



NOVA SCHOOL OF
SCIENCE & TECHNOLOGY

Ciência dos Materiais A

Departamento de Ciência dos Materiais

Margarida Lima (mmal@fct.unl.pt), Rui Borges (rcb@fct.unl.pt);

Carmo Lança (mcl@fct.unl.pt)

Departamento de Química

Ana Rita Duarte (ard08968@unl.pt)

FACULDADE DE CIÊNCIAS E TECNOLOGIA

UNIVERSIDADE NOVA DE LISBOA

Ano letivo de 2023-2024

Funcionamento da UC

- Aulas: exposição teórica, problemas e laboratoriais;
- Módulo 1 (DCM): TP1-Margarida Lima e Rui Borges; TP2-Carmo Lança
- Módulo 2 (DQ): Ana Rita Duarte; **23 de Outubro**
- Avaliação do Módulo 1: 1 teste e 1 ficha no moodle;
- Testes:
 - T1 (teste do Módulo 1 (**TP**)) - 4 de Novembro
 - Ficha (19h-19.30 Moodle) (**Lab.**) - 10 de Novembro
 - T2 (teste do Módulo 2 (**TP**)) - 12 de Dezembro
- Nota final: 50% Módulo 1 + 50% Módulo 2
- Nota do Módulo 1- 40% T1+ 10% ficha

Método de avaliação da UC – Módulo 1 (DCM)

- A avaliação contínua consiste em:
 - 1 teste escrito teórico e prático que corresponde a 40% da Nota final, e
 - 1 ficha de avaliação/relatório da componente laboratorial que corresponde a 10% da nota final.
 - Nota do Módulo 1- 40% T1+ 10% ficha
- A nota final resultante do teste e das ficha de avaliação laboratorial deverá ser igual ou superior a 10 valores. Frequência obrigatória pela presença nas aulas de laboratório.

Método de avaliação da UC

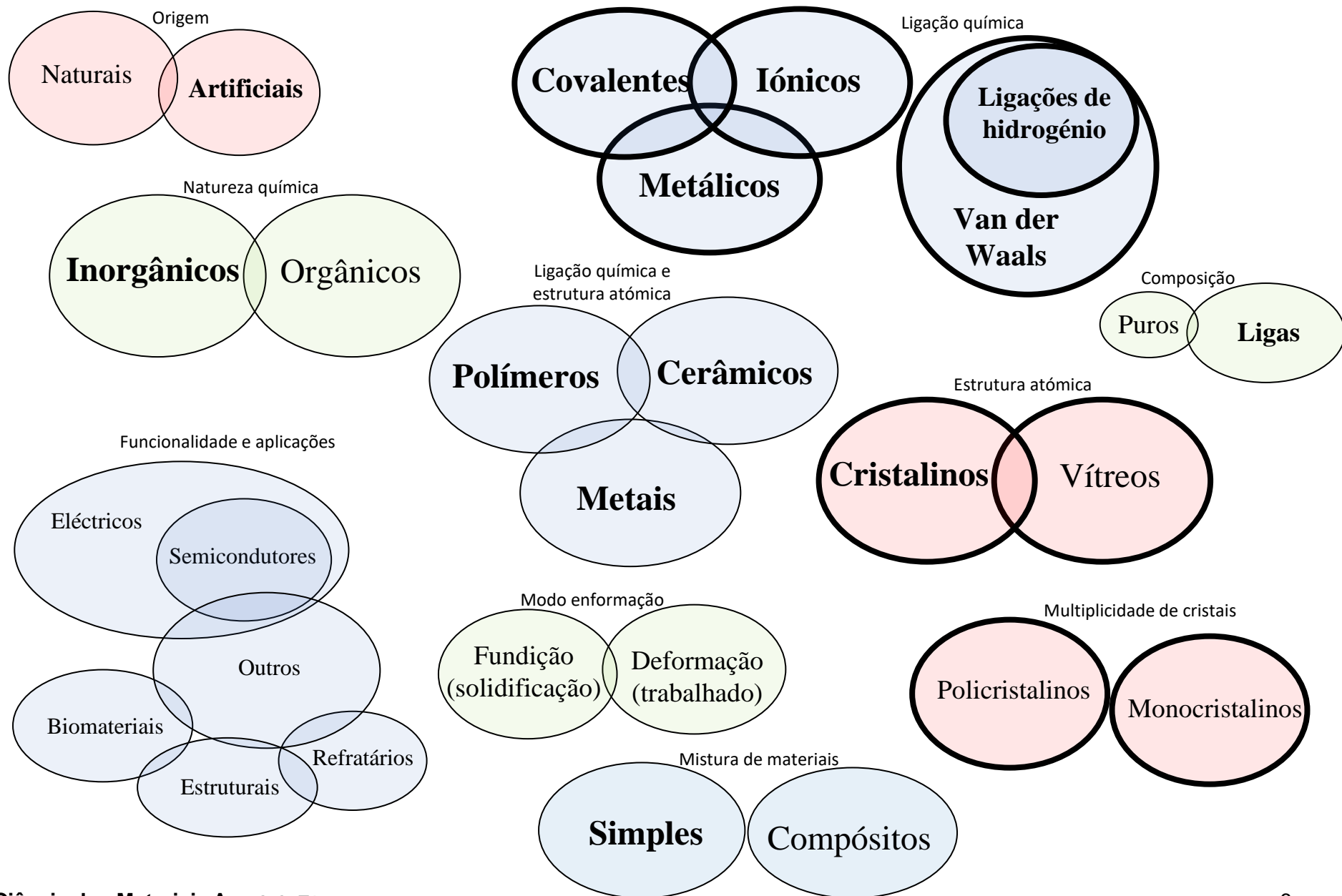
- Os alunos que pretendam fazer a disciplina unicamente por Exame (80% da Nota final) têm que frequentar obrigatoriamente as aulas de laboratório (20% da nota final).

Bibliografia (Módulo 1)

- Principles of Materials Science and Engineering, de W. F. Smith, McGraw-Hill, 3rd edition, New York, 1996; translated to Portuguese (“Princípios de Ciência e Engenharia dos Materiais”) published by McGrawHill de Portugal, Lisboa, 1998
- Fundamentals of Materials Science and Engineering. An Integrated approach, William Callister Jr, David G. Rethwisch, Wiley, 5th Edition, 2015
- Introduction to Materials Science for Engineers, James F. Shackelford, Pearson, 8th Edition, 2015

Conteúdo programático TP1

- Compreender a importância da relação "estrutura-propriedades" na seleção de materiais para diferentes aplicações,
- Identificar os principais tipos de sistemas cristalográficos, assim como as células unitárias das estruturas: cúbica simples, cúbica de corpo centrado, cúbica de faces centradas e hexagonal,
- Descrever a forma de empacotamento dos planos compactos das estruturas cristalinas do sistema cúbico de faces centradas e hexagonal,
- Relacionar a estrutura cristalina com o cálculo da densidade teórica.



Estrutura (Arranjo interno, subatômico, atômico, micro e macroscópico dos componentes)

Propriedades

(Resposta do material a um estímulo exterior independente da forma e da dimensão – características mecânicas, elétricas, térmicas, magnéticas, ópticas)

Materiais

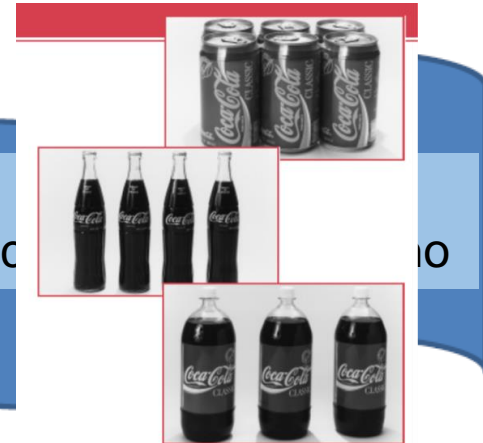
(Métodos de preparação dos materiais - dependem da estrutura pretendida e por isso das propriedades desejadas)

Processos de Transformação

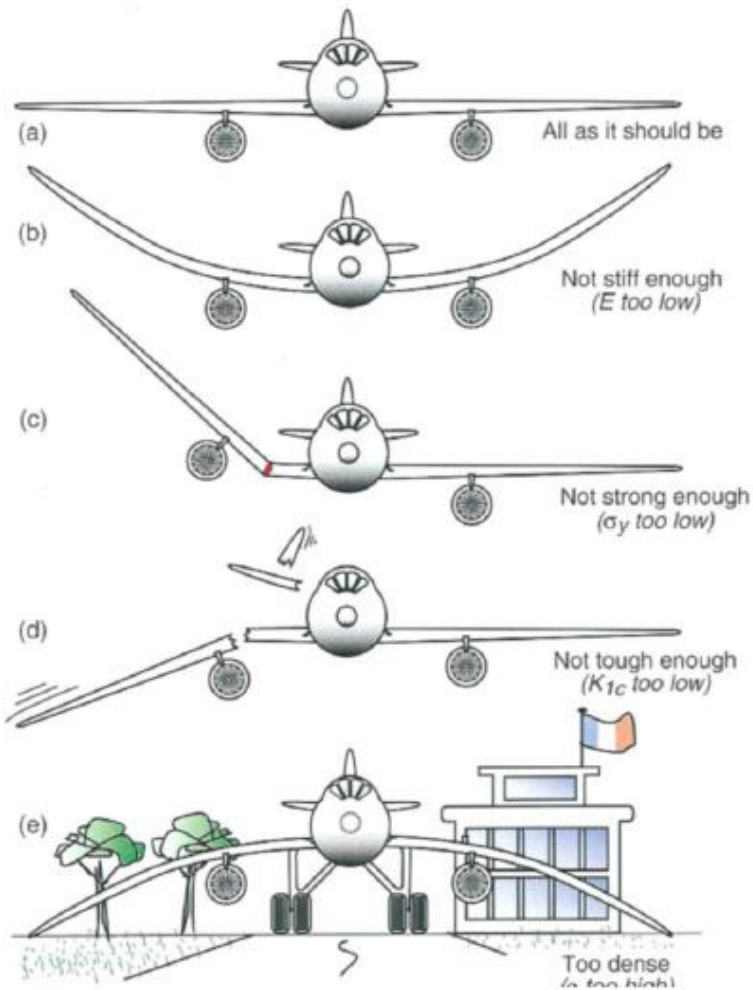
Engenharia

Aplicação

Desempenho/comportamento do material em determinadas aplicações



Exemplos ilustrativos (propriedades mecânicas) !



