Estrutura dos Sólidos

Cristal Ideal

- Um cristal ideal é um conjunto periódico de unidades estruturais, como átomos ou moléculas.
- Ele pode ser construído pela repetição infinita dessas unidades estruturais idênticas no espaço (células unitárias).
- A estrutura pode ser descrita em termos de uma rede, com um grupo de átomos anexados a cada ponto de rede. O grupo de átomos é a base.

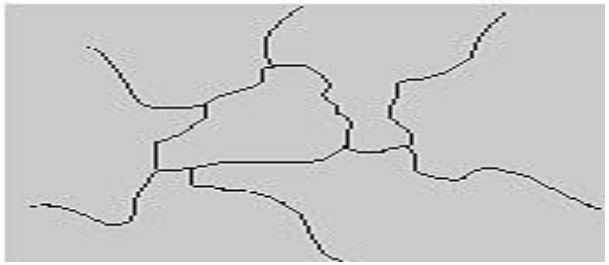
Tipos de Sólidos

Material cristalino: **arranjo periódico**

Cristal simples:

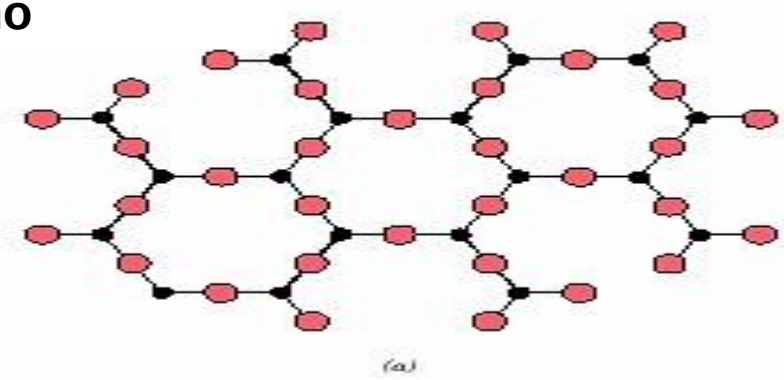
Matriz periódica em toda a extensão do material

Polycrystalline material: pequenos cristais ou grãos

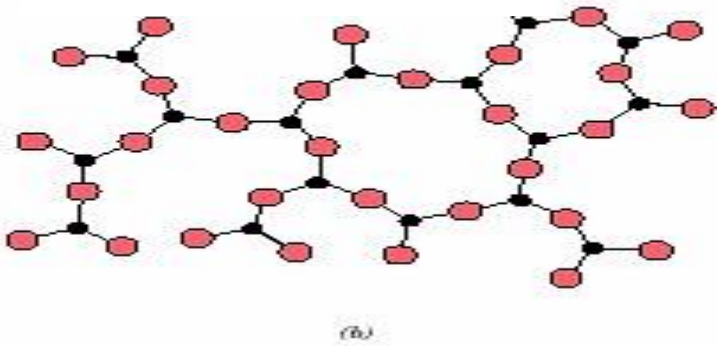


Amorfo: **sem um arranjo ordenado**

Cristalino



Amorfo

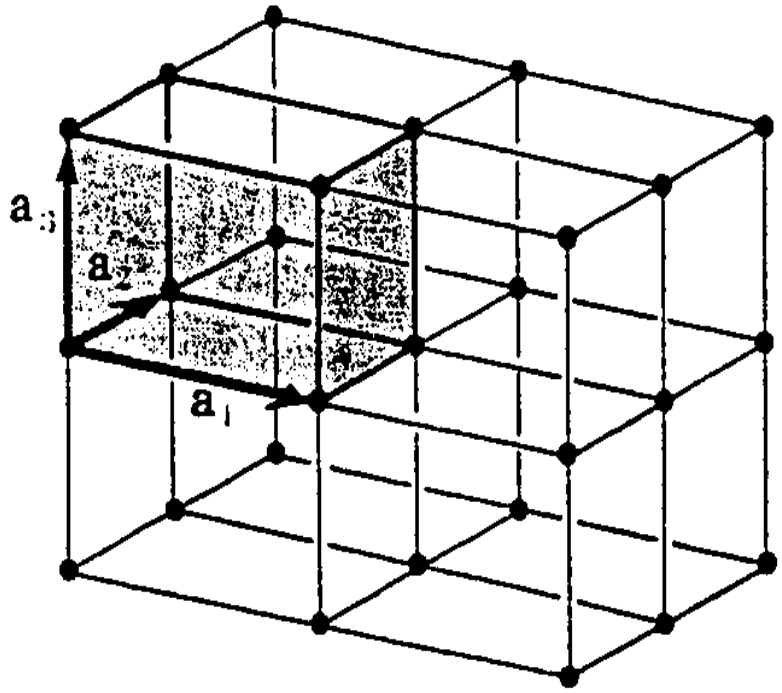


Estutura de Bravais

- Um conjunto infinito de pontos discretos com um arranjo e orientação que aparece exatamente o mesmo, de qualquer um dos pontos em que a matriz é visualizada.
- Uma rede de Bravais tridimensional consiste em todos os pontos com os vetores de posição R que podem ser escritos como uma combinação linear de vetores primitivos. Os coeficientes de expansão devem ser inteiros.

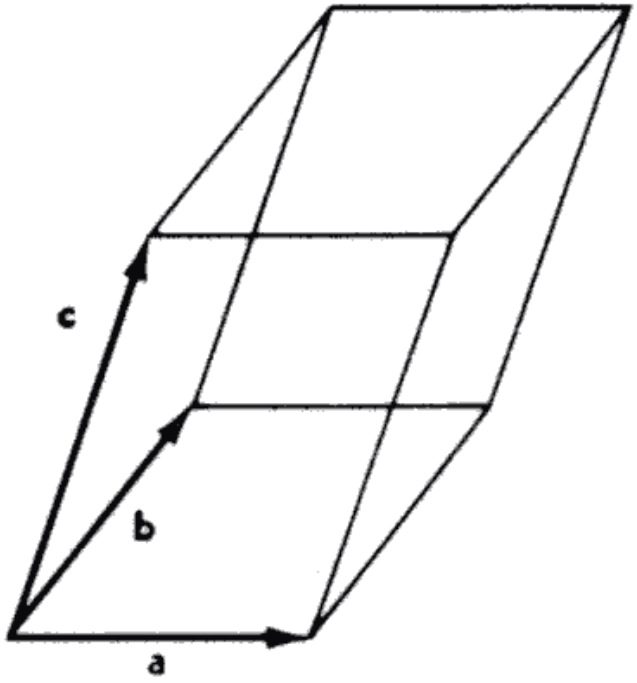
Célula unitária

- Uma célula primitiva ou uma célula unitária primitiva é um volume de espaço que quando traduzido através de todos os vetores em uma rede de Bravais apenas enche todo o espaço sem se sobrepor ou deixar vazios.
- Uma célula primitiva deve conter precisamente um ponto de rede.

