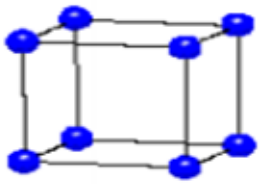
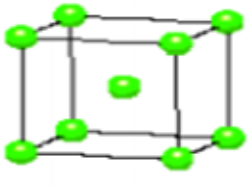
Tutorial Series No. 2

Exercise 1: Multiplicity

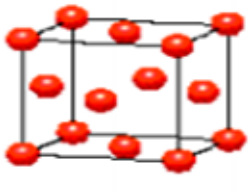
Find the number of atoms per unit cell (the multiplicity of the cell) for the three different crystalline structures: **simple cubic**, **centered cubic**, and **face-centered cubic**.



Simple cubic



Centered cubic



Face-centered cubic

Exercise 2: Density, Packing Factor, and Packing Rate of Pure Iron

When pure iron crystallizes, it adopts a **centered cubic (CC)** structure (a = b = c and α = β = γ = 90°) with **2 atoms per unit cell**.

Given data: M_{Fe}=55,85 g/mol ; a= 2,86x10^{-10}m ; r= 1,24A° ; N_A=6,023x10^{23}.

1. Calculate the density (ρ) of pure iron.
2. Calculate the packing factor (C) of pure iron.
3. Calculate the packing rate (τ).

Exercise 3: Density, Packing Factor, and Packing Rate of a Fe–Ni Alloy

The alloy contains **80% iron and 20% nickel by mass**, with a **centered cubic (CC)** crystal structure.

Both elements are uniformly distributed in the lattice.

Given data:

Fer	Nickel	N_A=6,023x10^{-23}
M_{Fe}= 55,85 g/mol r_{Fe}= 1,24A°	M_{Ni}= 58,69 g/mol R_{Ni}= 1,25A°	a= 2,86 A° z= 2

1. Calculate the density (ρ) of the Fe–Ni alloy.
2. Calculate the packing factor (C) for the Fe–Ni alloy.
3. Calculate the packing rate (τ) for the Fe–Ni alloy.

Exercise 4: Relationship Between the Lattice Edge Length (a) and Atomic Radius (r)

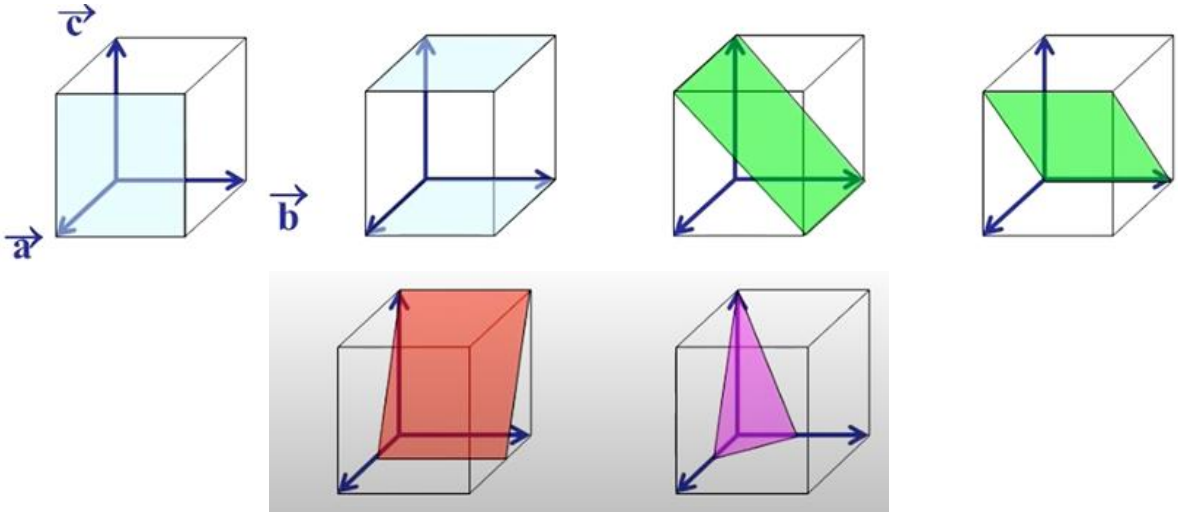
Consider a metallic crystal that can be modeled by one of the three cubic structures: **simple cubic (SC)**, **face-centered cubic (FCC)**, or **centered cubic (CC)**.

Given: r = 0.128 nm

1. Calculate the lattice edge length (a) for the three cubic structures.
2. Calculate the packing factor for each cubic structure.
3. Compare the packing factors of the three structures and draw a conclusion.

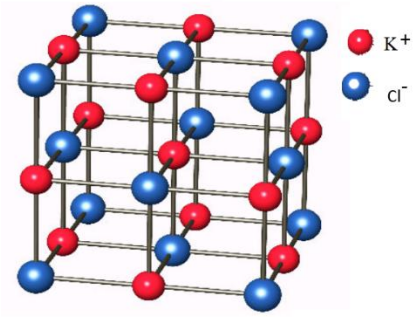
Exercise 5: Miller Indices

1. What are the indices of the crystallographic **direction** passing through the lattice node with coordinates: **(-4, 6, 2)**?
2. What are the **Miller indices** of the lattice plane that intersects the x, y, z axes at **4a**, **−6b**, and **2c**, respectively?
3. Sketch (represent) the lattice planes: **(111)**, **(110)**, **(321)** and **(131)**.
4. Determine the Miller indices of the following planes:



Exercise 6

Consider the crystal structure of potassium chloride (KCl).



Given: $r^+ = 0.130$ nm ; $r^- = 0.181$ nm ; V(KCl) = 0.144 nm^3.

1. What is the nature of the bonds between K and Cl atoms?
2. What Bravais lattice is formed by the Cl atoms?
3. What type of lattice sites do the K atoms occupy in this lattice?
4. Verify the electrical neutrality of the KCl crystal.
5. Calculate the coordination number of each ion.
6. What is the packing factor (compacity) of the KCl unit cell?
7. Calculate the theoretical density (mass per unit volume) of KCl in kg/m^3.