Solução adequada

Falta de rigidez

Falta de resistência

Falta de tenacidade

Peso excessivo

Dependendo do tipo **ligação química** predominante

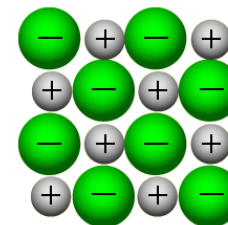
Covalentes

Iónicos

Metálicos

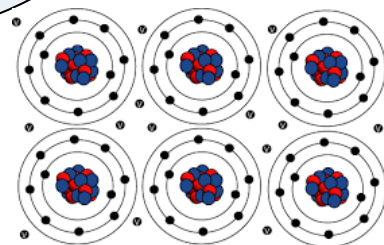


Electrões de valência partilhados nas ligações químicas: ligações direccionais



Ionização com electrões de valência transferidos para o elemento mais electronegativo. Ligações electrostáticas (ânion-catião)

Electrões de valência deslocalizados (partilha colectiva de electrões: nuvem electrónica): ligações pouco direccionais



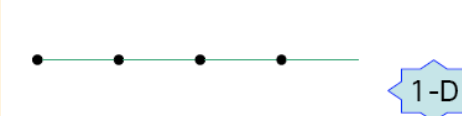
Tipo	Descrição	Ligação química	Propriedades	Aplicações
Metais	Maioritariamente compostos de um elemento metálico (Fe, Al, Cu, Ti, Au, Ni,...)	Ligação metálica	Cristalinos Densos, rígidos, resistentes (fractura e tracção), dúcteis Bons condutores eléctricos e térmicos	Materiais estruturais, condutores eléctricos e térmicos
Cerâmicos	Composto formado entre elementos metálicos e não-metálicos (maior parte óxidos, nitretos e carbonetos)	Ligação iónica (e covalente)	Cristalinos (cerâmico) ou amorfo (vidro) Rígidos, resistentes, frágeis e duros Quimicamente resistentes Isolantes térmicos (refractários) e eléctricos	Cerâmicos tradicionais: argilas (porcelanas), cimentos, vidros, tijolos, gesso Cerâmicos técnicos: vitrocerâmicos, instrumentos de corte, abrasivos, pyrex
Polímeros	Longas cadeias moleculares compostas de unidades que se repetem e tendo, a maior como base o elemento carbono (hidrocarbonetos)	Ligação covalente	Muito deformáveis (dúcteis); pouco resistentes à temperatura; quimicamente inertes, flexíveis e moldáveis	Indústria têxtil, automóvel, farmacêutica; construção civil; embalagens;

Estruturas cristalinas (Redes de Bravais)

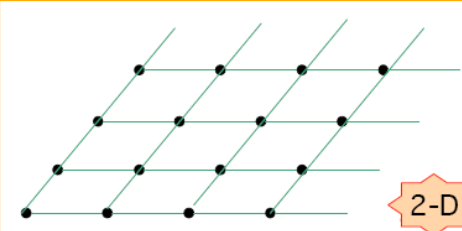
Os arranjos em sólidos cristalinos podem ser descritos por uma rede de linhas designada de rede espacial.

Crystal structure
Paolo Fornasini
Univ. Trento

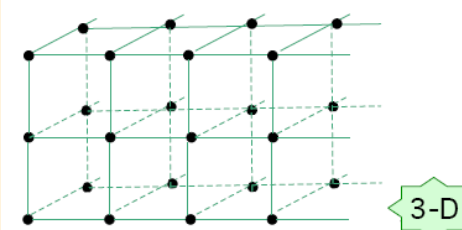
Bravais lattice



1-D




2-D




3-D

+

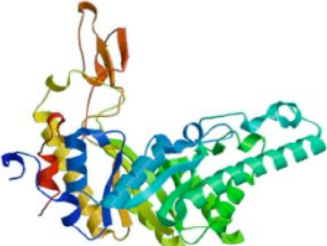
Basis



Atom



Molecule



Protein

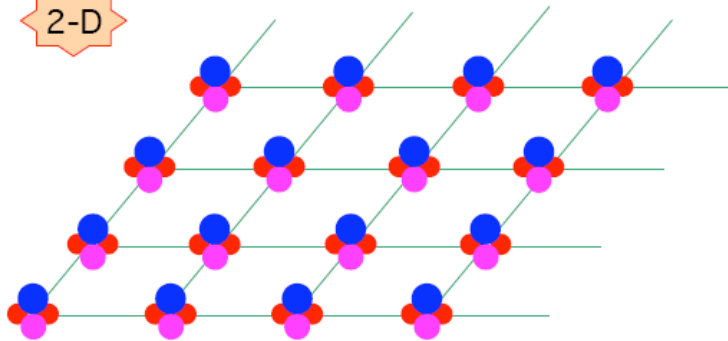
Bravais lattice + basis

Paolo
Fornasini
Univ. Trento

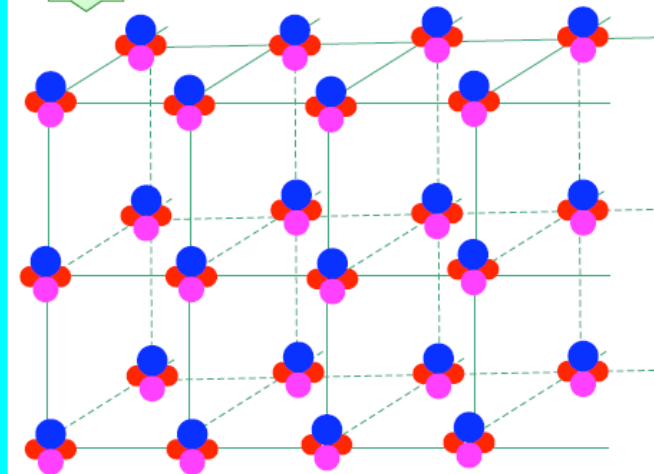


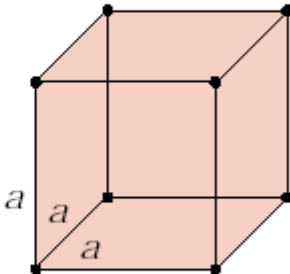
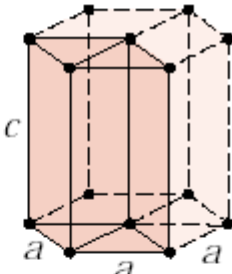
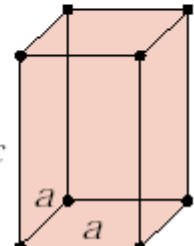
1-D

2-D



3-D

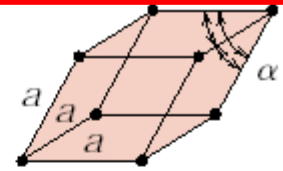


<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	

Rhombohedral

$$a = b = c$$

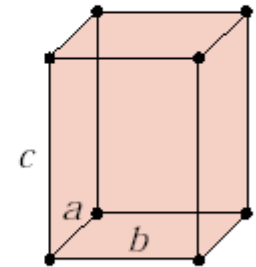
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

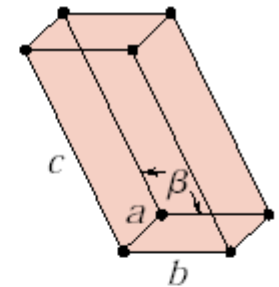
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

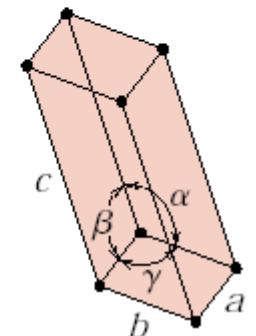
$$\alpha = \gamma = 90^\circ \neq \beta$$



Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



Estrutura Cúbica Simples (CS)

