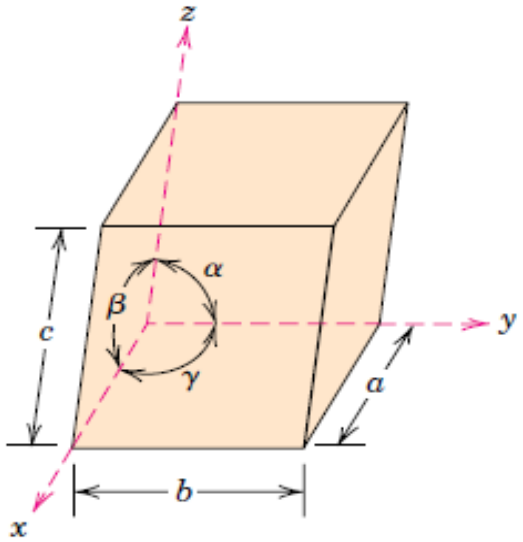
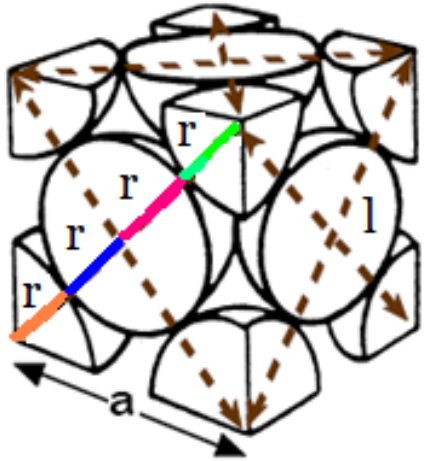
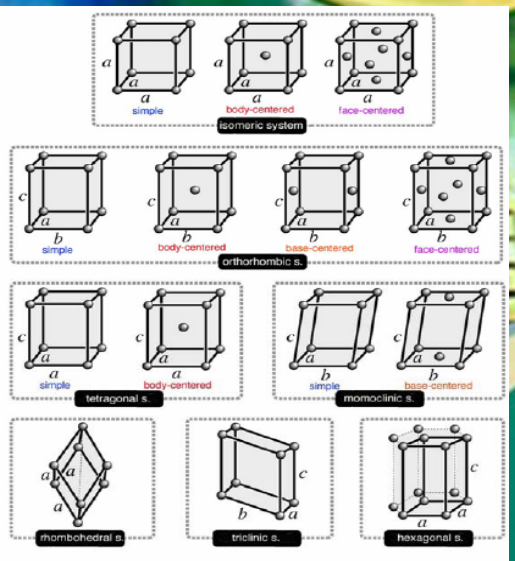
Struktur Kristal
(bagaian 2)







Oleh

Dr. H. Harun Nasrudin, M.S.

Samik, S.Si., M.Si.

Refresh materi sebelumnya.

Mari jawab pertanyaan sbb:

Untuk saat ini menjawab adalah emas (bukan diam) (:

1. Sebutkan hukum-hukum yang berkaitan dengan kristal?

2. Kenapa XRD bisa mengidentifikasi struktur kristal?

3. Apa perbedaan sel satuan (*unit cell*) dan kisi kristal (*crystal lattice*) ?

Struktur Kristal

Materi pertemuan ke 4

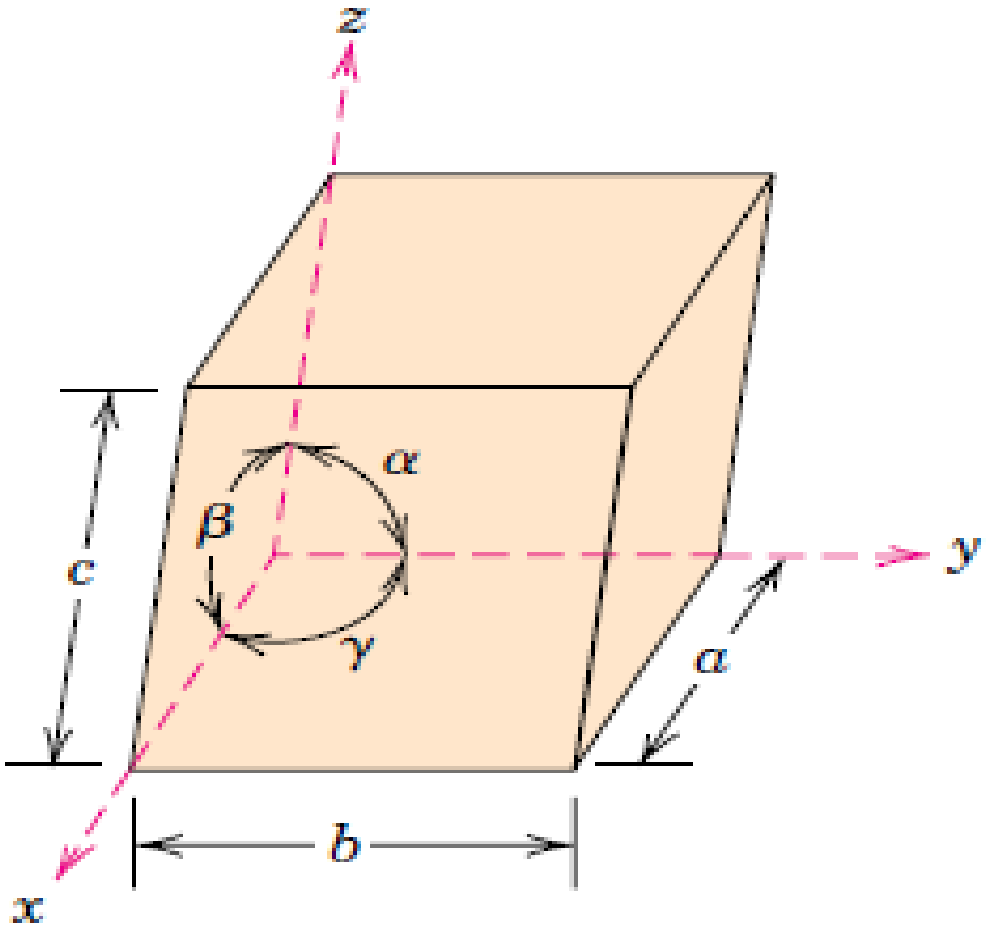
Mari jawab pertanyaan sbb:

