

INTRODUÇÃO A CIÊNCIA DOS MATERIAIS

seminários: quintas-feiras (13h30min às 15h30min)

exercícios e atendimento (combinaremos depois)

Prof. Aguinaldo M. Severino

Laboratório de Magnetismo e Materiais Magnéticos – UFSM

© Adalberto Fazzio – IF USP (2005-2007) NOTAS DE AULA

© WILLIAM D CALLISTER JR. Ciência e Engenharia dos Materiais: Uma Introdução

Bibliografia Principal

- HUMMEL, Rolf. E., Understanding Materials Science 2^a ed., New York, Springer Verlag, 2004, ISBN: 0-387-20939-5

- ★ CALLISTER JR., WILLIAM D., Ciência e Engenharia dos Materiais: Uma Introdução, 1^a ed., Rio de Janeiro, LTC, 2002, ISBN: 85-216-2188-5

Bibliografia Auxiliar

- VAN VLACK, LAWRENCE H., Princípios de Ciência e Tecnologia de Materiais, 1^a ed., São Paulo, Editora Campus, 1994, ISBN: 85-700-1480-5

- WHITE, Mary A., Properties of Materials, 1^a ed., New York, Oxford University Press, 1999, ISBN: 0-19-511331-4

- CALLISTER JR., WILLIAM D., Fundamentos da Ciência e Engenharia dos Materiais, 2^a ed., Rio de Janeiro, LTC, 2006, ISBN: 85-216-1515-9

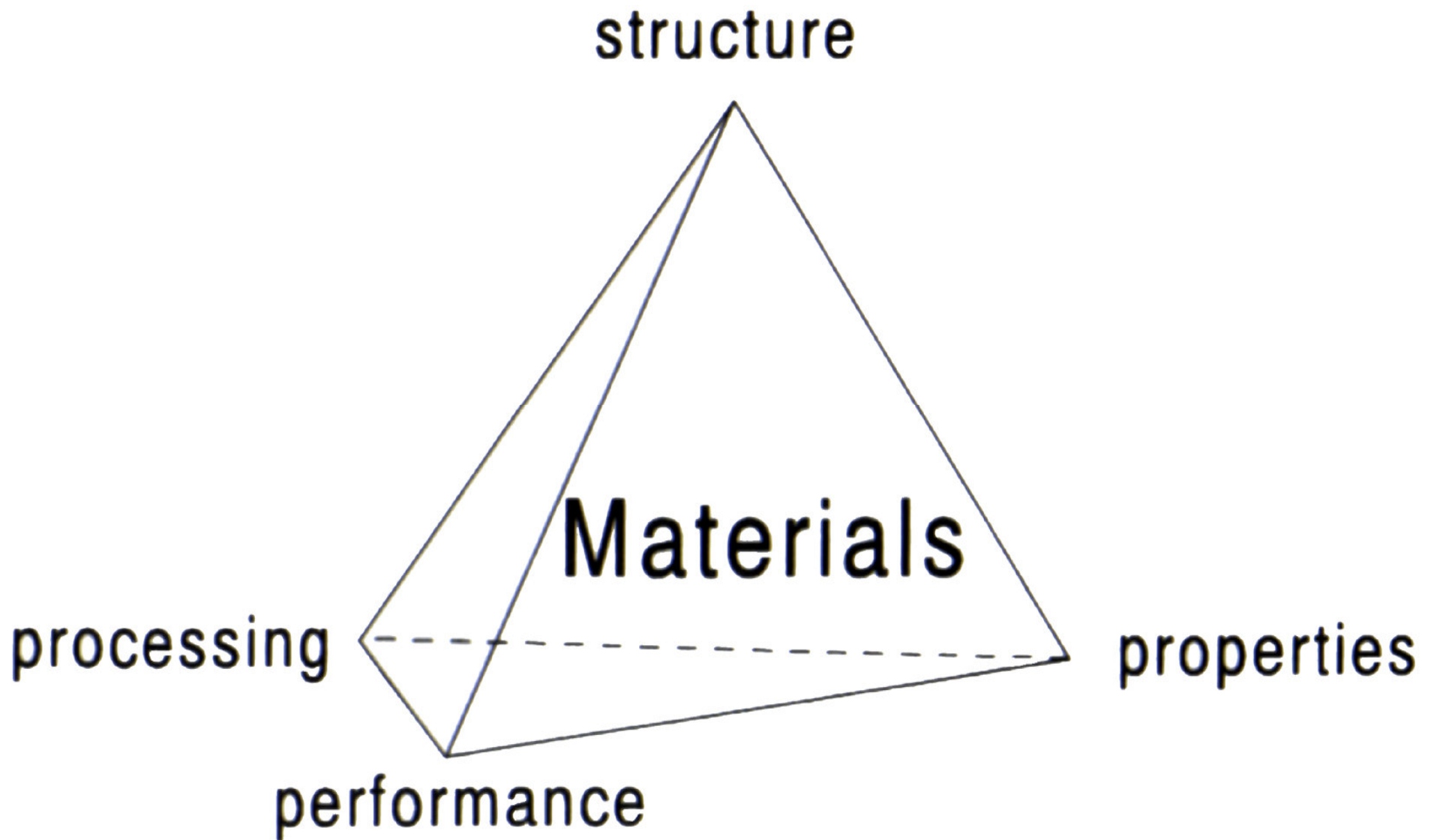


FIGURE 1.1 Materials science is the investigation of the relationships among structure, properties, processing, and performance of materials. (Mary Anne White. *Properties of Materials*.)