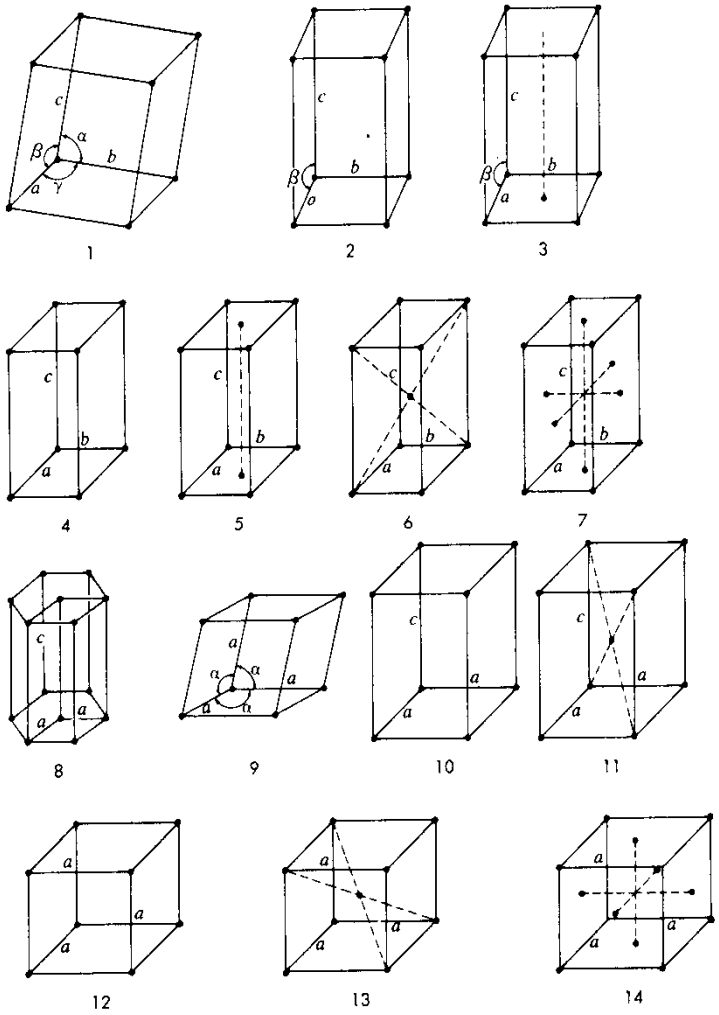


Célula unitária tridimensional

Existem 14 redes de pontos diferentes, chamadas de Bravais, compõem o sistema de cristal. Os comprimentos dos lados, a, b e c, e os ângulos entre eles podem variar para uma célula unitária particular.



System	Axes* and Interaxial Angles	Examples
Triclinic	Three axes not at right angles, of any length $a \neq b \neq c$† $\quad \alpha \neq \beta \neq \gamma \neq 90°$	$B(OH)_3$, $K_2S_2O_8$, Al_2SiO_5, $NaAlSi_3O_8$
Monoclinic	Three axes, one pair not at right angles, of any lengths $a \neq b \neq c \quad \alpha = \gamma = 90° \neq \beta$	$C_{18}H_{24}$, KNO_2, $K_2S_4O_6$, As_4S_4, $KClO_3$
Orthorhombic	Three axes at right angles, all unequal $a \neq b \neq c \quad \alpha = \beta = \gamma = 90°$	I, Ga, Fe_3C, FeS_2, $BaSO_4$
Tetragonal	Three axes at right angles, two equal $a = b \neq c \quad \alpha = \beta = \gamma = 90°$	In, TiO_2, $C_4H_{10}O_4$, KIO_4
Cubic	Three axes at right angles, all equal $a = b = c \quad \alpha = \beta = \gamma = 90°$	Cu, Ag, Ar, Si, Ni, NaCl, LiF
Hexagonal	Two axes of equal length at 120°, third axis at 90° to these $a = b \neq c \quad \alpha = \beta = 90° \quad \gamma = 120°$	Zn, Cd, Mg, NiAs
Rhombohedral	Three axes equally inclined, not at right angles, all equal $a = b = c \quad \alpha = \beta = \gamma \neq 90°$	Hg, Sb, Bi

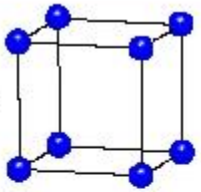


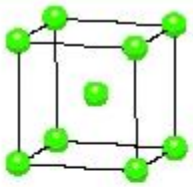
The 14 point lattices illustrated by a unit cell of each: (1) triclinic, simple; (2) monoclinic, simple; (3) monoclinic, base centered; (4) orthorhombic, simple; (5) orthorhombic, base centered; (6) orthorhomic, body centered; (7) orthorhombic, face centered; (8) hexagonal; (9) rhombohedral; (10) tetragonal, simple; (11) tetragonal, body centered; (12) cubic, simple; (13) cubic, body centered; (14) cubic, face centered.

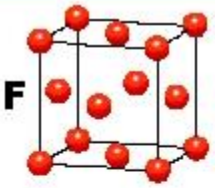
CUBIC

$a = b = c$

$\alpha = \beta = \gamma = 90°$

P 

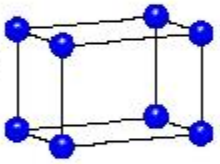
I 

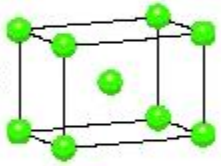
F 

TETRAGONAL

$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

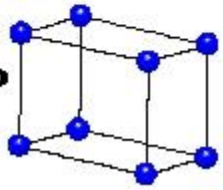
P 

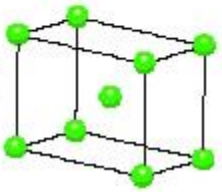
I 

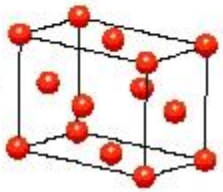
ORTHORHOMBIC

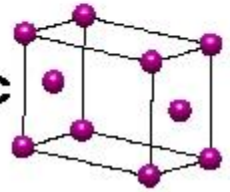
$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

P 

I 

F 

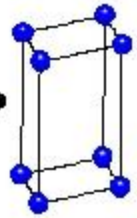
C 

HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

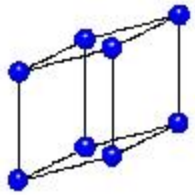
$\gamma = 120°$

P 

TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

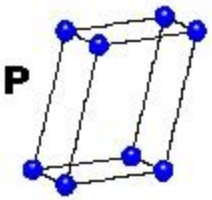
P 

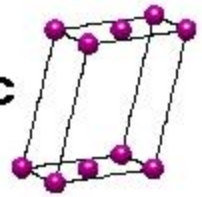
MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