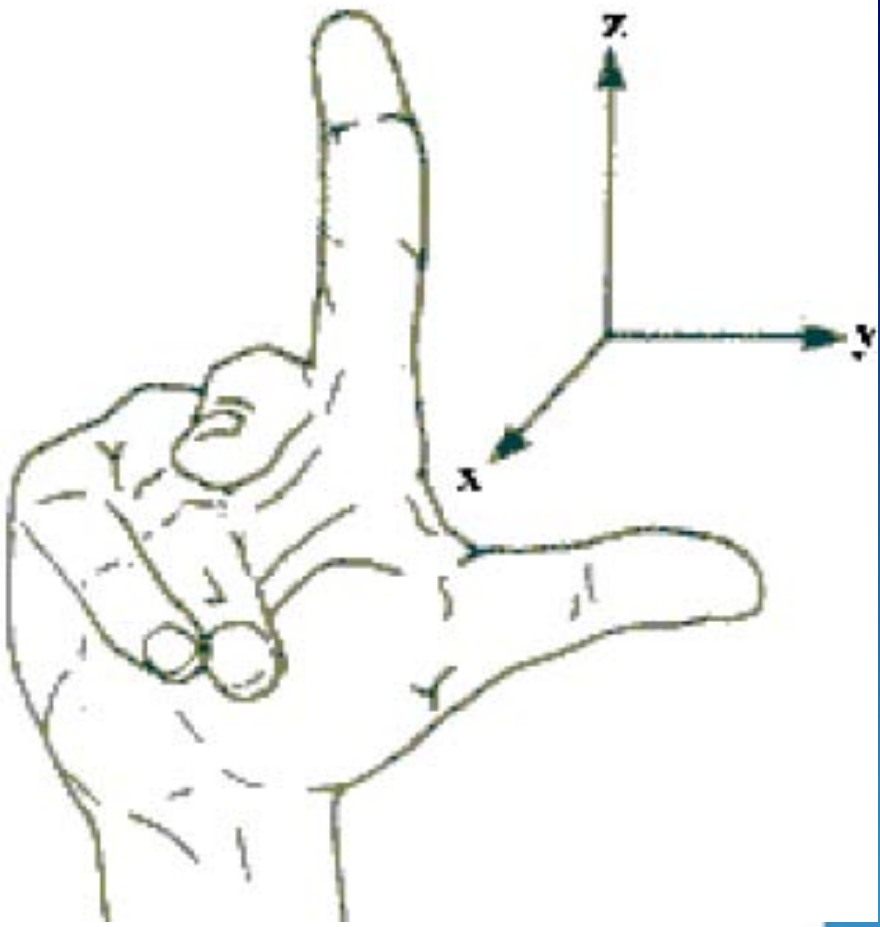
Untuk saat ini menjawab adalah emas (bukan diam) (:

1. Apa yang anda ketahui tentang kisi Bravais dan sistem kristal?

2. Apa perbedaan kubus sederhana, kubus berpusat badan, dan kubus berpusat muka?

3. Bagaimana cara menghitung jumlah atom per sel satuan, massa sel satuan dan kerapatan?

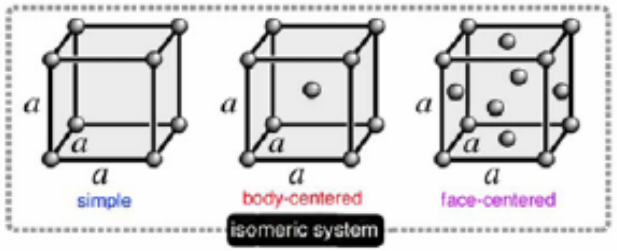


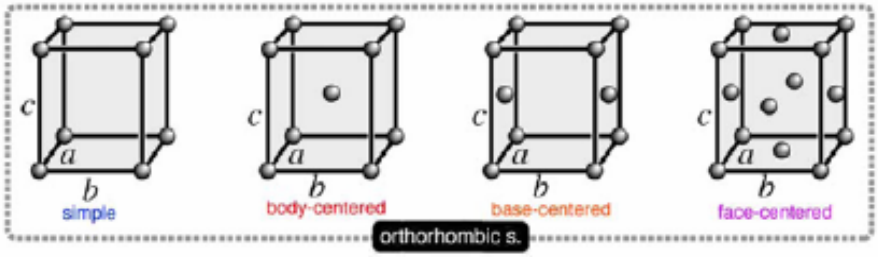


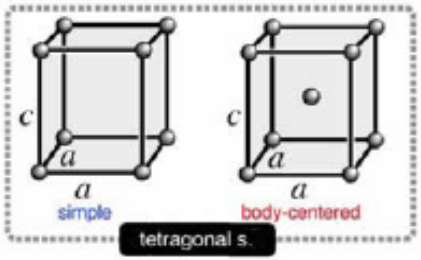
Sel satuan dapat dicirikan oleh parameter berikut:

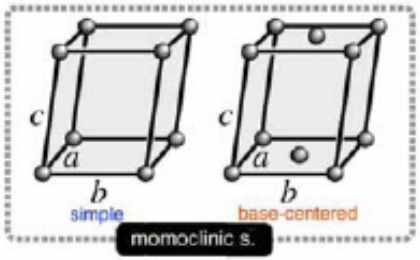
1. Panjang relatif tepi sepanjang tiga sumbu (*a*, *b*, *c*)

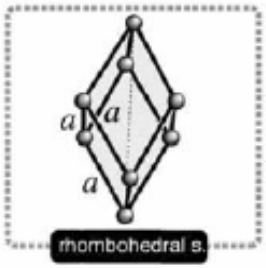
2. Tiga sudut antara tepi (α, β, γ).