CHAPTER 1: MATERIALS SCIENCE & ENGINEERING

Materials are...

engineered structures...not blackboxes!

Structure...has many dimensions...

Structural feature	Dimension (m)
atomic bonding	$< 10^{-10}$
missing/extra atoms	10^{-10}
crystals (ordered atoms)	10^{-8} - 10^{-1}
second phase particles	10^{-8} - 10^{-4}
crystal texturing	$> 10^{-6}$

SUMMARY

Course Goals:

- Use the right material for the job.
- Understand the relation between **properties**, **structure**, and **processing**.
- Recognize new design opportunities offered by materials selection.

CHAPTER 2: BONDING AND PROPERTIES

- **What promotes bonding?**
- **What types of bonds are there?**
- **What properties are inferred from bonding?**

SUMMARY: BONDING

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional semiconductors , ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

SUMMARY: PRIMARY BONDS

Ceramics

(Ionic & covalent bonding):

Large bond energy

large T_m

large E

small α

Metals

(Metallic bonding):

Variable bond energy

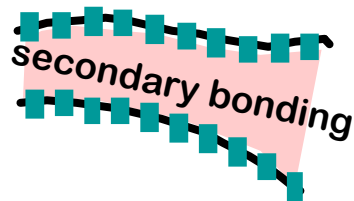
moderate T_m

moderate E

moderate α

Polymers

(Covalent & Secondary):



Directional Properties

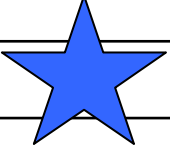
Secondary bonding dominates

small T

small E

large α

READING SCHEDULE

Reading Schedule		week	chapter
Introduction		0	-
	General Introduction Atomic Bonding	1	1 e 2
	Crystalline Structure; Imperfections	2	3 e 4
	Diffusion; Mechanical Properties	3	5 e 6
Strengthening Mechanisms; Failure		4	7 e 8
Phase Diagrams		5	9
Kinetics & Phase Transformations		6	10
Processing & Applications of Metals		7	11
Structure, Properties, Process and Applications of Ceramics		8	12 e 13
Structure, Properties, Process of Polymers and Composites		9	15 e 16
Corrosion; Electrical & Thermal Properties		10	17, 18 e 19
Magnetic & Optical Properties		11	20 e 21
Economic & Environmental Issues; Materials Selection		12	22

CALLISTER JR., WILLIAM D., Ciência e Engenharia dos Materiais: Uma Introdução, 1ª ed., Rio de Janeiro, LTC, 2002, ISBN: 85-216-2188-5

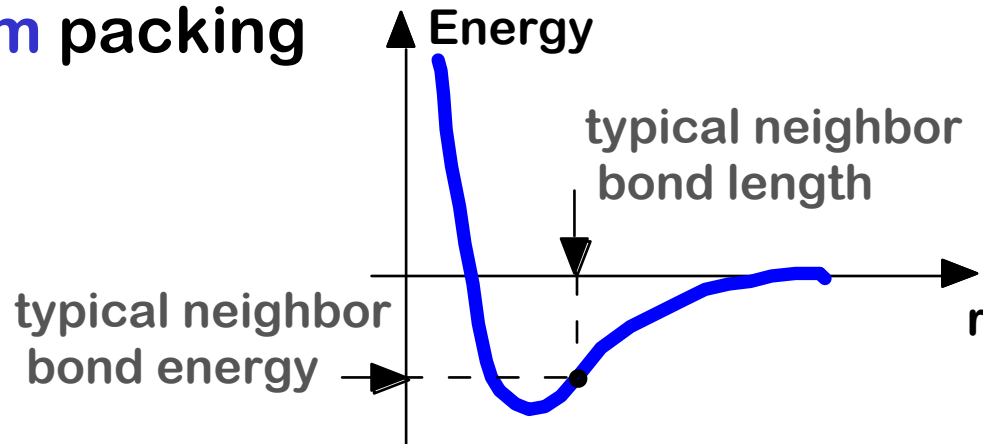
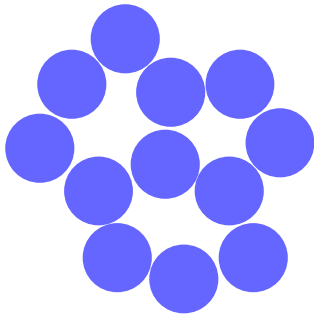
CHAPTER 3: CRYSTAL STRUCTURES & PROPERTIES

ISSUES TO ADDRESS...