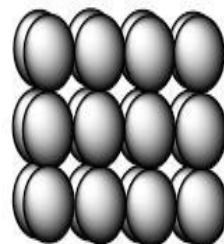
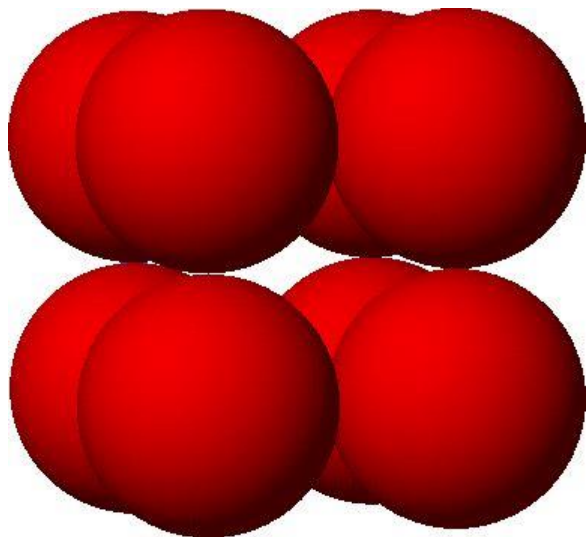


Figure 3a:
Square Array Layering

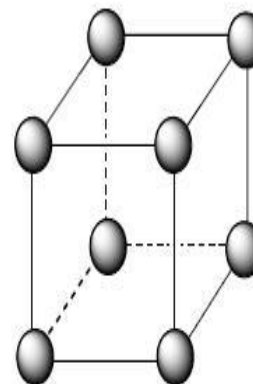


Figure 3b:
Simple Cubic

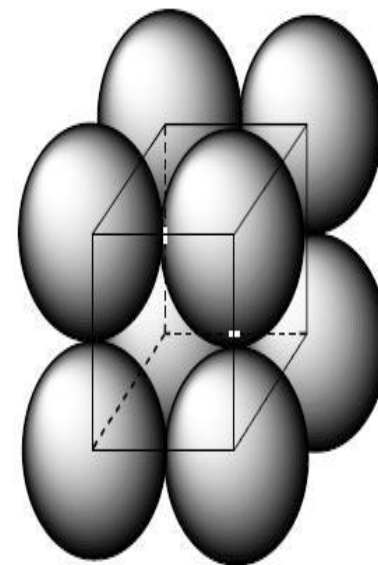
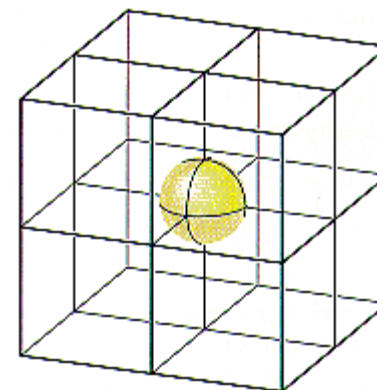
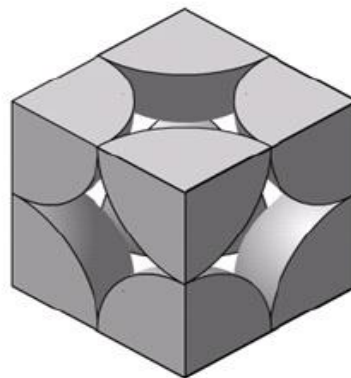
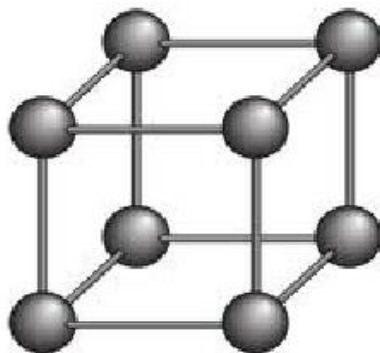


Figure 3c:
Space Filling Simple Cubic

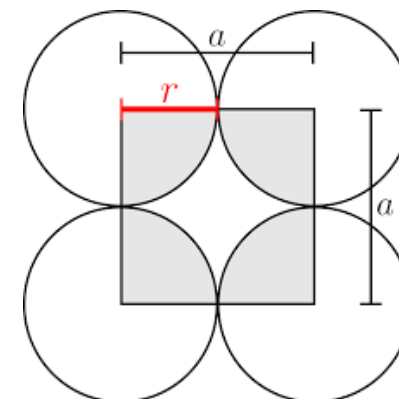
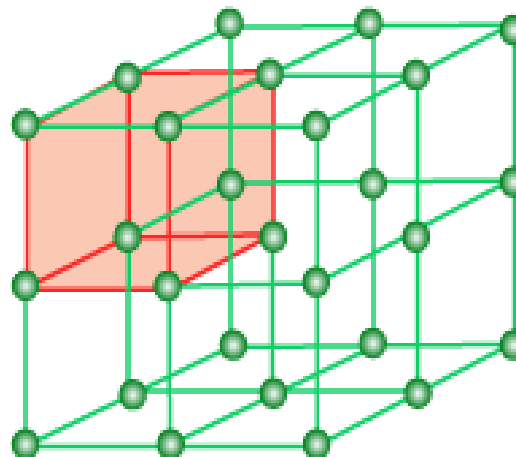
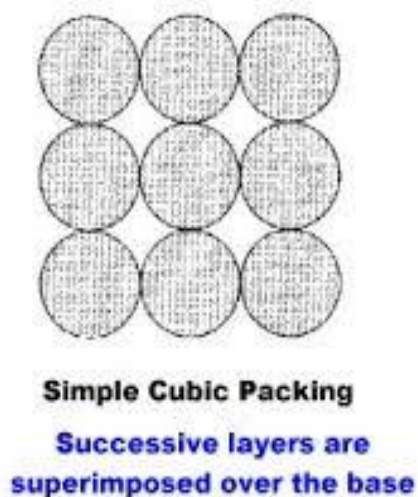
empilhamento AAA (empilhamento de planos não compactos)

Número de átomos por célula unitária

- Simple cubic (SC) structures: In these structures there are 8 atoms corresponding to 8 corners and there are no atoms on the faces or in the interior of the unit cell. Therefore, $N_c = 8$, $N_f = 0$ and $N_i = 0$
Using above eqn. we get, $N_{av} = 8/8 + 0/2 + 0/1 = 1$



Parâmetro de rede vs raio atômico - CS

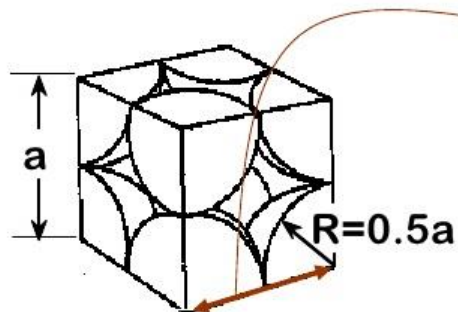


$$a=2r$$

Factor de empacotamento atómico- CS (52%)

$$\text{APF} = \frac{\text{Volume of atoms* in unit cell}}{\text{Volume of unit cell}}$$

*assume hard spheres



There are 8 of 1/8 atoms.

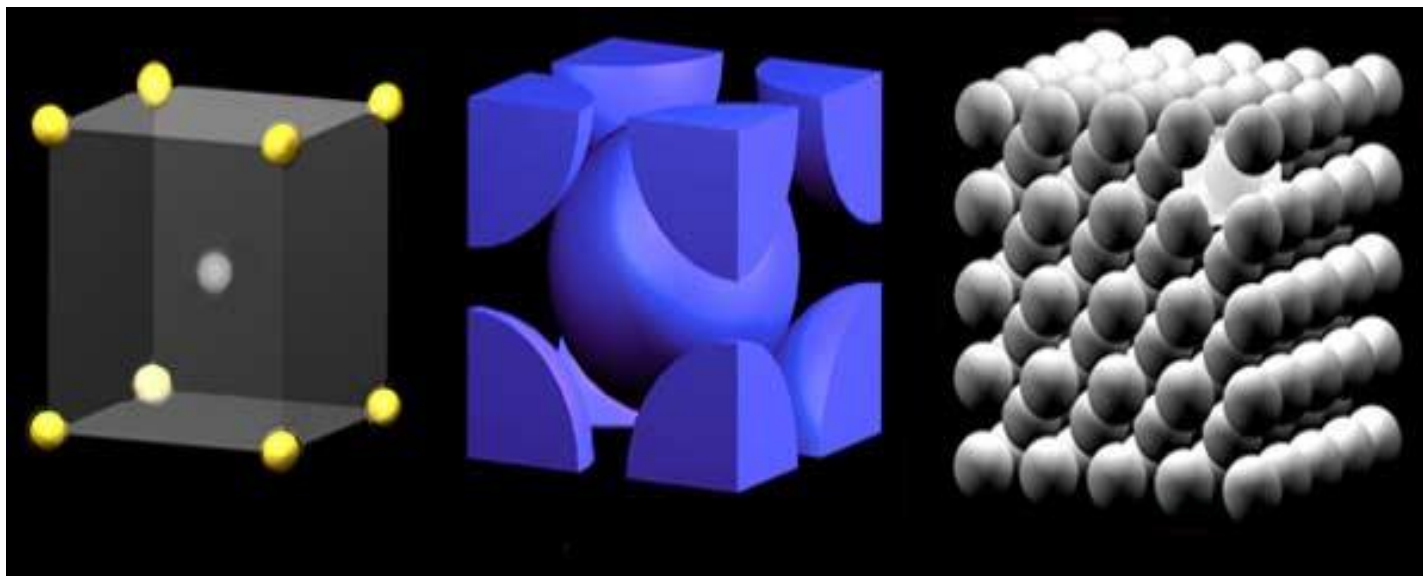
1 atom/unit cell

Close-packed direction:

$$a = 2R$$

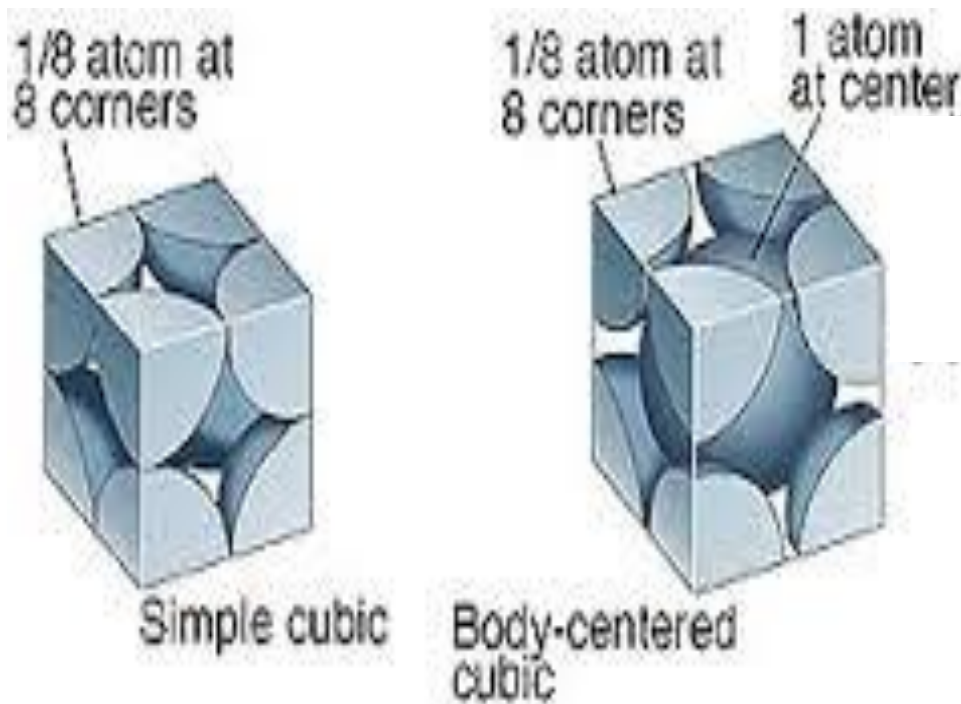
$$\text{APF} = \frac{\text{atoms/unit cell} \times \text{volume/atom}}{\text{volume/unit cell}} = \frac{1 \times \frac{4}{3} \pi (0.5a)^3}{a^3} = 0.52$$

Estrutura Cúbica de Corpo Centrado (CCC)

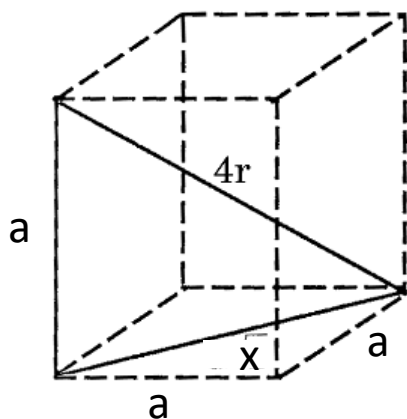


empilhamento ABA (empilhamento de planos não compactos)

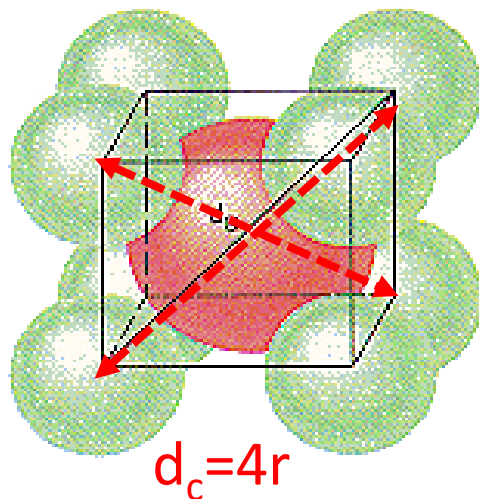
Número de átomos por célula unitária



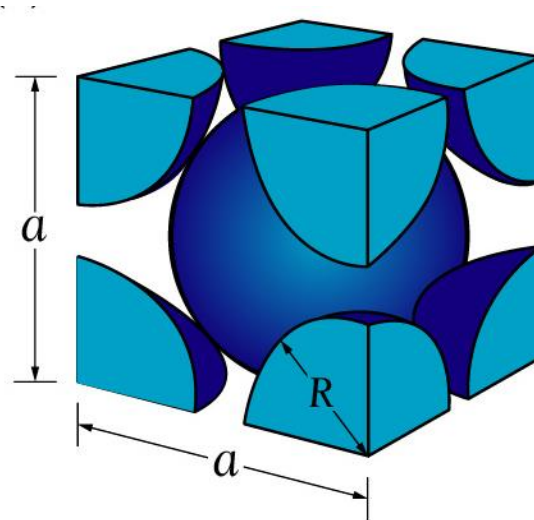
Parâmetro de rede vs raio atômico - CCC



$$\begin{aligned}a^2 + a^2 &= x^2 \\2a^2 &= x^2 \\x &= \sqrt{2}a\end{aligned}$$

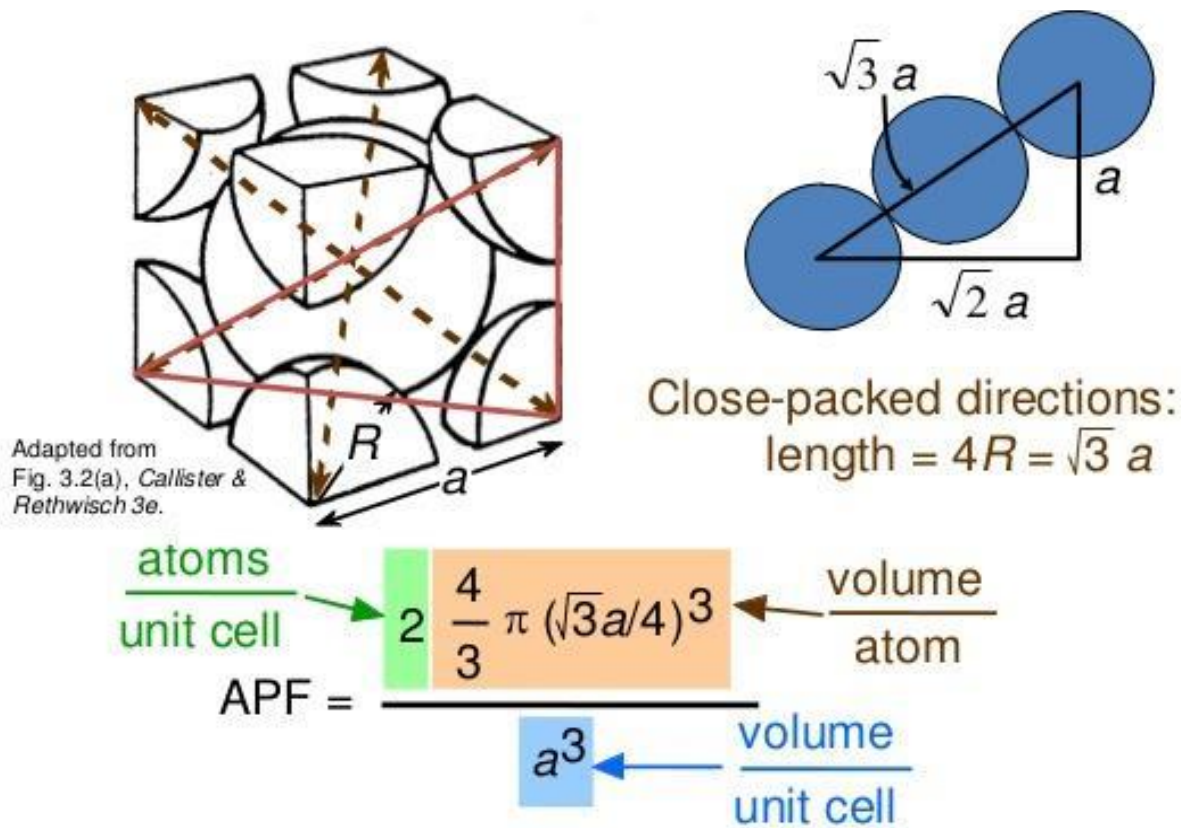


$$\begin{aligned}a^2 + (\sqrt{2}a)^2 &= (4r)^2 \\3a^2 &= 16r^2 \\a^2 &= \frac{16}{3}r^2\end{aligned}$$