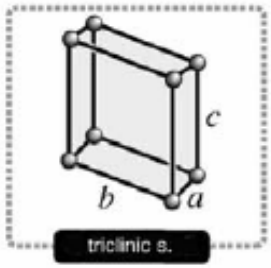


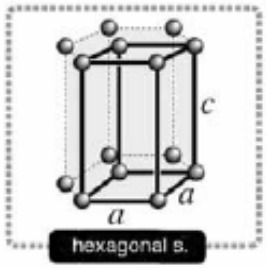


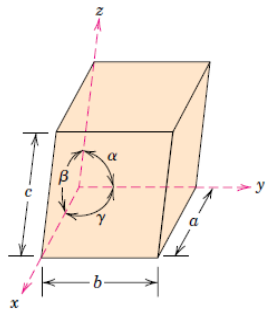












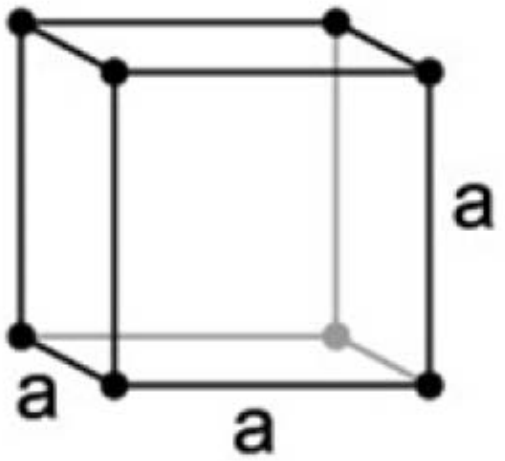
Tabel 2.1. Tujuh sel satuan Bravais

Sistem Kristal	Panjang Relatif Aksial	Sudut	Contoh
Kubus (isometrik)	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	Na^+Cl^-, Cs^+Cl^-, $Ca^{2+}(F^-)_2$, $Ca^{2+}O^{2-}$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	$(K^+)_2PtCl_6^{2-}$, $Pb^{2+}WO_4^{2-}$, $NH_4^+Br^-$
Ortorhombik	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	$(K^+)_2SO_4^{2-}$, $K^+NO_3^-$, $Ba^{2+}SO_4^{2-}$, $Ca^{2+}CO_3^{2-}$ (aragonit)
Rombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	$Ca^{2+}CO_3^{2-}$ (kalkit), $Na^+NO_3^-$
Heksagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$	AgI, SiC, HgS
Monoklinik	$a \neq b \neq c$	$\alpha = \beta = 90^\circ$, $\gamma \neq 90^\circ$	$Ca^{2+}SO_4^{2-}.\ 2H_2O$, $K^+ClO_3^-$, $(K^+)_4Fe(CN)_6^{4-}$
Triklinik	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	$Cu^{2+}SO_4^{2-}.5H_2O$, $(K^+)_2Cr_2O_7^{2-}$

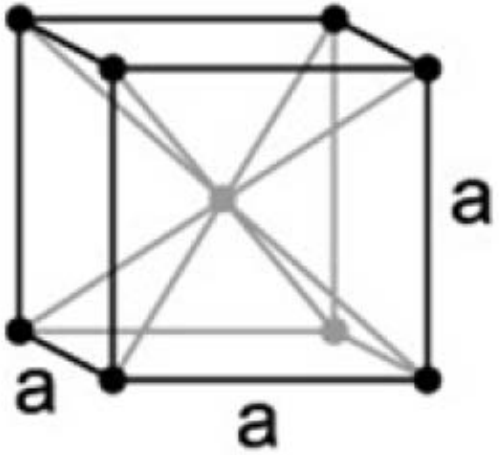
(Bahl, 2002).

Auguste Bravais, mengklasifikasikan kisi kristal berdasarkan simetrinya, dan menemukan bahwa terdapat 14 kisi kristal dan 7 sistem kristal.

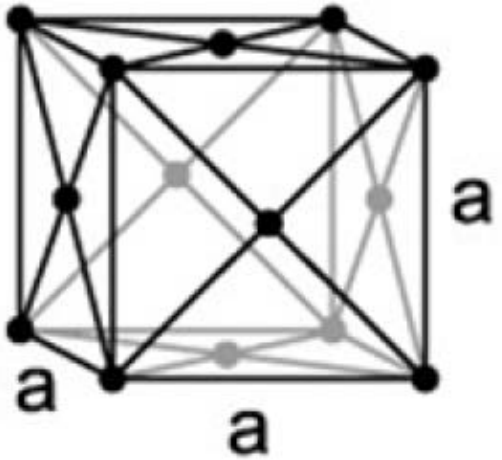
Ada tiga jenis sel satuan kubus yaitu:



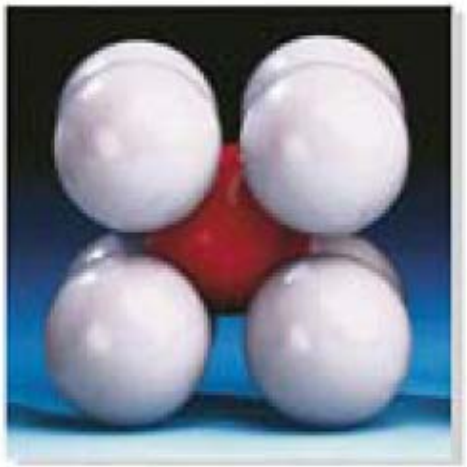
Kubus Sederhana

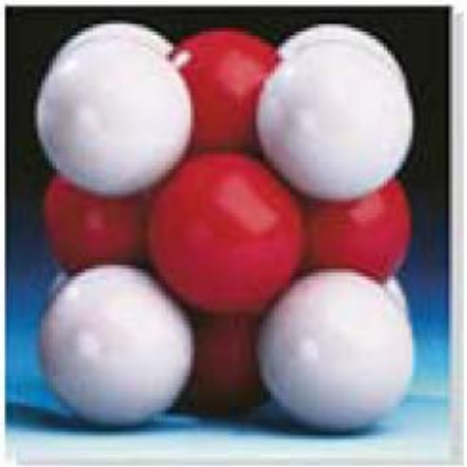


Kubus Berpusat Badan



Kubus Berpusat Muka





How to Compute Atoms or Points in a Unit Cell ?

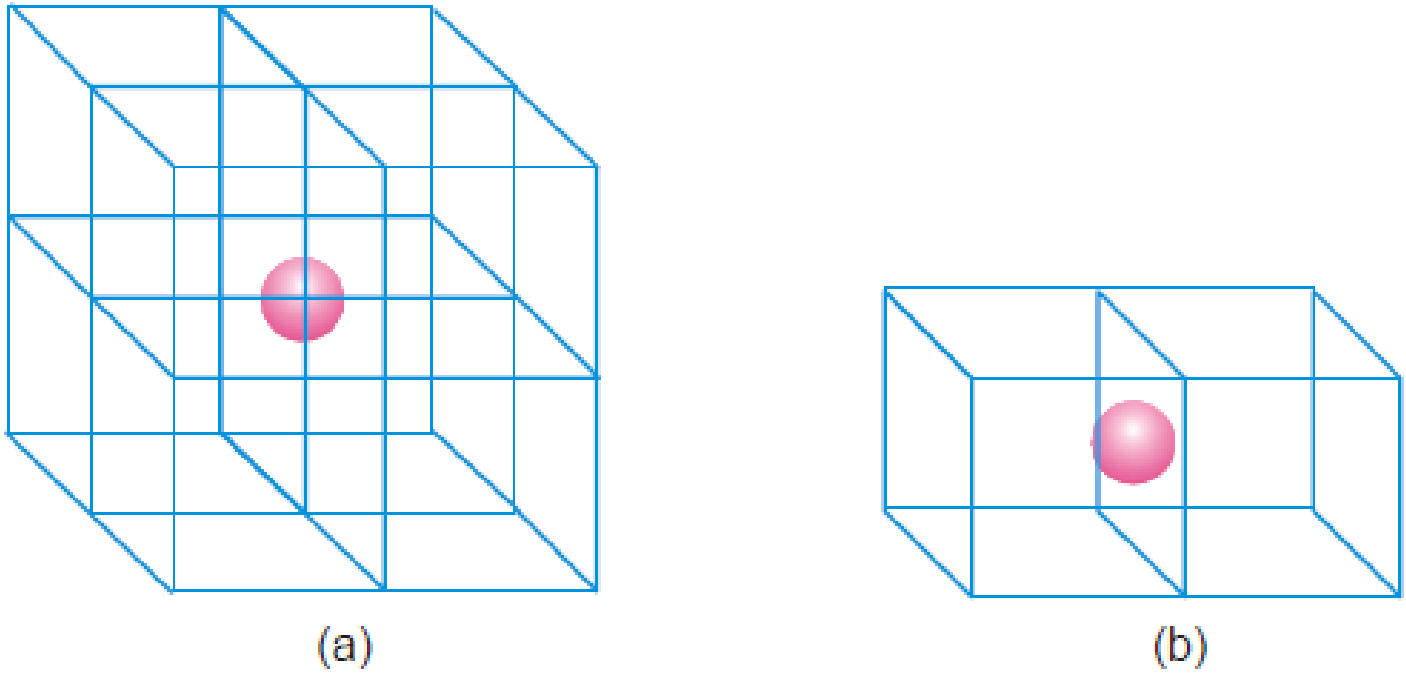
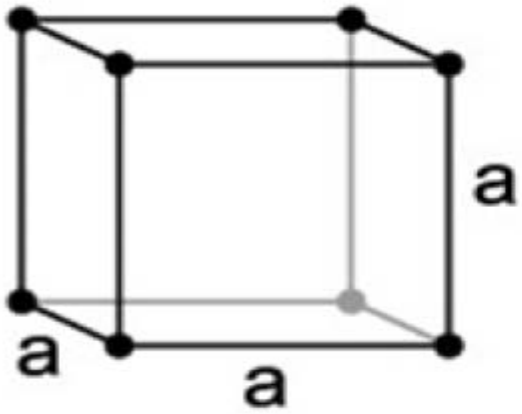


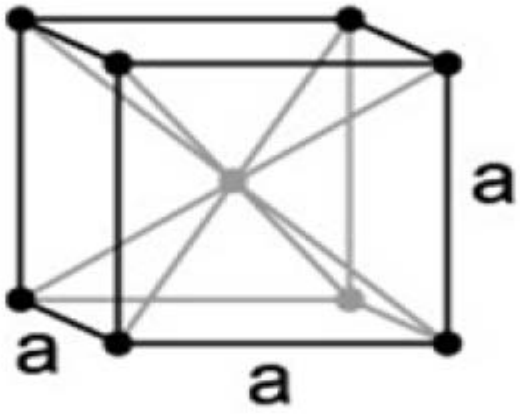
Figure 12.12

(*a*) In the simple cubic cell, each corner atom is shared by 8 cells; (*b*) In the face-centred cell, each atom in a face is shared by 2 cells.