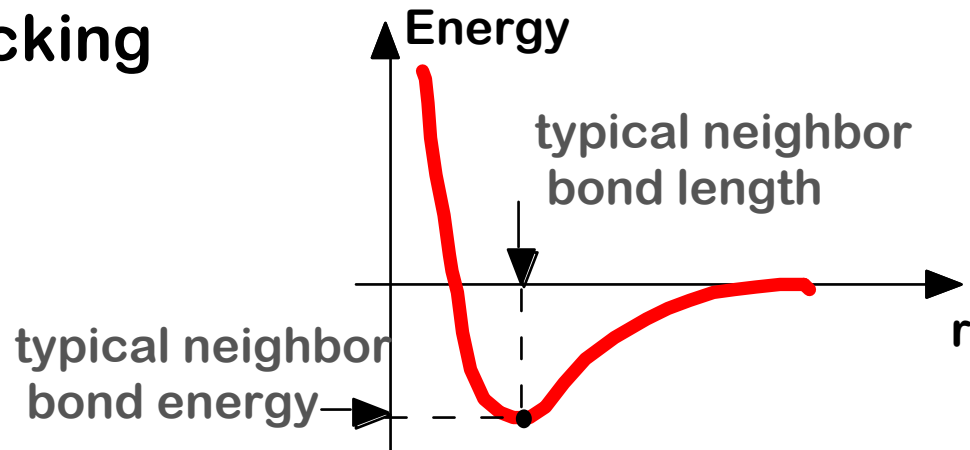
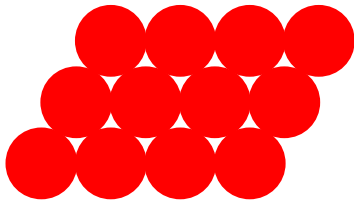
- How do atoms assemble into solid structures?
(for now, focus on metals)
- How does the density of a material depend on its structure?
- When do material properties vary with the sample (i.e., part) orientation?

ENERGY AND PACKING

- Non dense, **random** packing



- Dense, **regular** packing

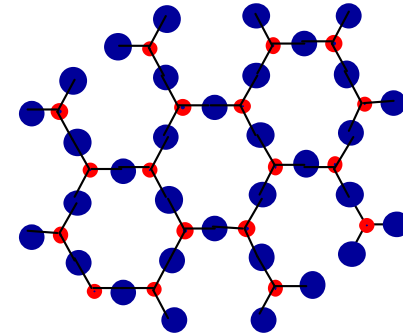


Dense, regular-packed structures tend to have lower energy.

MATERIALS AND PACKING

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
-many ceramics
-some polymers



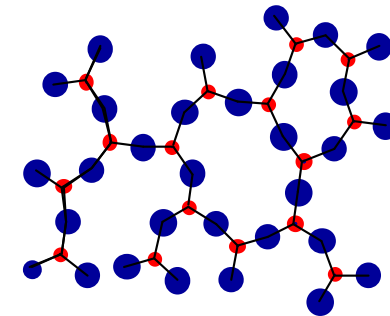
crystalline SiO₂

Adapted from Fig. 3.18(a),
Callister 6e.

• Si • Oxygen

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: -complex structures
-rapid cooling



noncrystalline SiO₂

Adapted from Fig. 3.18(b),
Callister 6e.

"Amorphous" = Noncrystalline

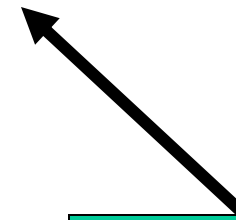
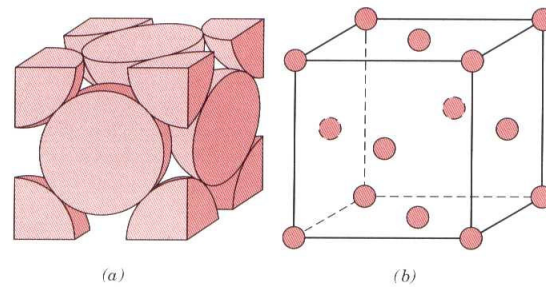
METALLIC CRYSTALS

- tend to be densely packed.
- have several reasons for dense packing:
 - Typically, only one element is present, so all atomic radii are the same.
 - Metallic bonding is not directional.
 - Nearest neighbor distances tend to be small in order to lower bond energy.
- have the simplest crystal structures.

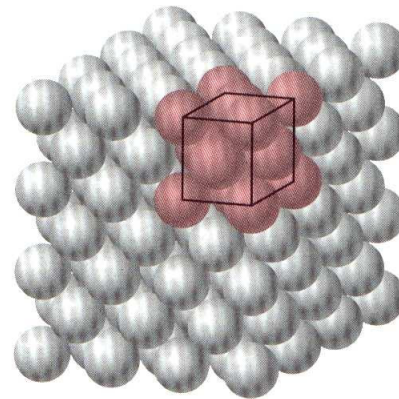
We will look at three such structures...

CÉLULA UNITÁRIA

(unidade básica repetitiva da estrutura tridimensional)



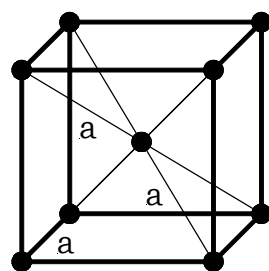
Célula Unitária



Os átomos são representados como esferas rígidas

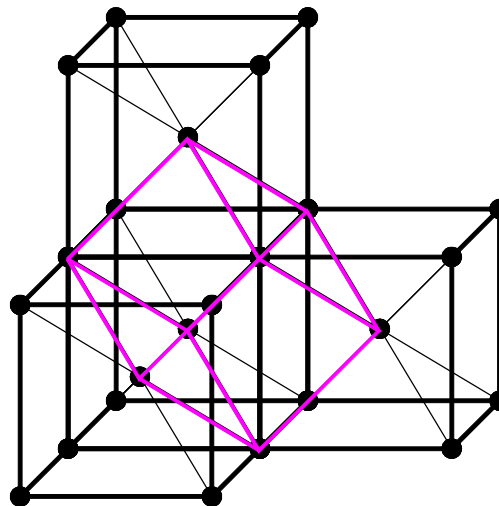
Unit Cell vs. Primitive Cell

A volume of space that when translated through all the vectors in a Bravais lattice just fills all of space without overlapping or leaving voids is called a *primitive cell* of the lattice. A primitive cell contains just one Bravais lattice point (recall that a crystal lattice is formed by placing one or more atoms at each Bravais lattice point). The primitive cell is the smallest cell that can be translated throughout space to completely recreate the entire lattice. There is not one unique shape to a primitive cell and many possible shapes fulfill the definition. The primitive cell for the simple cubic lattice is equal to the simple cubic unit cell (they are identical in shape). A common choice for the primitive cell of the body-centered cubic lattice is shown below.