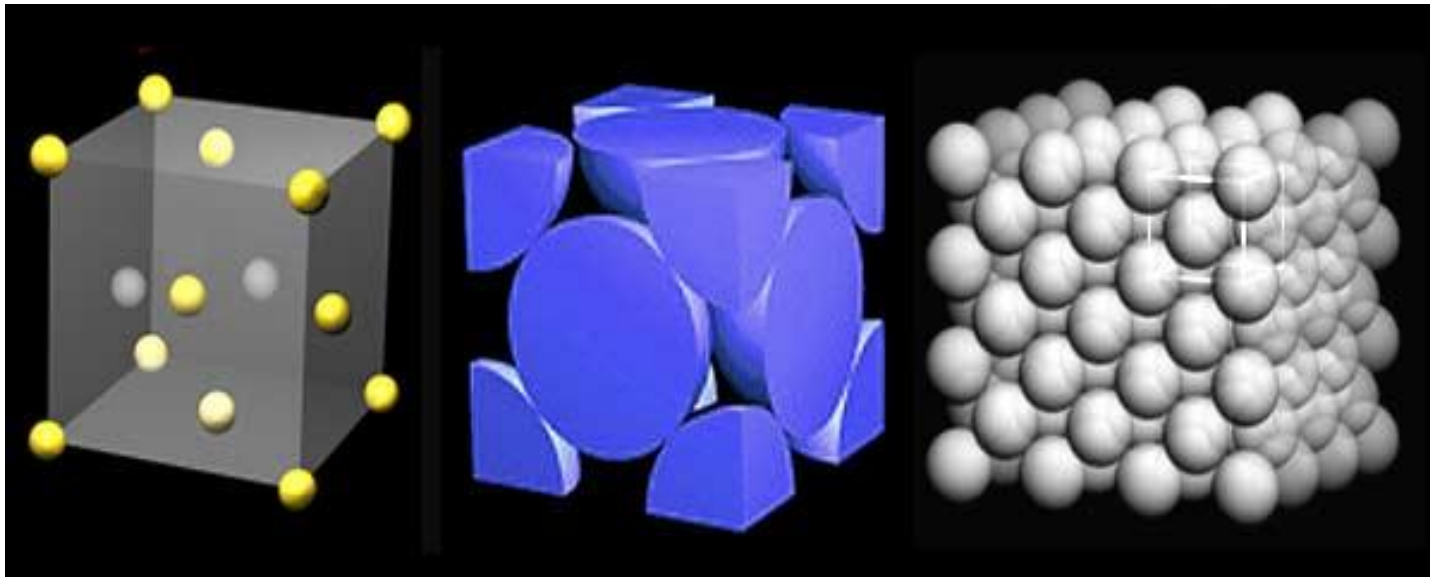
$a = \frac{4}{\sqrt{3}}r$	ou	$a = \frac{4\sqrt{3}}{3}r$
---------------------------	----	----------------------------

Factor de empacotamento atómico- CCC (68%)



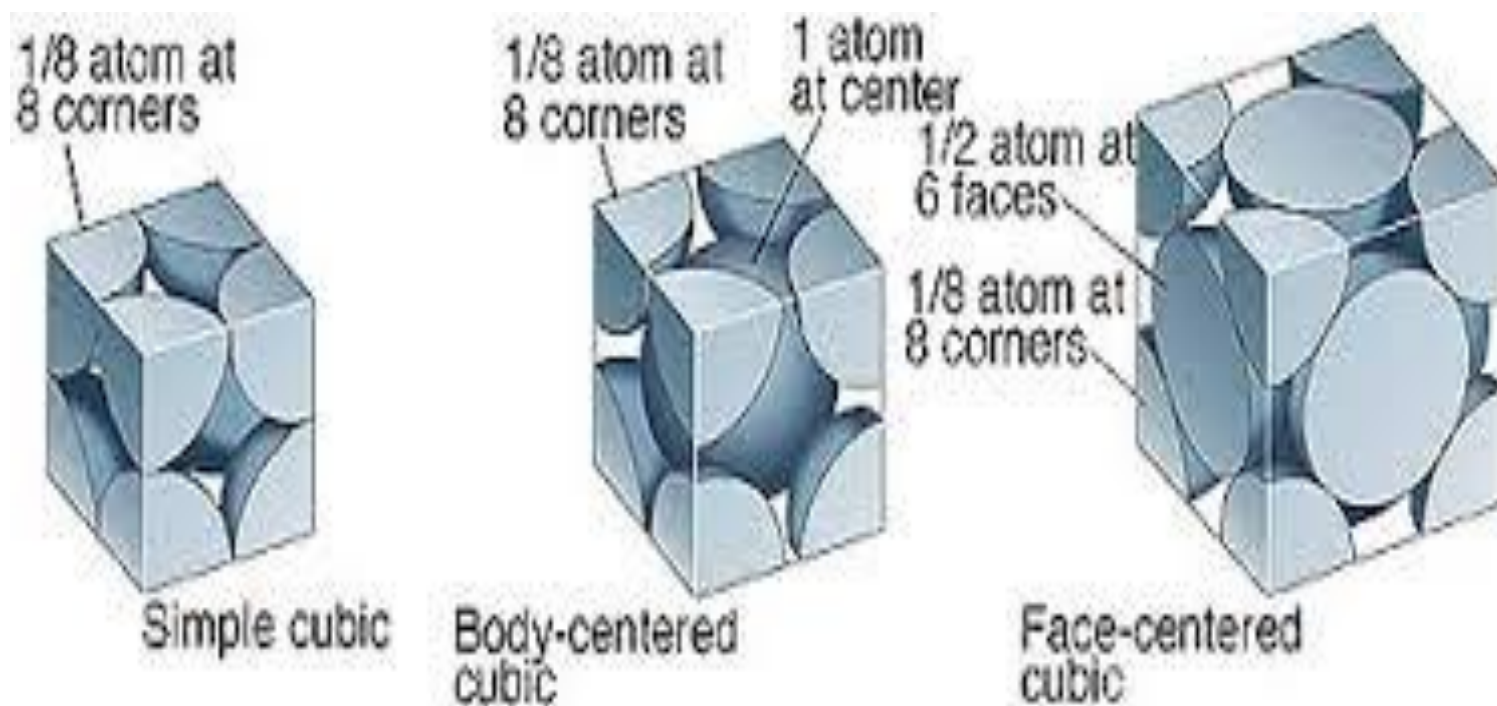
23

Estrutura Cúbica de Faces Centradas (CFC)

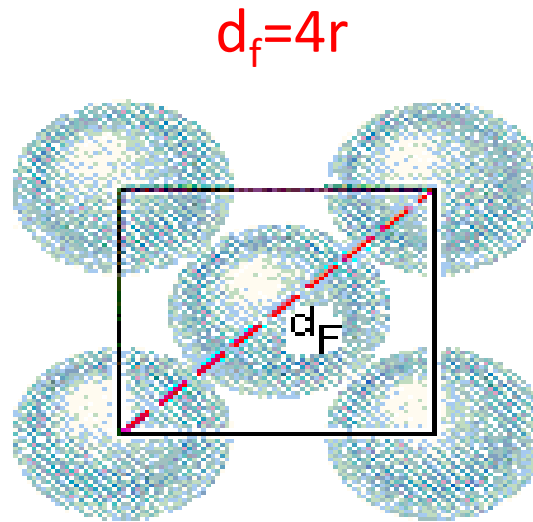
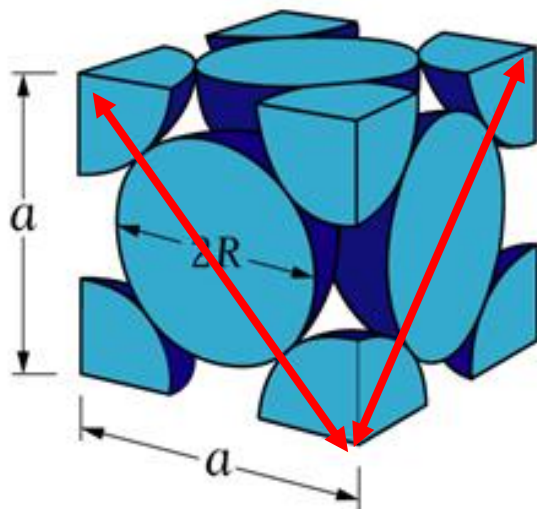


empilhamento ABC (empilhamento de planos compactos)

Número de átomos por célula unitária



Parâmetro de rede vs raio atômico - CFC



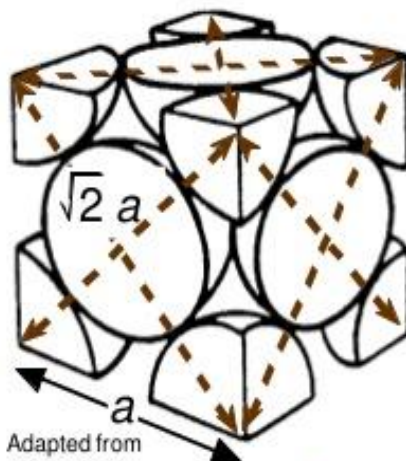
$$a^2 + a^2 = (4r)^2$$

$$2a^2 = 16r^2$$

$$a = \sqrt{8}r$$

$$a = 2\sqrt{2}r$$

Factor de empacotamento atómico- CFC (74%)



Adapted from
Fig. 3.1(a),
Callister &
Rethwisch 3e.