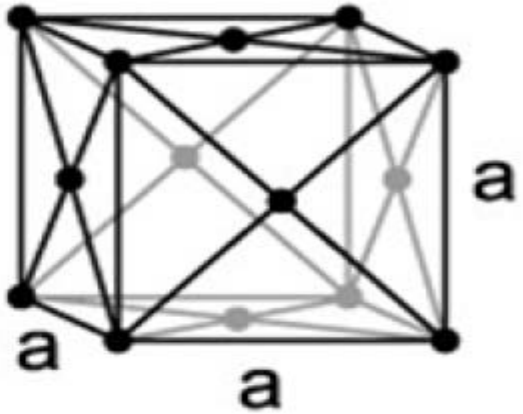
Compute Atoms or Points in a Unit Cell !



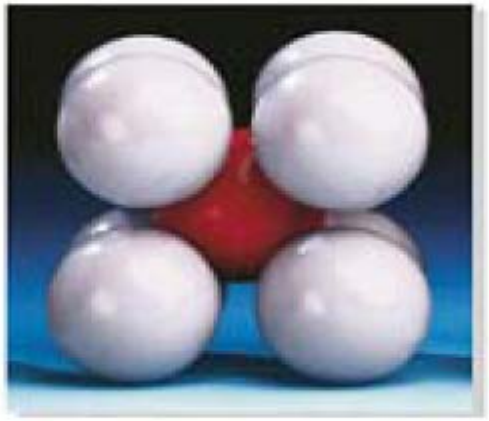
Kubus Sederhana

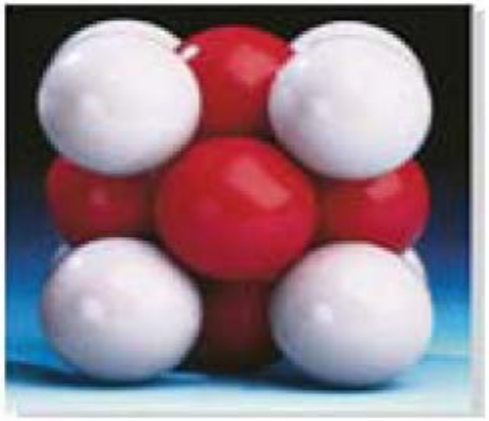


Kubus Berpusat Badan



Kubus Berpusat Muka





1/8 x 8 = 1 ; 1+1 = 2 ; (1/8 x 8) + (1/2 x 6) = 4

$$\text{Thus the mass of one atom} = \frac{\text{molar mass of the substance}}{\text{Avogadro's number}}$$

SOLVED PROBLEM 1. The unit cell of metallic gold is face-centred cubic.

(*a*) How many atoms occupy the gold unit cell ?

(*b*) What is the mass of a gold unit cell ?

SOLUTION

eight corners at 1/8 atom each = 1 atom

six faces at 1/2 atom each = 3 atoms

$\therefore$ 4 atoms occupy the gold unit cell.

$$\text{Mass of gold atom} = \frac{\text{molar mass}}{\text{Avogadro's number}}$$

$$\frac{197 \text{ g/mol}}{6.022 \times 10^{23} \text{ Au atoms/mol}} \times \frac{1}{4} = \mathbf{8.178 \times 10^{-23}\ g}$$

Mass of a gold unit cell = $\frac{197 \text{ g/mol}}{6.022 \times 10^{23} \text{ Au atoms/mol}}$ x 4 = 130.85 x 10^{-23} g

Characteristics of Crystal Structure

- **Coordination Number** (CN): number of nearest-neighbor or touching atoms

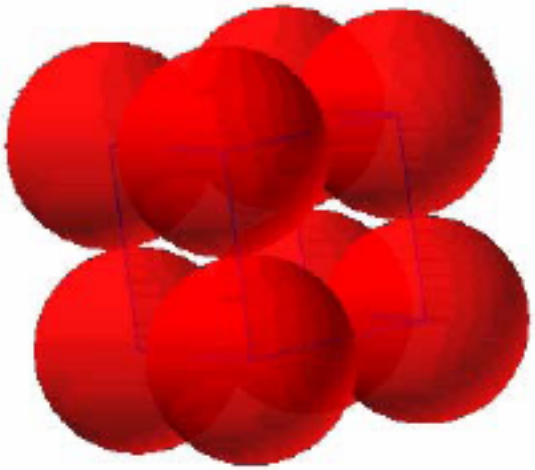
- **Atomic Packing Factor** (APF): fraction of solid atoms volume in a unit cell

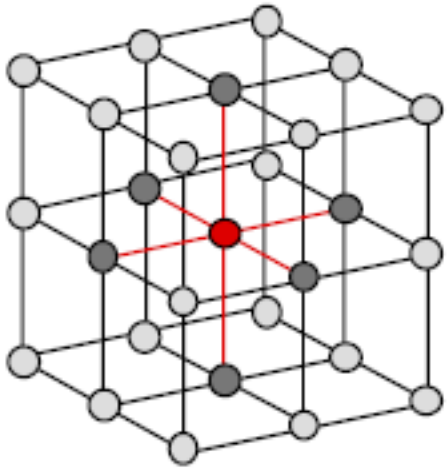
$$APF = \frac{\text{volume of atoms in a unit cell } *}{\text{total unit cell volume}}$$

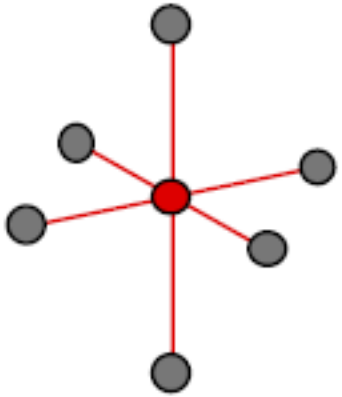
* assume hard sphere

Simple Cubic Structure (SC)

- Rare due to poor packing (only Po has this structure)
- Close-packed directions are cube edges.