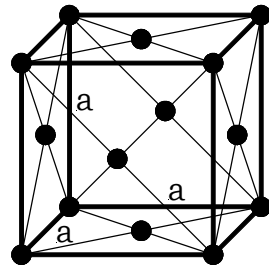
Body-Centered
Cubic (I)

Unit Cell



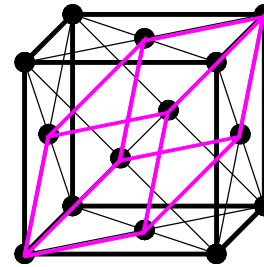
Primitive Cell (magenta)

Unit Cell vs. Primitive Cell

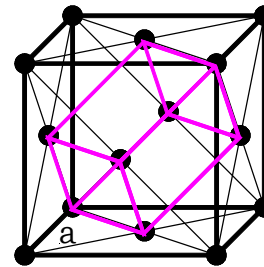


Face-Centered
Cubic (F)

Unit Cell



Primitive Cell



Rotated 90°

The primitive cell is smaller or equal in size to the unit cell. The unit cells help to remind us of the symmetry (ie. Cubic).

Bravais Lattice

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$$

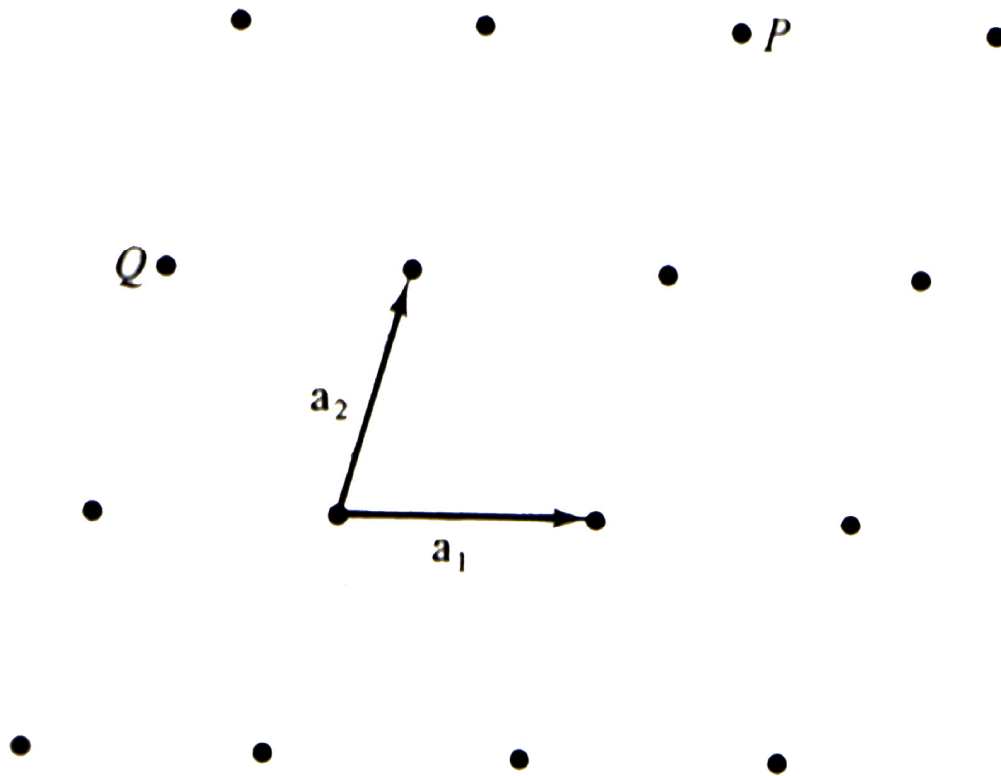


FIGURE A general two-dimensional Bravais lattice of no particular symmetry: the oblique net. Primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are shown. All points in the net are linear combinations of these with integral coefficients; for example, $\mathbf{P} = \mathbf{a}_1 + \mathbf{a}_2$, and $\mathbf{Q} = -\mathbf{a}_1 + \mathbf{a}_2$. (Ashcroft, Neil W. *Solid state physics*.)