maximum achievable APF

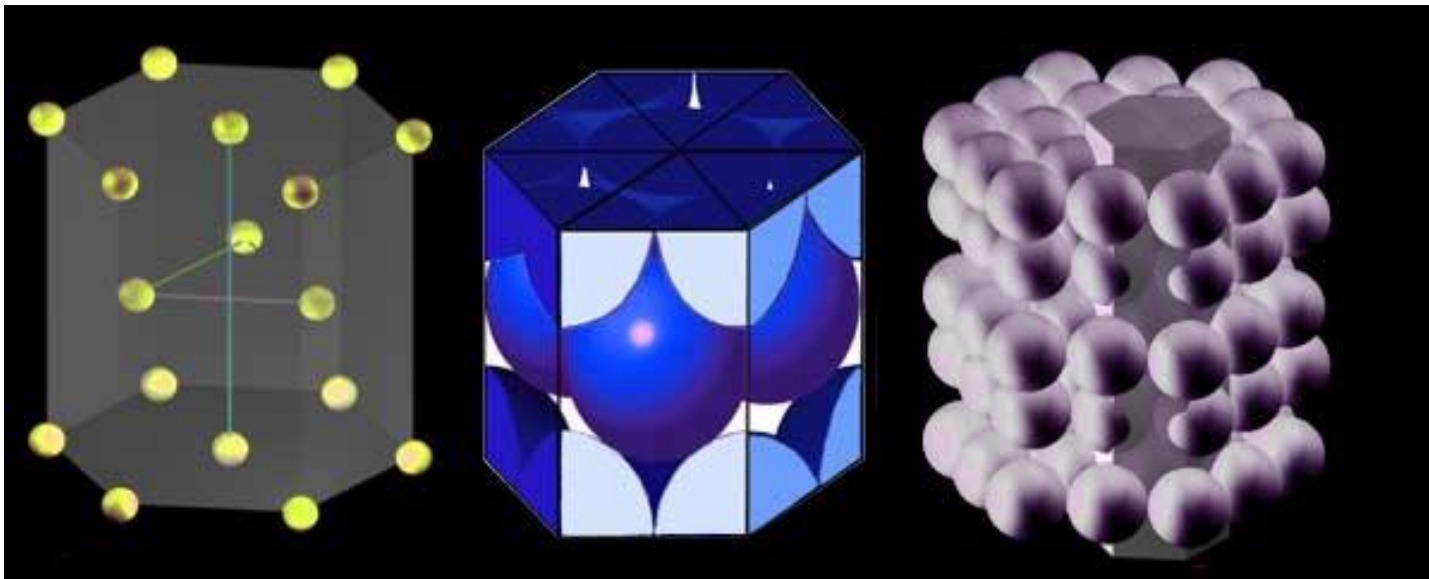
Close-packed directions:
length = $4R = \sqrt{2} a$

Unit cell contains:

$$6 \times 1/2 + 8 \times 1/8 \\ = 4 \text{ atoms/unit cell}$$

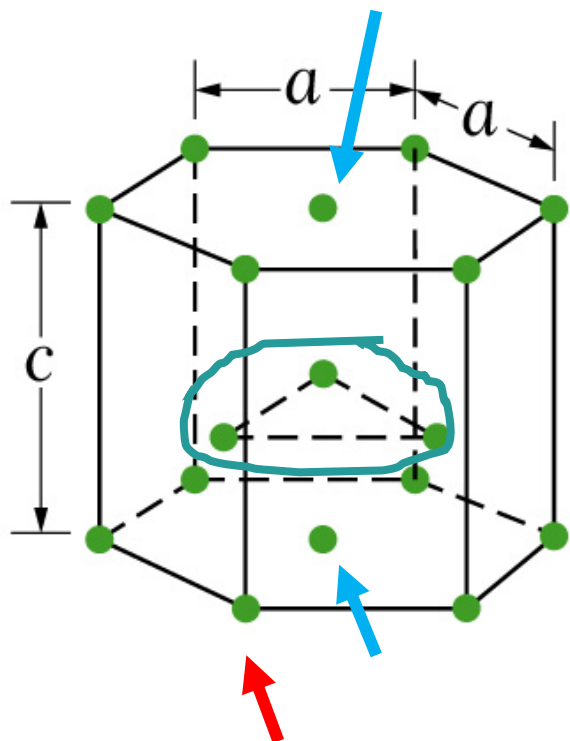
$$\text{APF} = \frac{\begin{array}{c} \text{atoms} \\ \text{unit cell} \end{array} \quad 4 \quad \frac{4}{3} \pi (\sqrt{2}a/4)^3 \quad \begin{array}{c} \text{volume} \\ \text{atom} \end{array}}{\begin{array}{c} \text{volume} \\ \text{unit cell} \end{array} \quad a^3}$$

Estruturas Hexagonal Compacta



empilhamento ABA (empilhamento de planos compactos)

Cada átomo no centro dos planos hexagonais contribui para a célula unitária com $\frac{1}{2}$ átomo

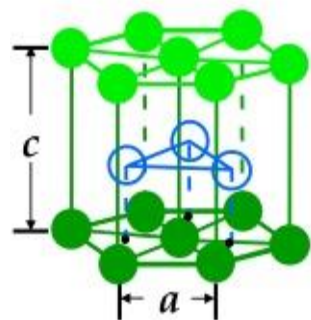


Cada átomo de cada vértice dos planos hexagonais contribui para a célula unitária com $\frac{1}{6}$ de átomo.

Há que considerar ainda 3 átomos no interior da célula unitária

$$\text{Número de átomos por célula unitária} = 12 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3 = 6$$

Factor de empacotamento atómico- HC (74%)



A sites

$$C = 1.633a$$

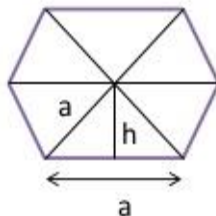
B sites

Number of atoms in HCP unit cell=
 $(12 \times 1/6) + (2 \times 1/2) + 3 = 6 \text{ atoms}$

A sites

Vol. of HCP unit cell =
area of the hexagonal face \times height of the hexagonal
Area of the hexagonal face = area of each triangle $\times 6$

$$a = 2r$$



$$\text{Area of triangle} = \frac{bh}{2} = \frac{ah}{2} = \frac{1}{2}a \cdot \frac{a\sqrt{3}}{2}$$

$$\text{Area of hexagon} = 6 \cdot \frac{a^2\sqrt{3}}{4}$$

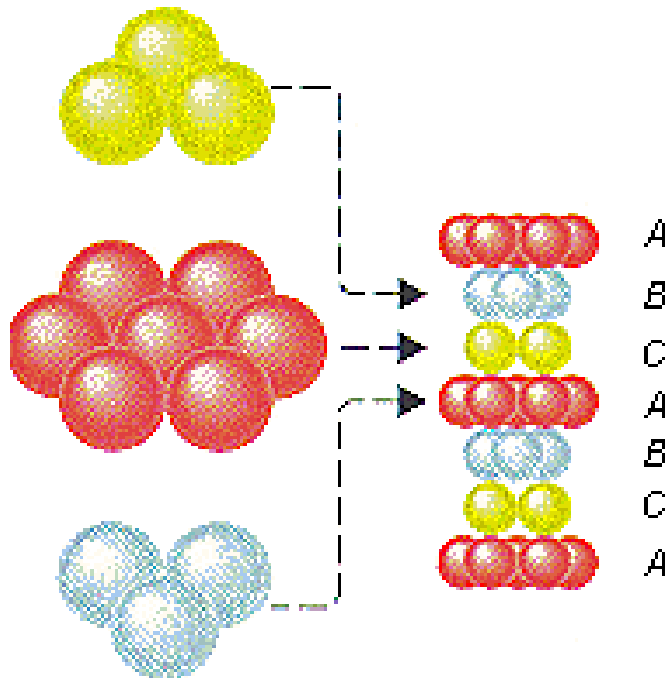
$$\text{Volume of HCP} = 6 \cdot \frac{a^2\sqrt{3}}{4} \cdot C = 6 \cdot \frac{a^2\sqrt{3}}{4} \cdot 1.633a$$

$$\text{APF} = 6 \cdot \frac{4\pi r^3}{3} / \left(\frac{\sqrt{3}}{4} \cdot 6 \cdot 1.633 \cdot a^3 \right)$$