$\beta \neq 120°$

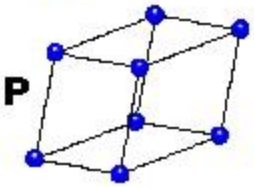
P 

C 

TRICLINIC

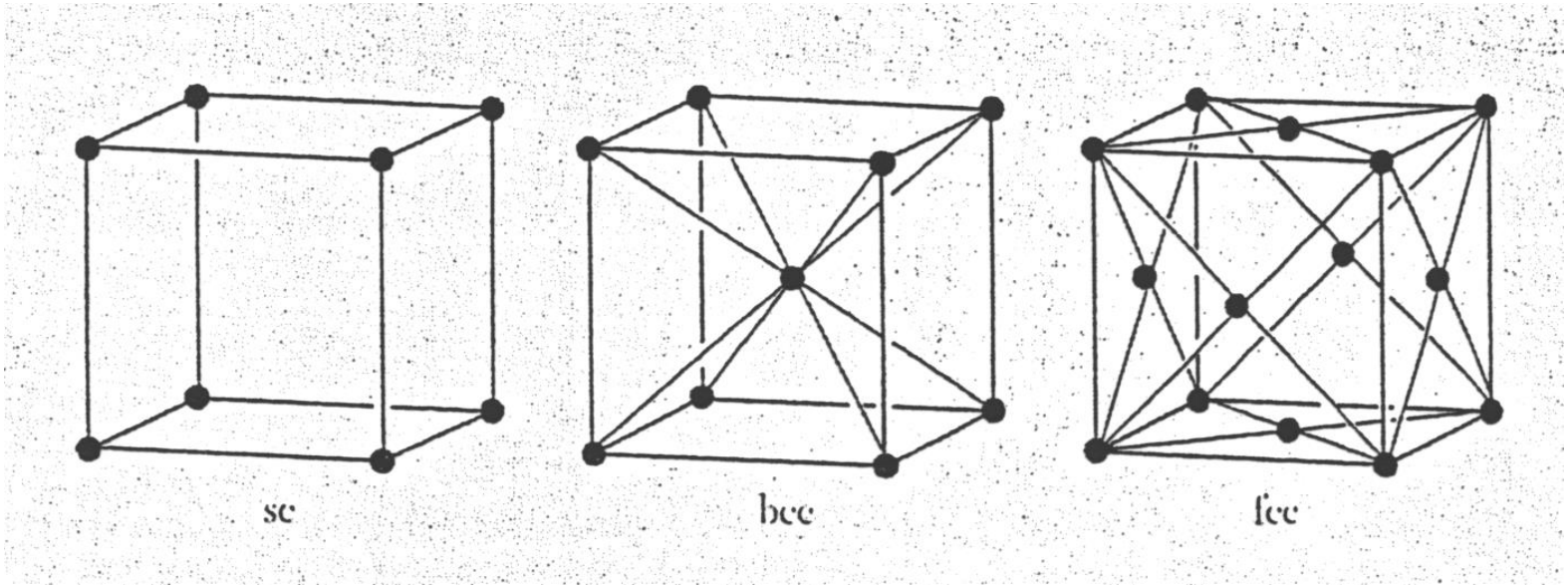
$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$

P 

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

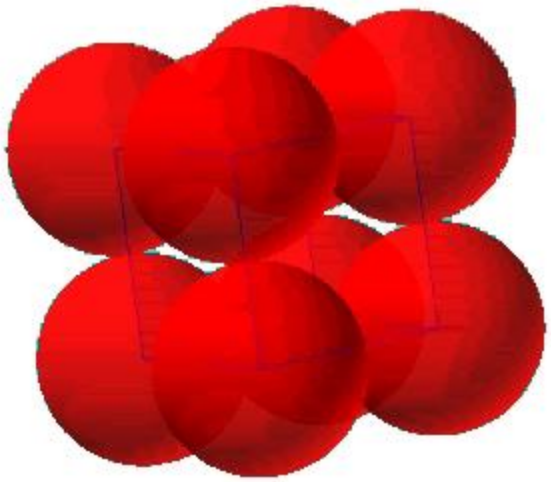
Retículo Cubico



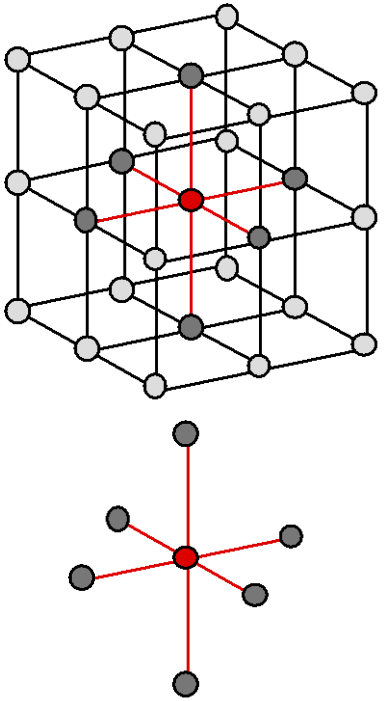
SC = cúbico simples
BCC = cúbico de face centrada
FCC = cúbico de corpo centrado

ESTRUTURA CUBICA SIMPLES (SC)