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

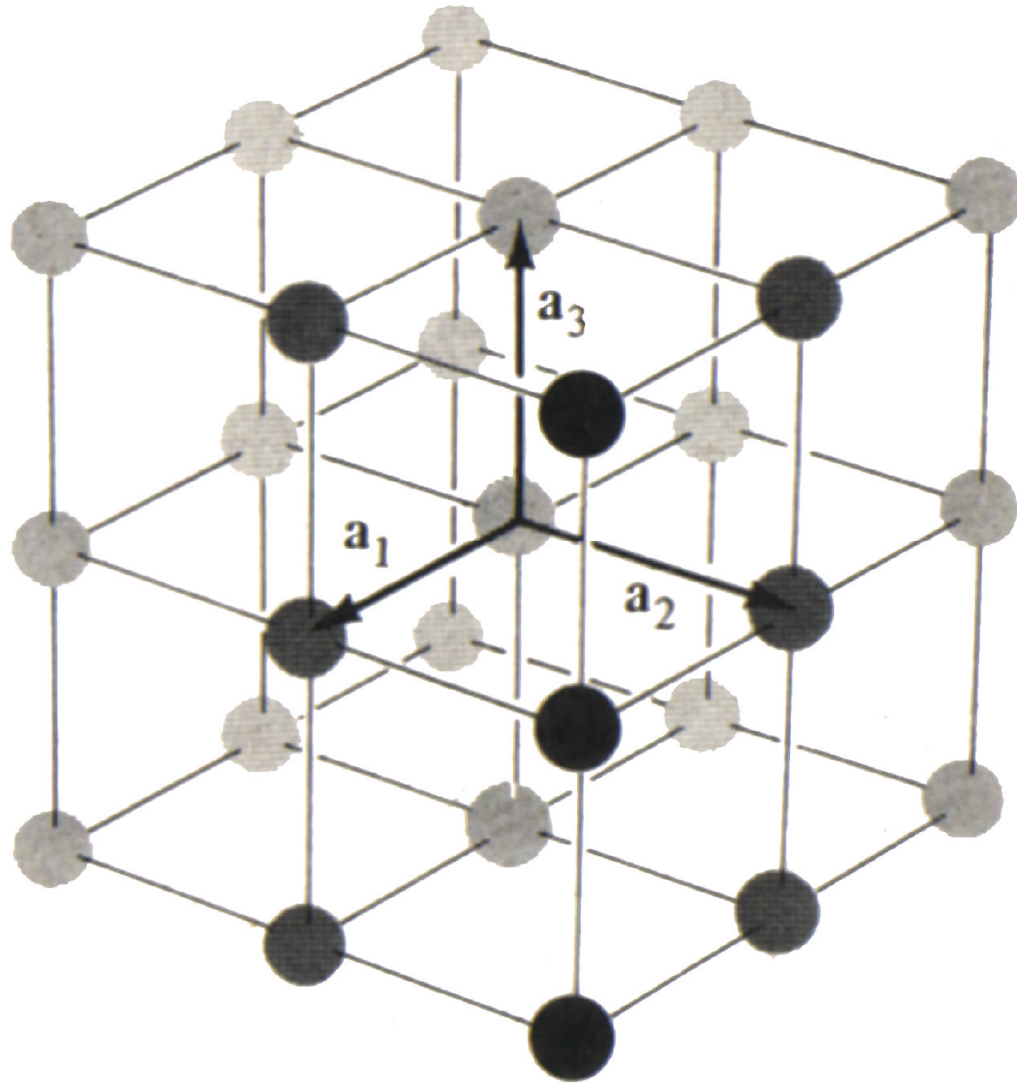


FIGURE A simple cubic three-dimensional Bravais lattice. The three primitive vectors can be taken to be mutually perpendicular, and with a common magnitude. (Ashcroft, Neil W. *Solid state physics*.)