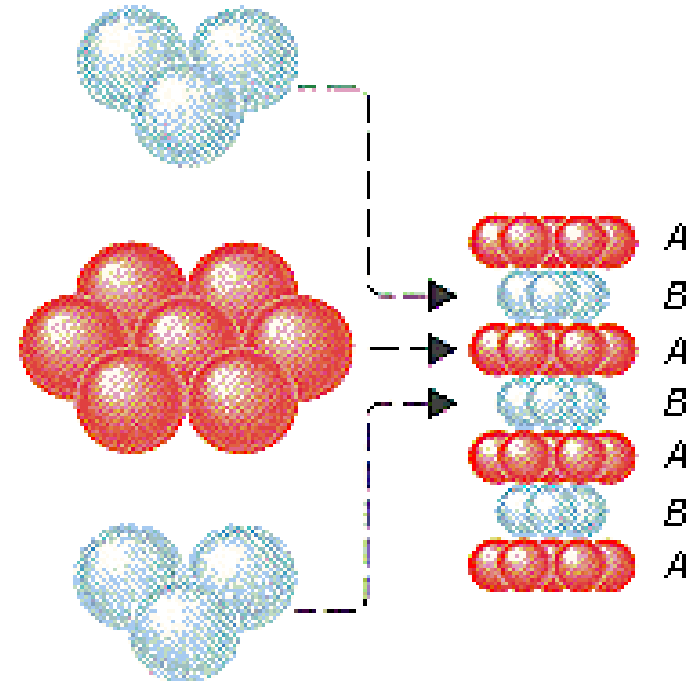
$$\text{APF} = 0.74$$

Hari Prasad

Empilhamento das camadas

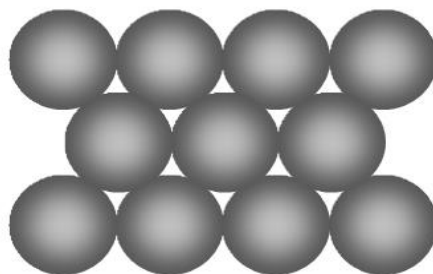


Cubic
closest packed
structure

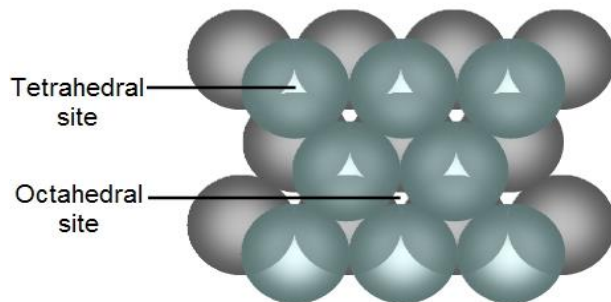


Hexagonal
closest packed
structure

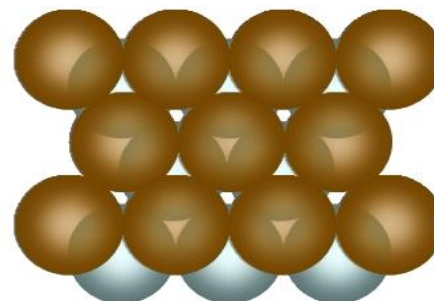
Empilhamento das camadas



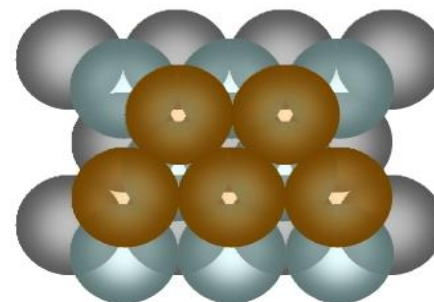
A) a layer of close-packed spheres
(note hexagonal arrangement)



B) Addition of a second layer, sitting in
the depressions between the lower
layer, as close together as they can get

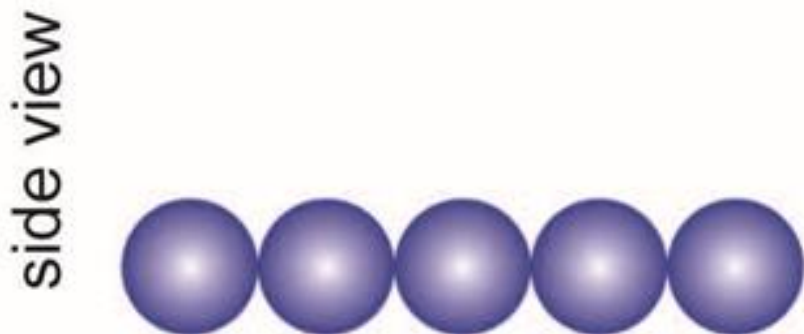
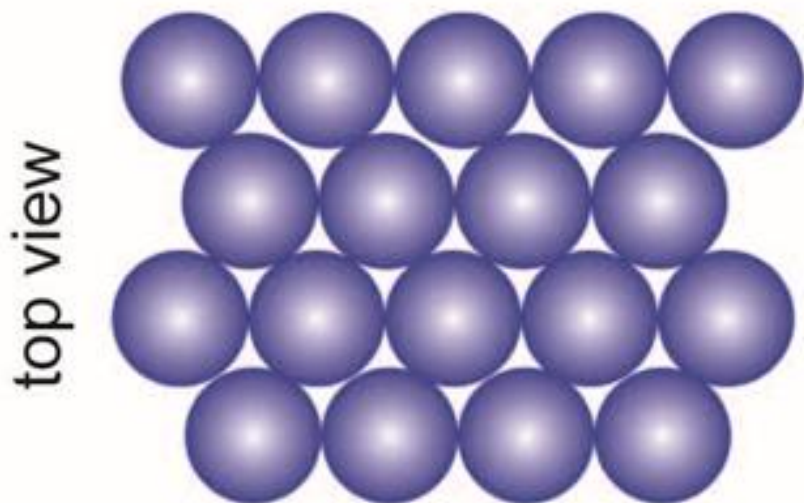


C) Adding a third layer directly over
the first/bottom layer (ABAB...) hcp

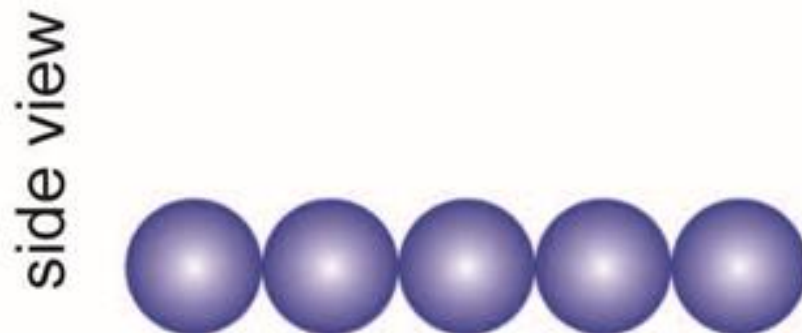
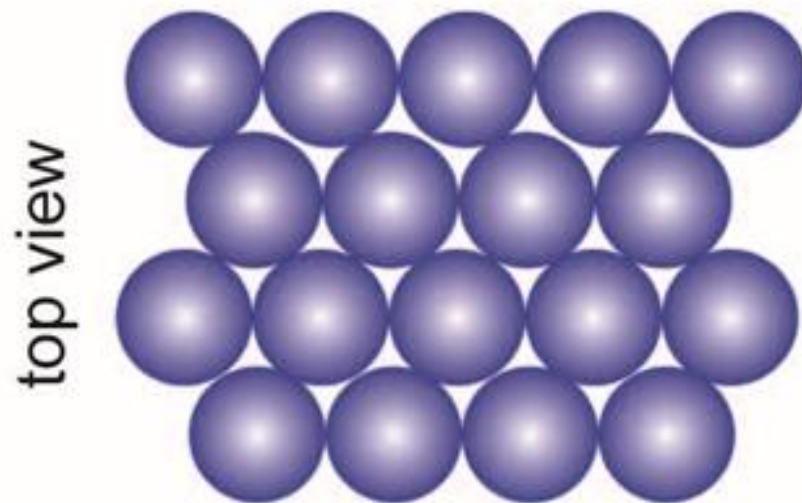


D) Adding a third layer over the
octahedral sites (ABCABC...) ccp
or fcc (face-centred cubic)