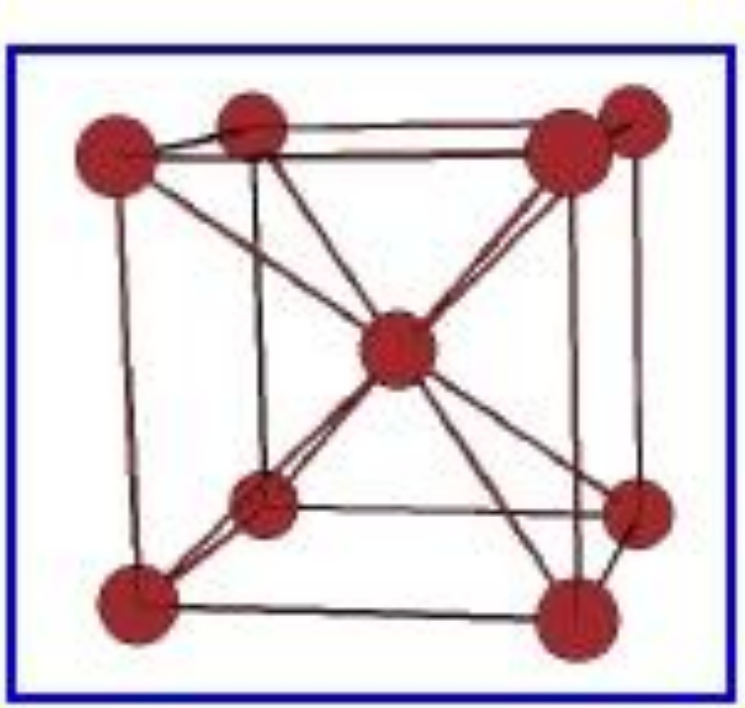
- Raro (somente Po)
- Bordas de um cubo



- Coordenação = 6

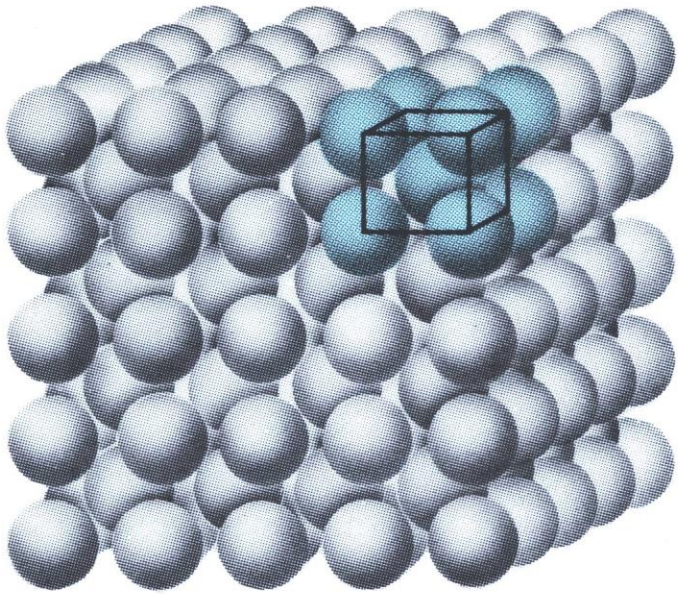


Estrutura BCC



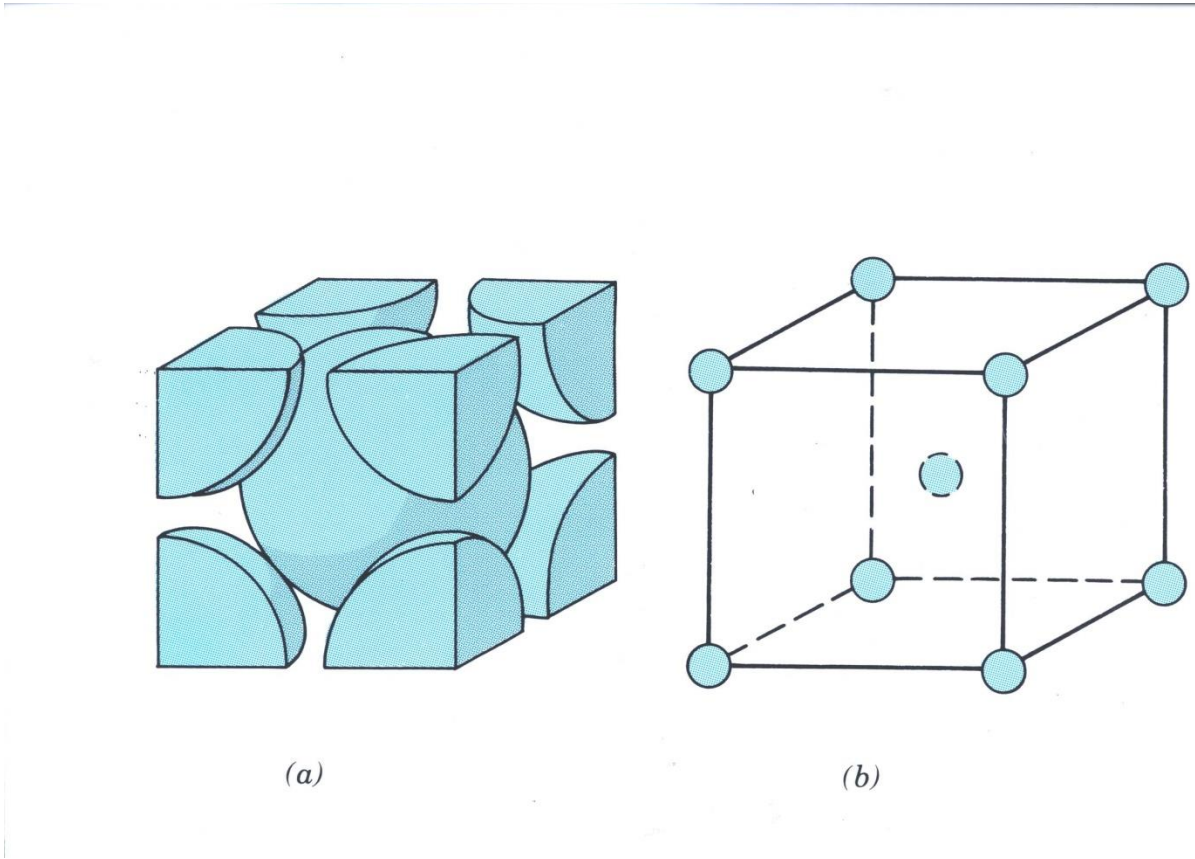
Cristal BCC

(a) (b)



(c)

BCC



(a)

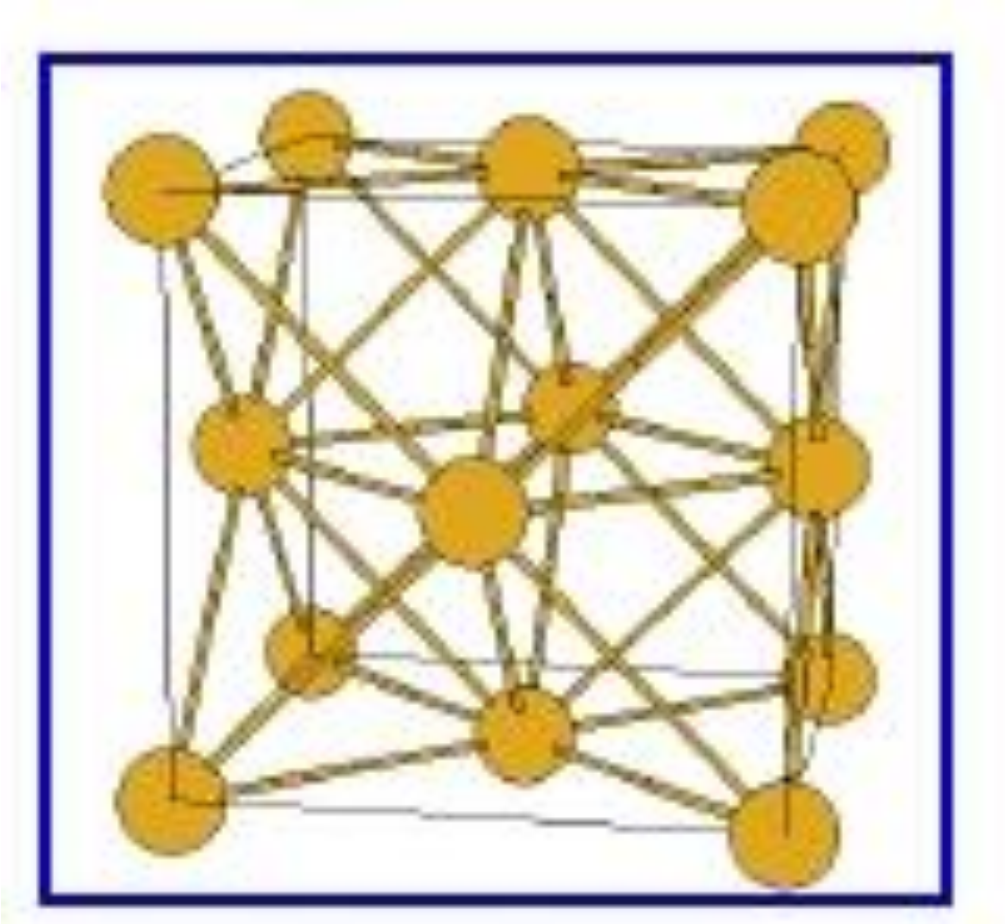
(b)