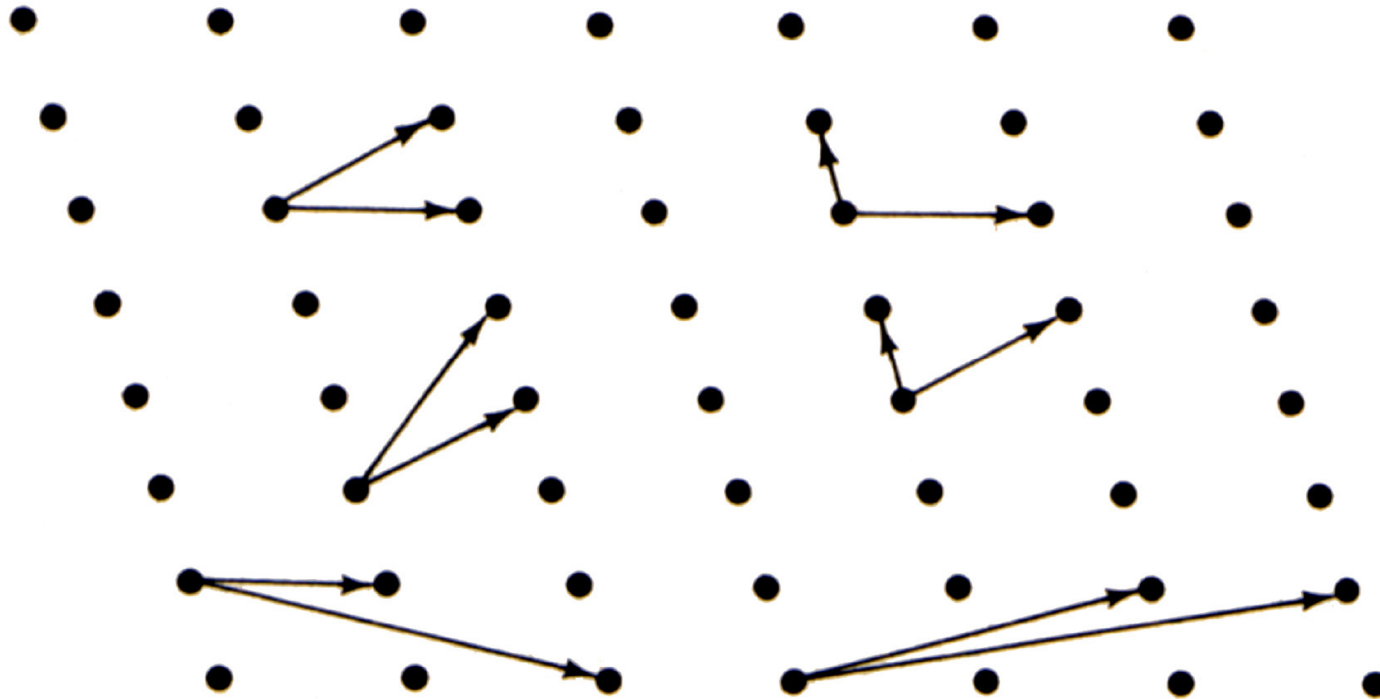


FIGURE Several possible choices of pairs of primitive vectors for a two-dimensional Bravais lattice. They are drawn, for clarity, from different origins. (Ashcroft, Neil W. *Solid state physics*.)

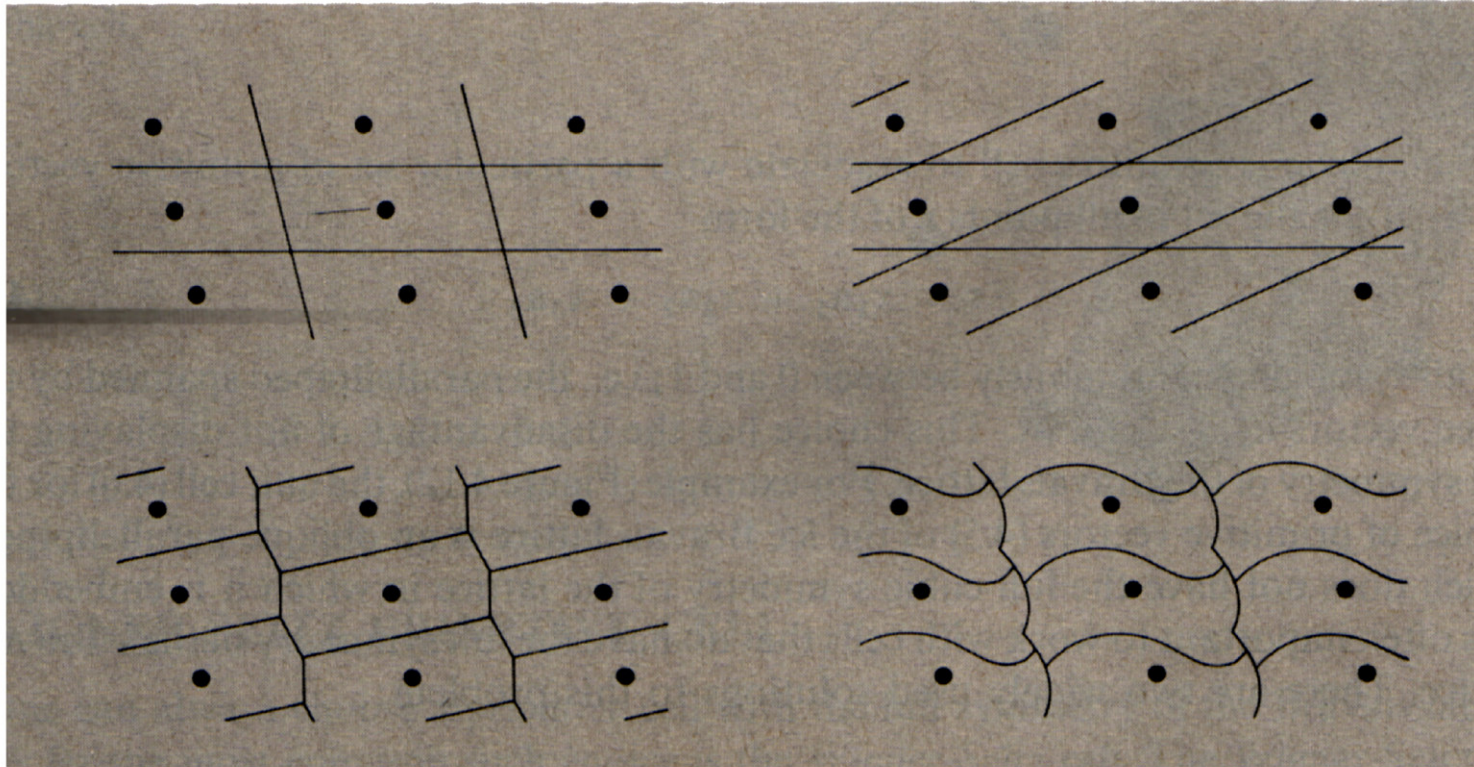
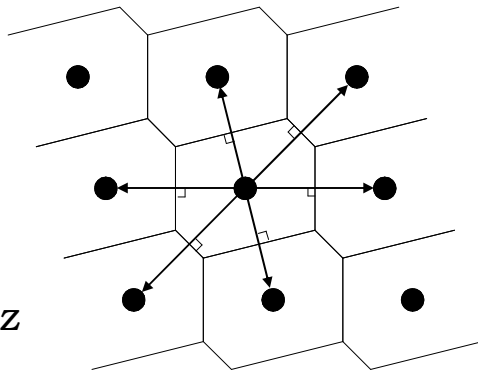
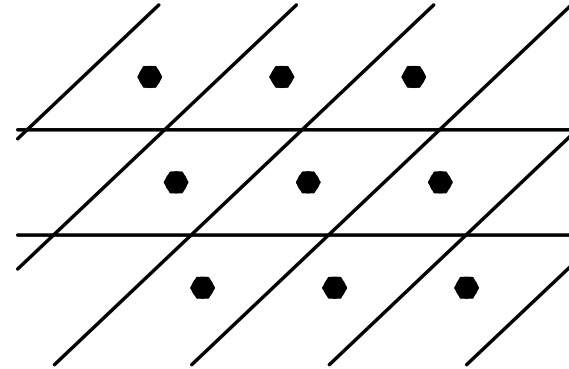
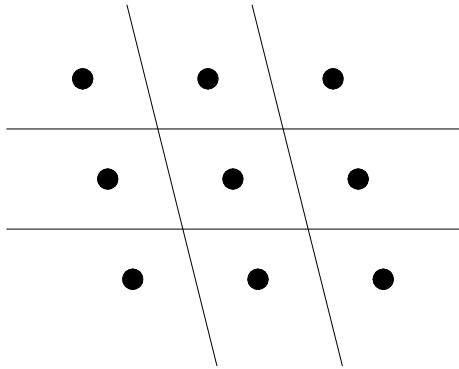