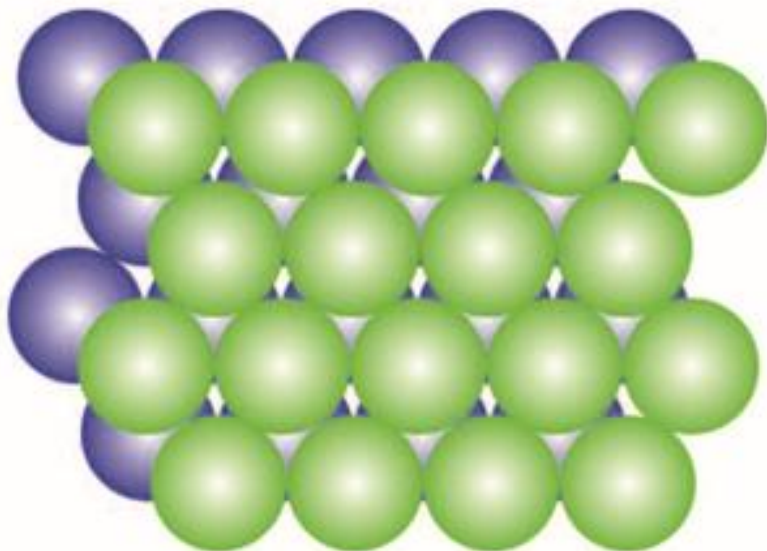
1s close-packed layer



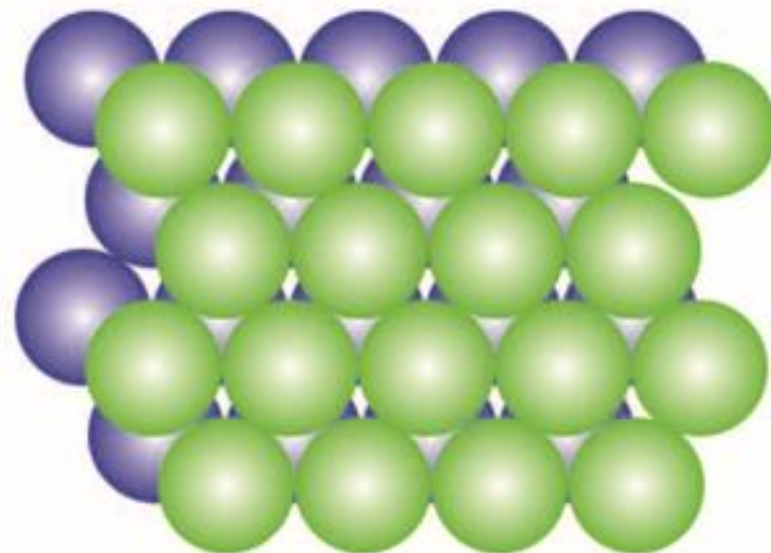
1s close-packed layer



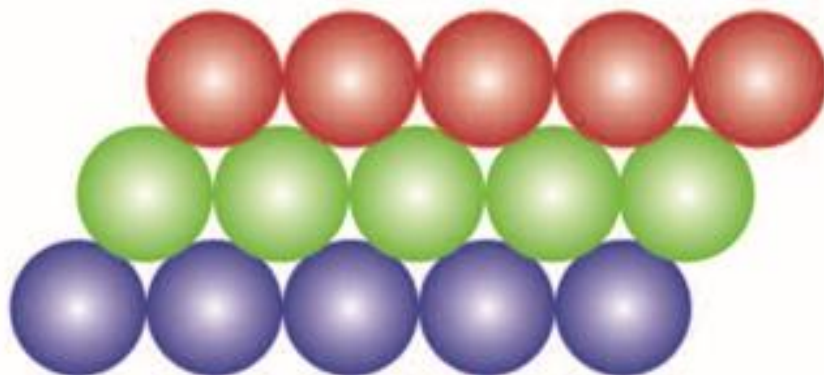
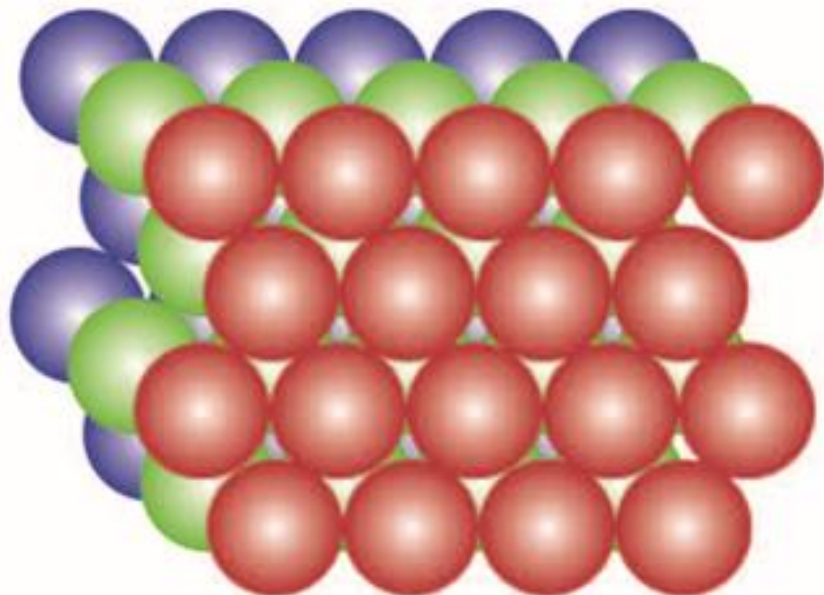
2nd close-packed layer



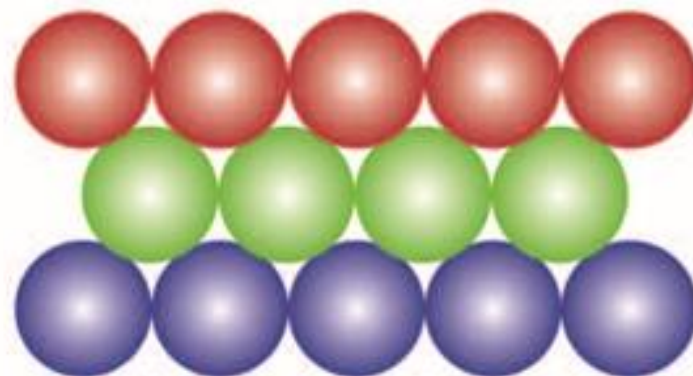
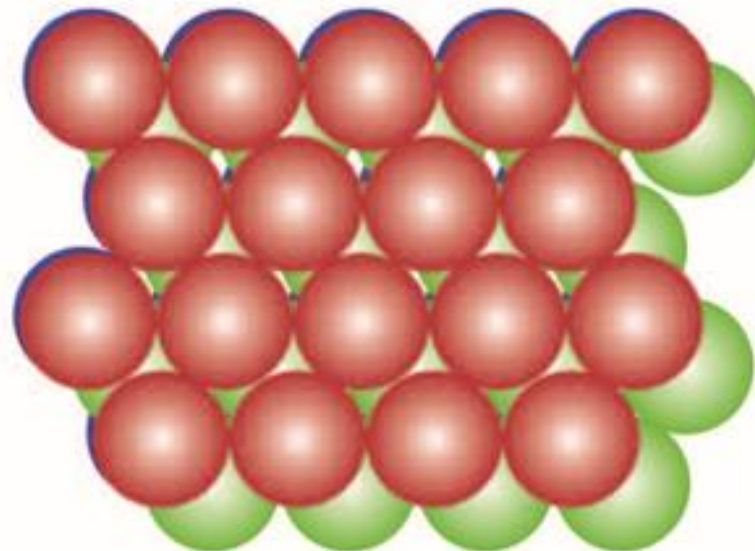
2nd close-packed layer

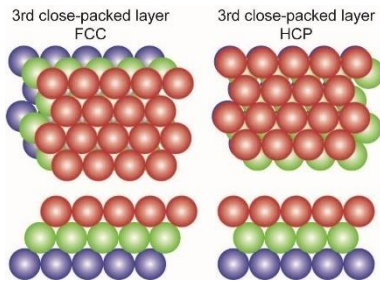


3rd close-packed layer
FCC



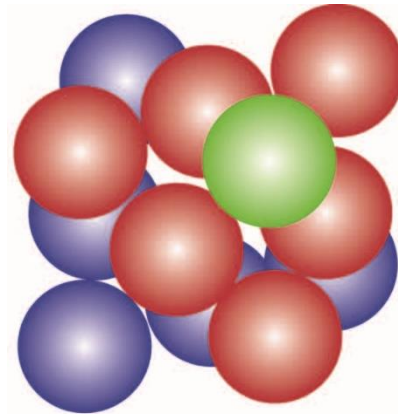
3rd close-packed layer
HCP



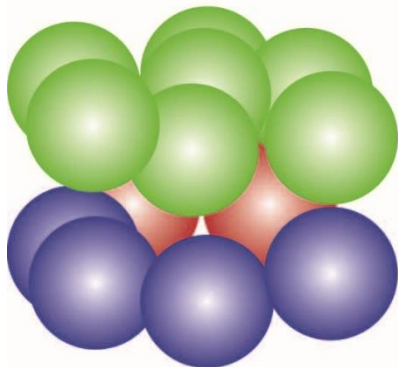
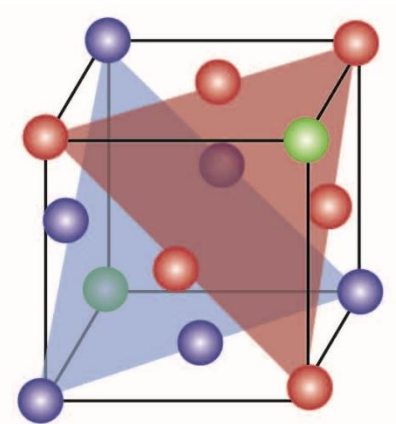


Estruturas compactas

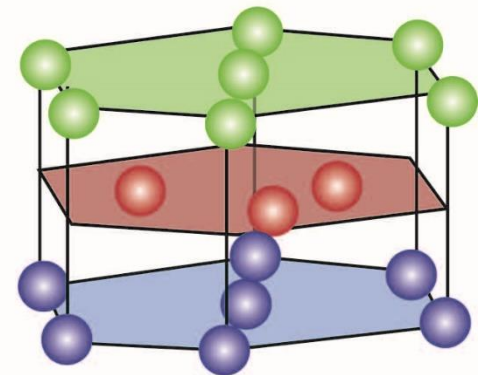
(estruturas de máxima compacidade)



Cúbica de fases centradas (cfc)


















Hexagonal compacta (hc)



Estruturas cristalinas de metais (25°C)

Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431
Cadmium	HCP	0.1490
Chromium	BCC	0.1249
Cobalt	HCP	0.1253
Copper	FCC	0.1278
Gold	FCC	0.1442
Iron (Alpha)	BCC	0.1241
Lead	FCC	0.1750
Magnesium	HCP	0.1599
Molybdenum	BCC	0.1363
Nickel	FCC	0.1246
Platinum	FCC	0.1387
Silver	FCC	0.1445
Tantalum	BCC	0.1430
Titanium (Alpha)	HCP	0.1445
Tungsten	BCC	0.1371
Zinc	HCP	0.1332

<https://www.nde-ed.org/EducationResources/CommunityCollege/Materials/Structure>

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
														
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
