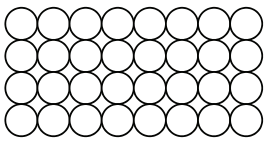
6. Equilibrium Number of Vacancies

- **Equilibrium number of vacancies**

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$ **(6 points)**

- N_v: Number of defects
- Q_v: Activation energy
- N: Number of potential defect sites
- T: Absolute temperature
- k: Boltzmann's constant (1.38 ×10-23 J/atom-K)

Each lattice site is a potential vacancy site. **(2 points)**



$$N = \frac{N_A \rho_{Fe}}{A_{Fe}} \times 10^6$$

$$\therefore N_v = N\exp\left(\frac{-Q_v}{kT}\right) = \frac{N_A \rho_{Fe}}{A_{Fe}} \times 10^6 \times \exp\left(\frac{-Q_v}{1000k}\right)$$ **(6 points)**