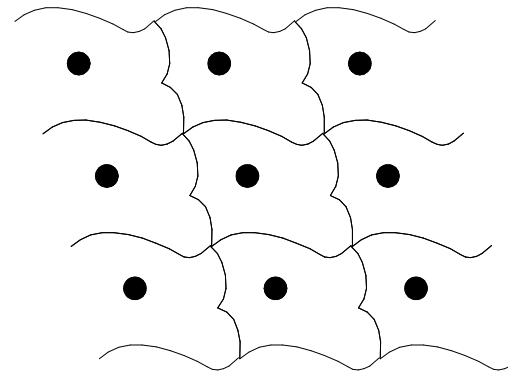
FIGURE Several possible choices of primitive cell for a single two-dimensional Bravais lattice. (Ashcroft, Neil W. *Solid state physics*.)

CÉLULA PRIMITIVA

Two Dimensional Lattice



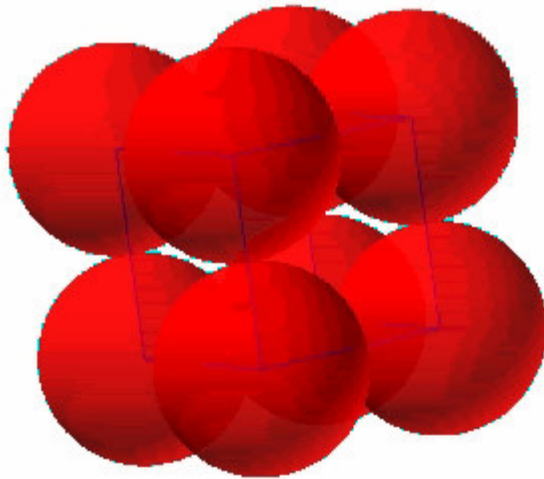
Wigner-Seitz



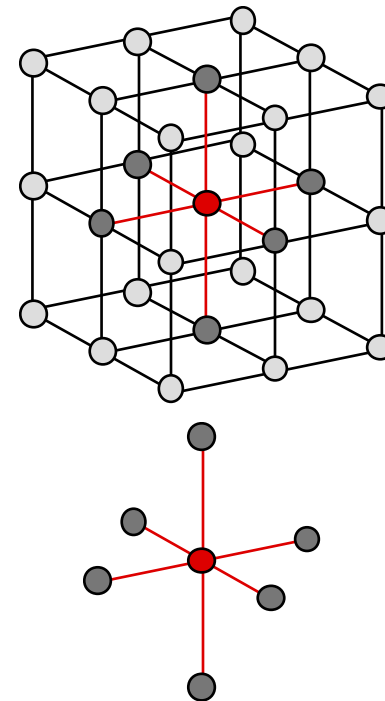
Possible choices of primitive cell for a single 2D Bravais lattice.

SIMPLE CUBIC STRUCTURE (SC)

- Rare due to poor packing (only Po has this structure)
- **Close-packed directions** are cube edges.
- **Coordination # = 6**
(# nearest neighbors)



(Courtesy P.M. Anderson)