Table 4.2

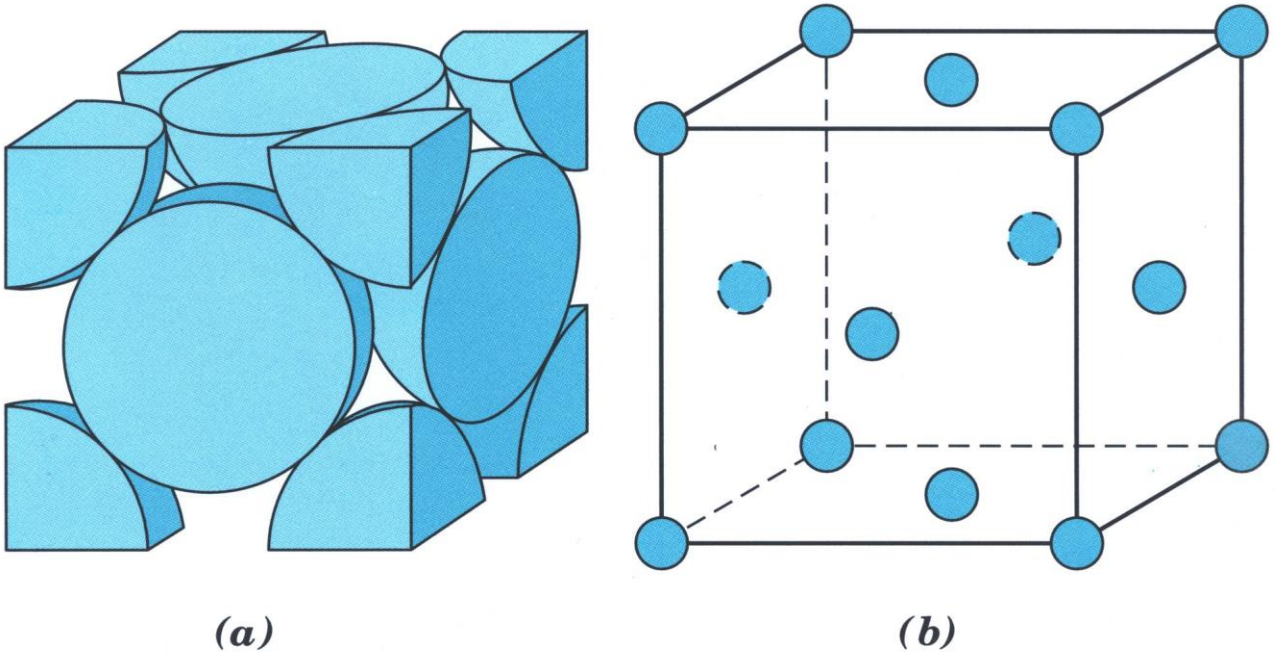
ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

Estrutura FCC



Estrurura FCC



FCC

Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

NaCl

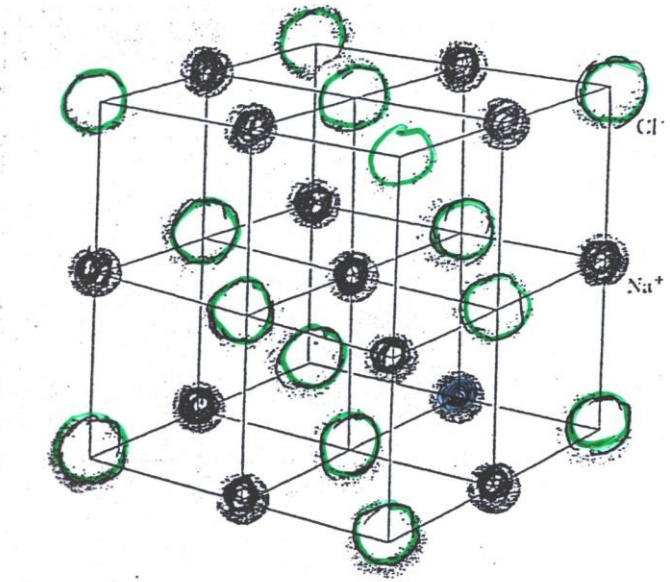
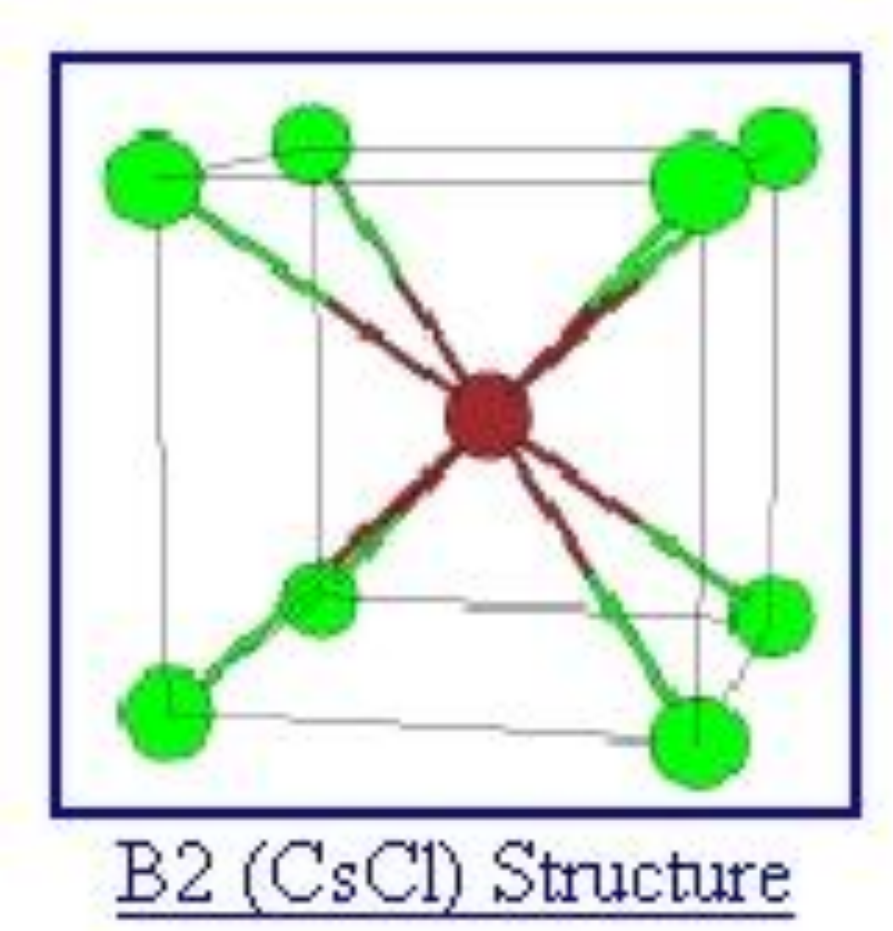


Figure 17 We may construct the sodium chloride crystal structure by arranging Na^+ and Cl^- ions alternately at the lattice points of a simple cubic lattice. In the crystal each ion is surrounded by six nearest neighbors of the opposite charge. The space lattice is fcc, and the basis has one Cl^- ion at 000 and one Na^+ ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. The figure shows one conventional cubic cell. The ionic diameters here are reduced in relation to the cell in order to clarify the spatial arrangement.