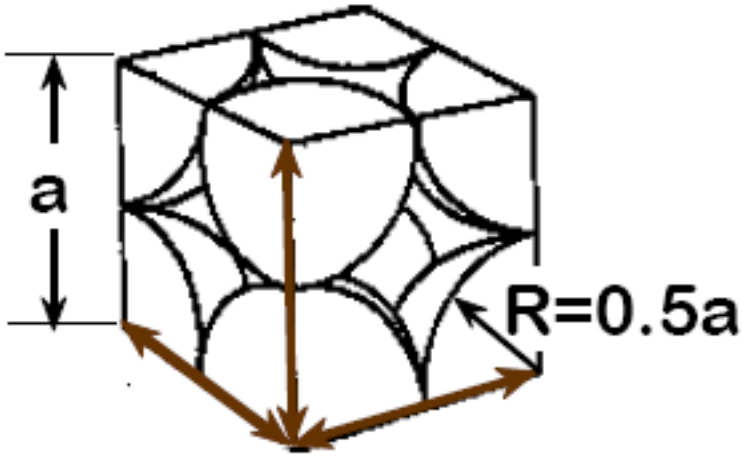




Coordination # = 6
(# nearest neighbors)

Atomic Packing Factor: SC

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

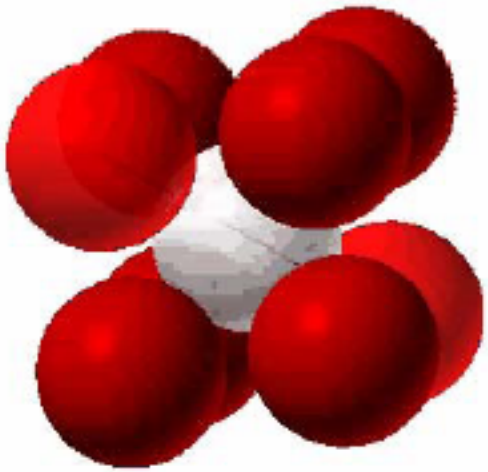
1 atom/unit cell

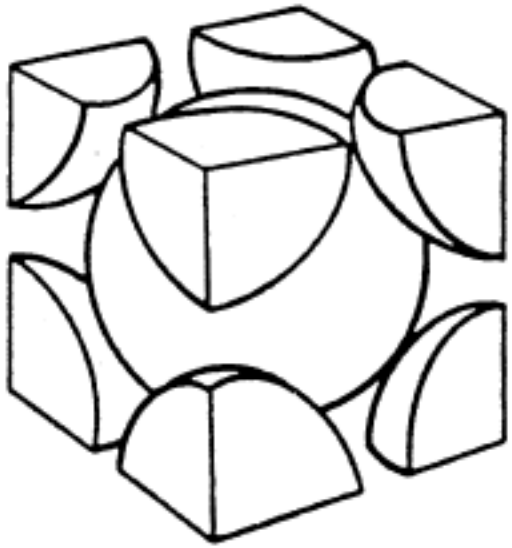
$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

Body Centered Cubic (BCC)

- Close packed directions are cube diagonals.

  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

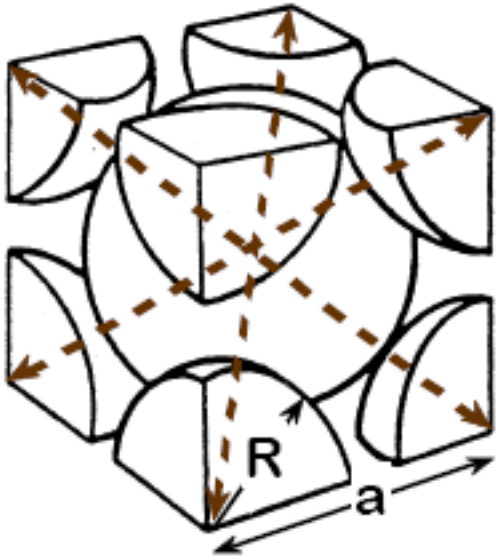




Coordination # = 8

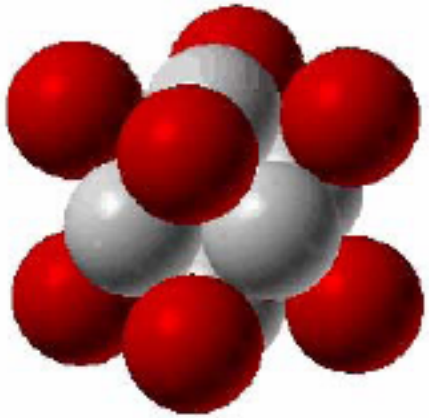
Atomic Packing Factor: BCC

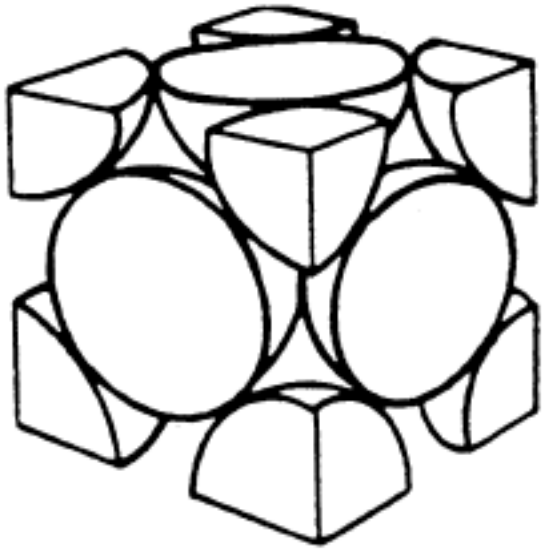
- APF for a body-centered cubic structure = 0.68



Face Centered Cubic (FCC)

- Close packed directions are face diagonals.
  --Note: All atoms are identical; the face-centered atoms are shaded differentlv onlv for ease of viewing.