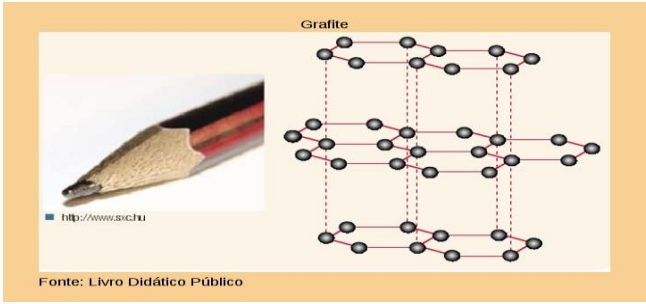
CsCl

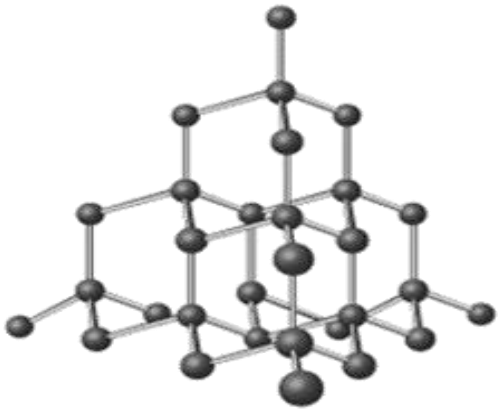


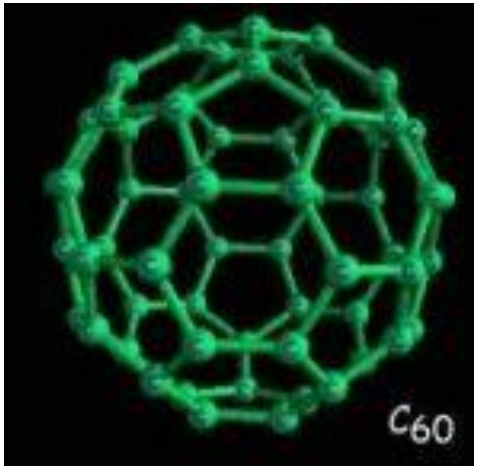
A ALOTROPIA NO CARBONO

Carbono (C)

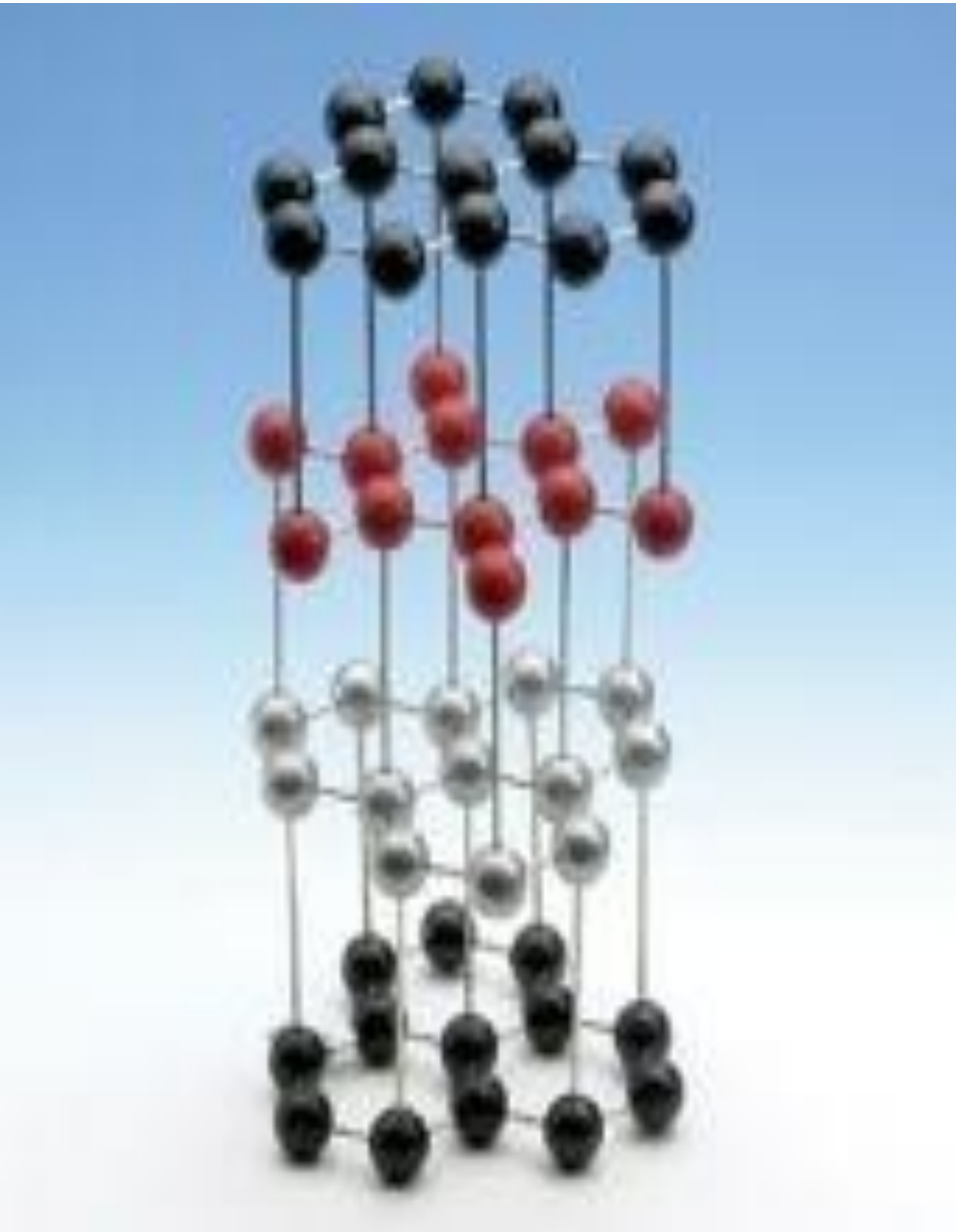
- **C (gr) = grafite**
- **C(d) = diamante**
- **C(n) = fulerenos**