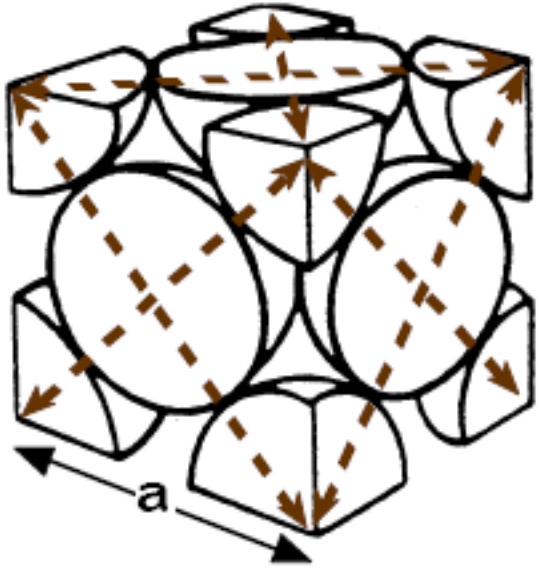




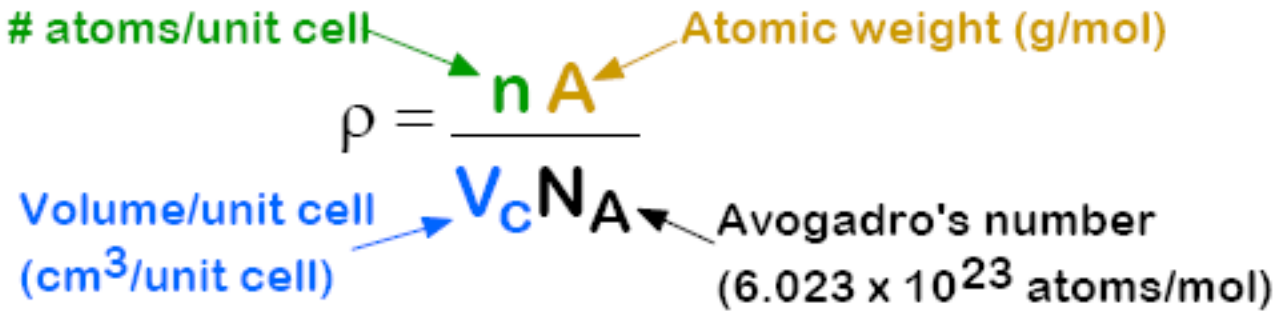
Coordination # = 12

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74



Theoretical Density, ρ



Example: Copper

crystal structure = FCC: 4 atoms/unit cell
atomic weight = 63.55 g/mol atomic radius R = 0.128 nm

$V_C = a^3$; for FCC, $a = 4R/\sqrt{2}$ $\Rightarrow$ **$V_C = 4.75 \times 10^{-23}$ cm^3**

Result: theoretical, $\rho_{Cu} = 8.89$ g/cm^3
compare to actual, $\rho_{Cu} = 8.94$ g/cm^3

Contoh soal:

Tembaga mengkristal dalam bentuk kubus berpusat muka dan mempunyai kerapatan 8,96 g/cm^3 (L= 6,023 x 10^{23} atom/mol; Ar. Cu = 63,5 gram/mol). Berdasarkan data tersebut, hitunglah:

a) Hitung jumlah atom Cu dalam setiap sel satuan,

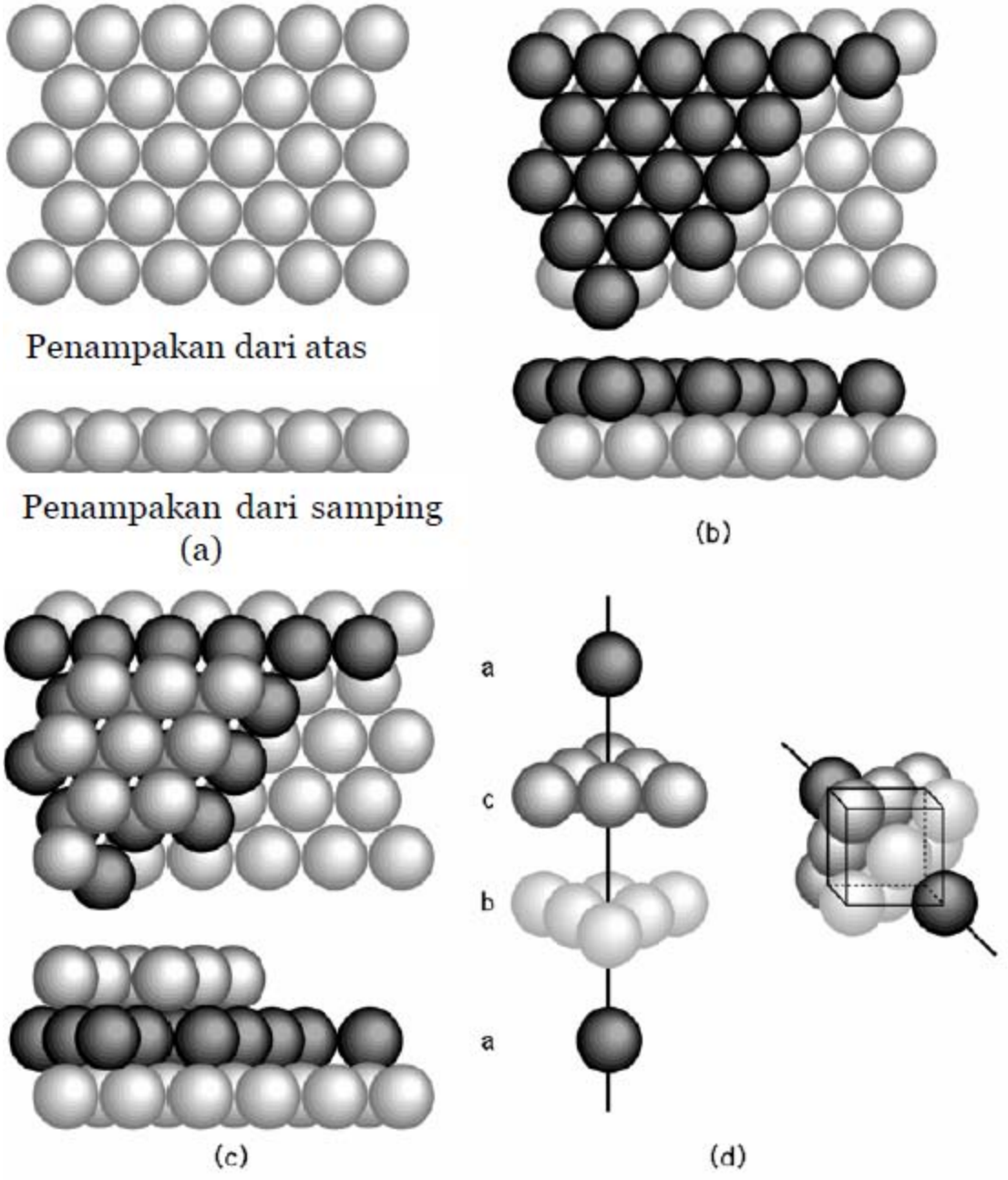
b) Massa sel satuan

c) Hitung panjang rusuk sel satuan (a),

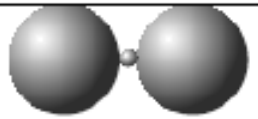
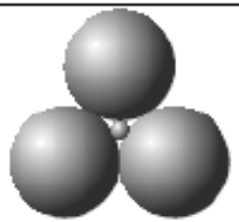
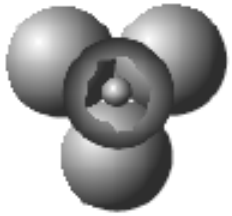
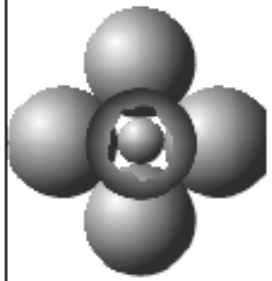
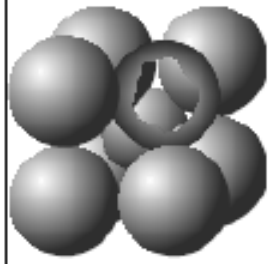
d) Hitung jari jari atom Cu. ?

Susunan terjejal

Gambar. Struktur terjejal
(a) Satu lapisan khas,
(b) Lapisan kedua,
(c) setiap bola di lapisa ketiga akan terletak persis di atas lapisan pertama (susunan aba),
(d) setiap bola di lapisan ketiga terletak di atas lubang lapisan pertama yang tidak digunaka oleh lapisan kedua (susunan abc)



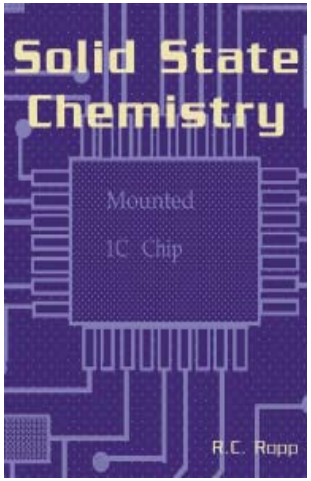
Tabel 2.2. Hubungan antara rasio radius dengan bilangan koordinasi (BK) dan kemungkinan geometri disekitar kation

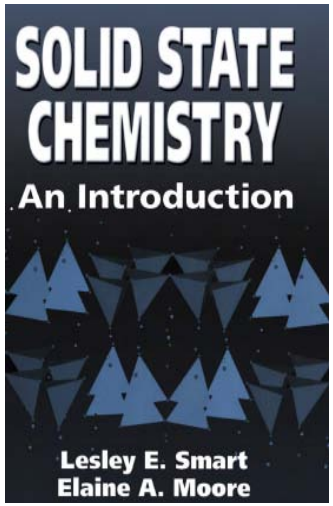
r_+/r_-	BK Kation	Geometri disekitar kation	Gambar
< 0,155	2	Linier	
0,155-0,225	3	Trigonal	
0,225-0,414	4	Tetrahedral	
0,414- 0,732	6	Oktahedral	
> 0,732	8	Kubus	

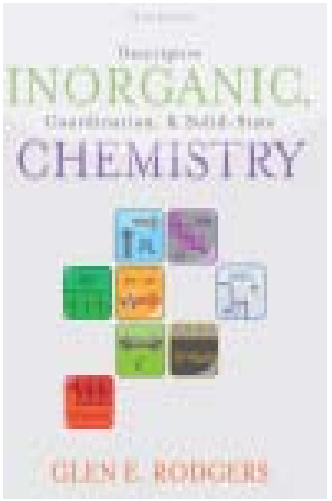
(Modifikasi dari berbagai literatur: Effendy, 2004; Mitchell, 2004; Rodgers, 2012)

Referensi

Buku ajar kimia zat padat,
buku referensi lainnya, dan artikel ilmiah







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October 12-13th, 2016, Bali, Indonesia

CHARACTERIZATION of MESOPOROUS NaZSM-5 and K_3PO_4/NaZSM-5 from ADSORPTION and DESORPTION ISOTHERMS

[1]Samik*, [2]Ratna Ediati, and [3]Didik Prasetyoko

TERIMAKASIH

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