Carbono (grafite)



APLICAÇÕES

. contatos elétricos,

. equipamentos para altas temperaturas,

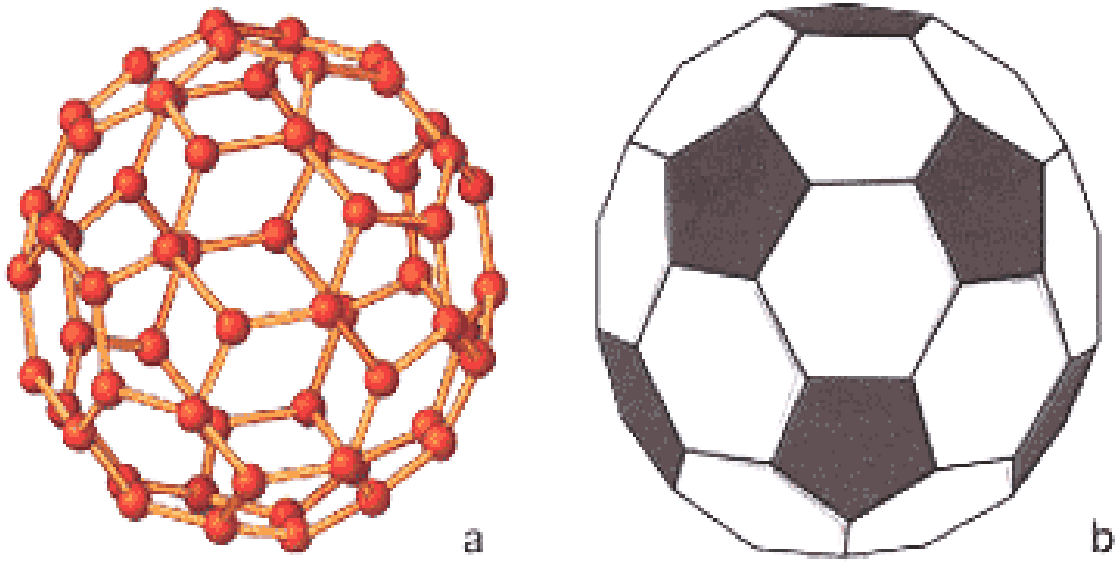
. lubrificantes sólidos.

. bom condutor de calor e eletricidade ao longo das camadas.

Carbono (diamante)

O diamante possui uma estrutura com átomos extremamente unidos, sendo a substância natural mais dura existente no mundo.

FULERENOS – C(n)



Os fulerenos são formados por uma rede de pentágonos e hexágonos unidos na forma de uma esfera. Os carbonos possuem hibridização sp^2, formando ligações simples com três outros átomos de carbono, restando um elétron de cada carbono, que fica deslocalizado num sistema que atribui à molécula o caráter aromático.

FULERENOS – C(n)

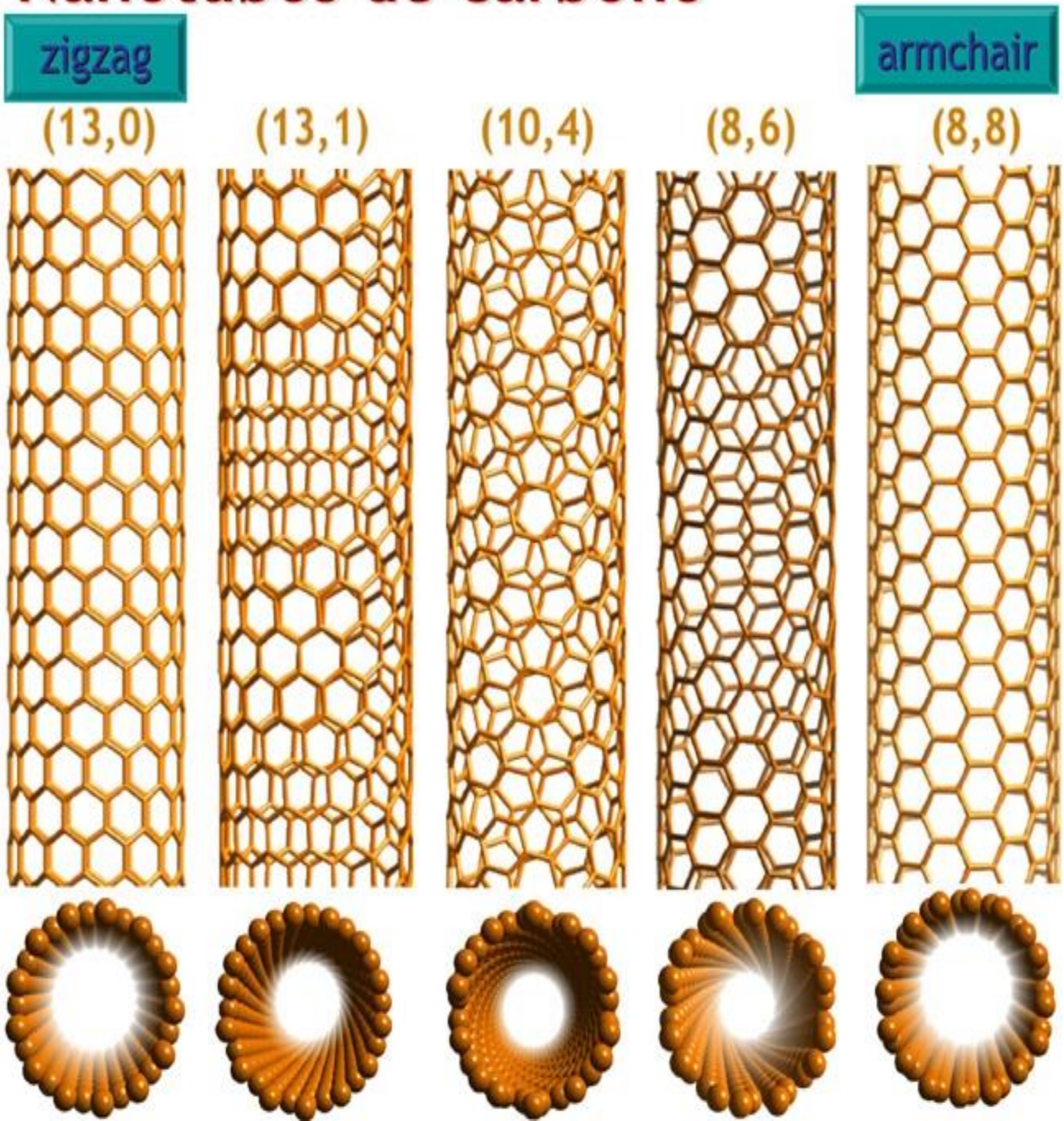
Existem fulerenos com quantidades diferentes de átomos de carbono.

C_{20},C_{60}, C_{70}, C_{100}, C_{180}, C_{240}, C_{540}.

APLICAÇÕES DOS FULERENOS

. lubrificantes,
. semicondutores,
. supercondutores,
. ponto de partida na síntese de novos fármacos.

Nanotubos de carbono



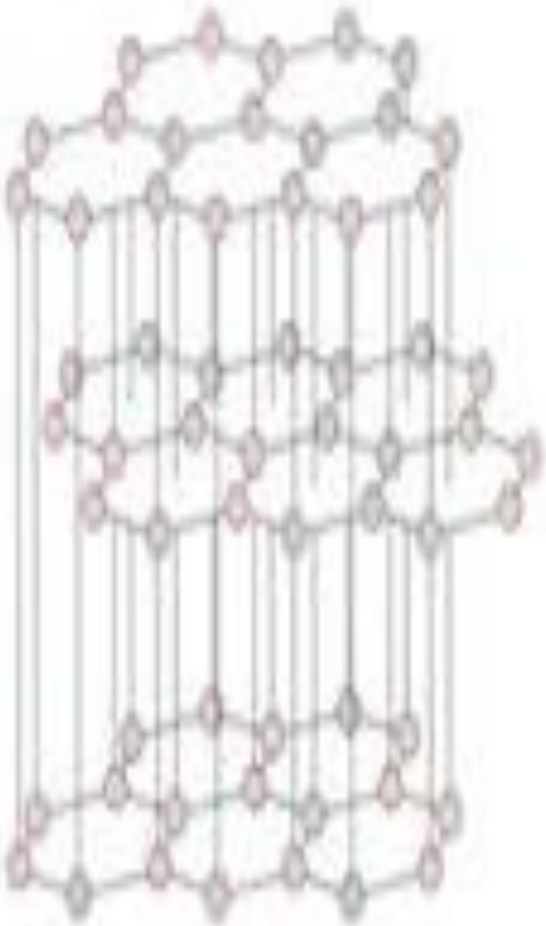
. 1000X MELHOR CONDUTOR DE ELETRICIDADE QUE O COBRE.

. 100X MAIS RESISTENTES À TRAÇÃO QUE O AÇO.

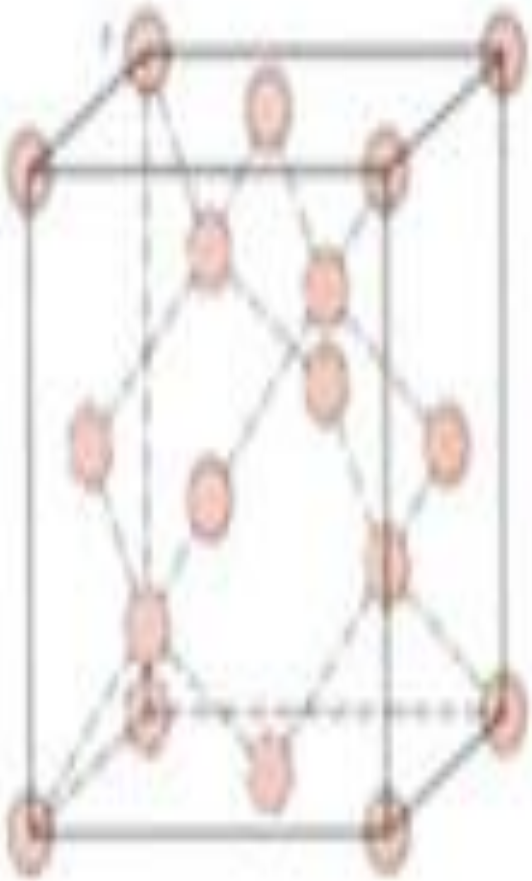
. NANOPROCESSADO-

-RES MAIS RÁPIDOS QUE OS ATUAIS DE SILÍCIO.

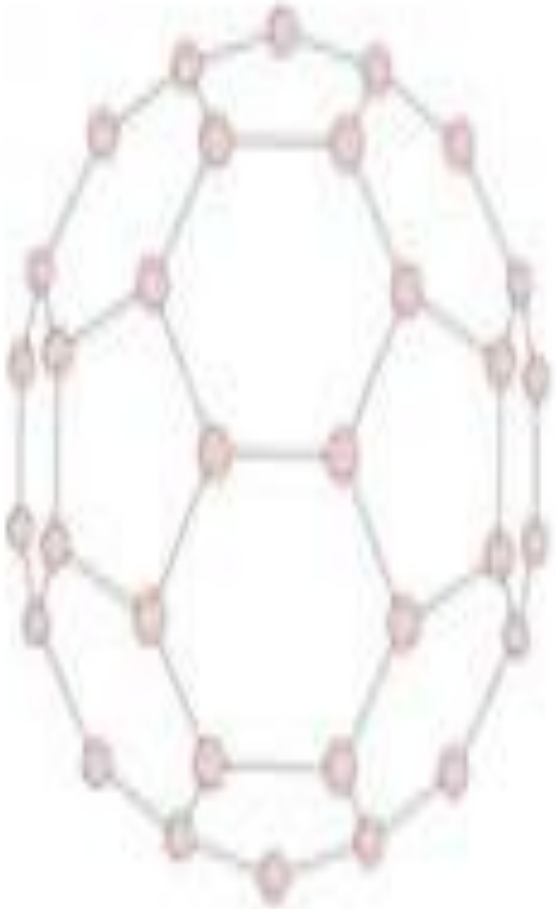
. COLETES À PROVA DE BALA E ROUPAS ESPACIAIS.



Grafite



Diamante



Fulereno

Characteristics of Selected Elements at 20C

Element	Symbol	At. Weight (amu)	Density (g/cm^3)	Crystal Structure	Atomic radius (nm)
Aluminum	Al	26.98	2.71	FCC	0.143
Argon	Ar	39.95	------	------	------
Barium	Ba	137.33	3.5	BCC	0.217
Beryllium	Be	9.012	1.85	HCP	0.114
Boron	B	10.81	2.34	Rhomb	------
Bromine	Br	79.90	------	------	------
Cadmium	Cd	112.41	8.65	HCP	0.149
Calcium	Ca	40.08	1.55	FCC	0.197
Carbon	C	12.011	2.25	Hex	0.071
Cesium	Cs	132.91	1.87	BCC	0.265
Chlorine	Cl	35.45	------	------	------
Chromium	Cr	52.00	7.19	BCC	0.125
Cobalt	Co	58.93	8.9	HCP	0.125
Copper	Cu	63.55	8.94	FCC	0.128
Flourine	F	19.00	------	------	------
Gallium	Ga	69.72	5.90	Ortho.	0.122
Germanium	Ge	72.59	5.32	Dia. cubic	0.122
Gold	Au	196.97	19.32	FCC	0.144
Helium	He	4.003	------	------	------
Hydrogen	H	1.008	------	------	------

Adapted from Table, "Characteristics of Selected Elements", inside front cover, *Callister 6e.*