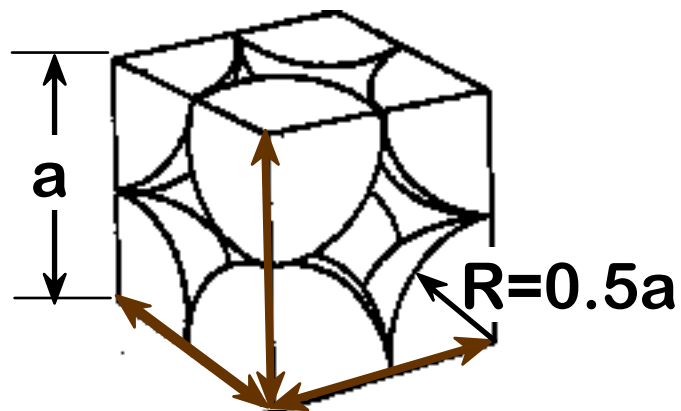


ATOMIC PACKING FACTOR

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

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains $8 \times 1/8 =$

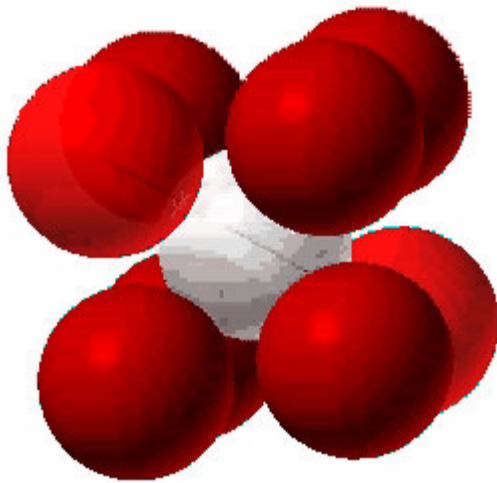
1 atom/unit cell

Adapted from Fig. 3.19,
Callister 6e.

$$APF = \frac{\overbrace{1}^{\text{atoms}} \overbrace{\frac{4}{3} \pi (0.5a)^3}^{\text{volume atom}}}{\underbrace{a^3}_{\text{volume unit cell}}}$$

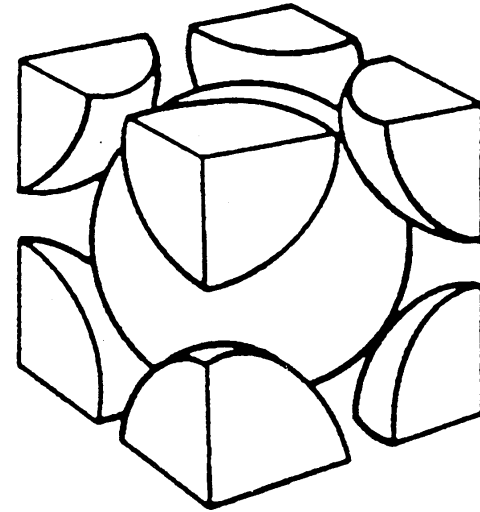
BODY CENTERED CUBIC STRUCTURE (BCC)

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

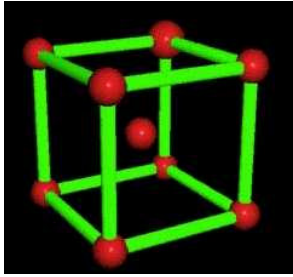


(Courtesy P.M. Anderson)

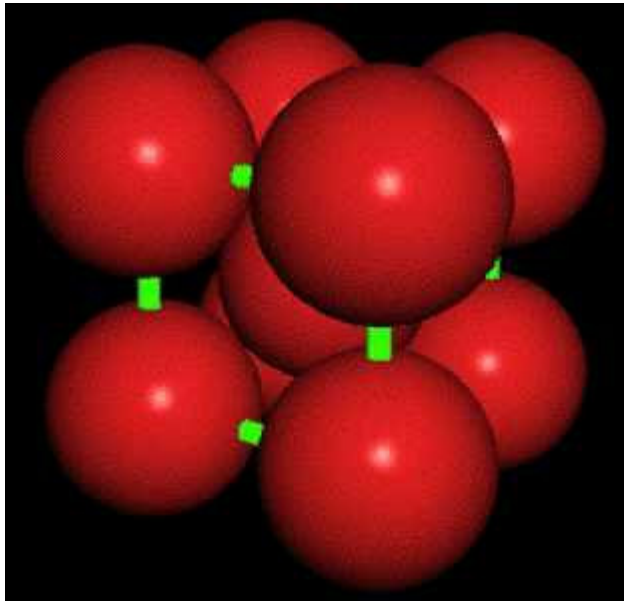
- Coordination # = 8



Adapted from Fig. 3.2,
Callister 6e.



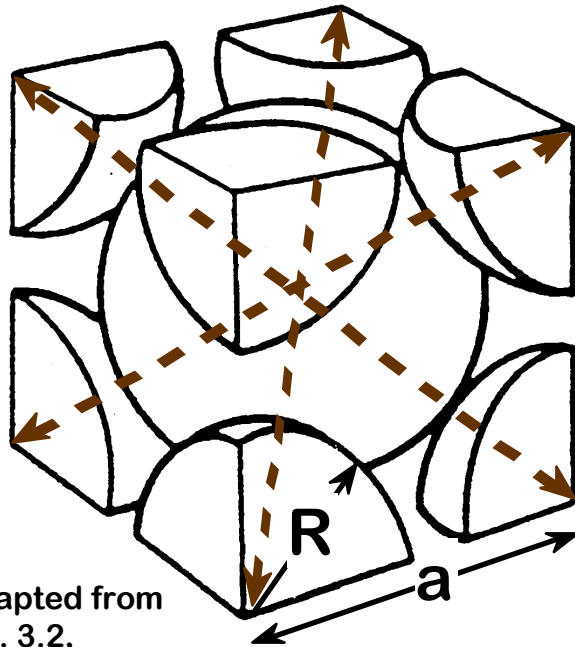
EST. CÚBICA DE CORPO CENTRADO



- Na est. ccc cada átomo dos vertices do cubo é dividido com 8 células unitárias
- Já o átomo do centro pertence somente a sua célula unitária.
- Cada átomo de uma estrutura ccc é cercado por 8 átomos adjacentes
- Há 2 átomos por célula unitária na estrutura ccc
- O Fe, Cr, W cristalizam em ccc

ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



Adapted from
Fig. 3.2,
Callister 6e.

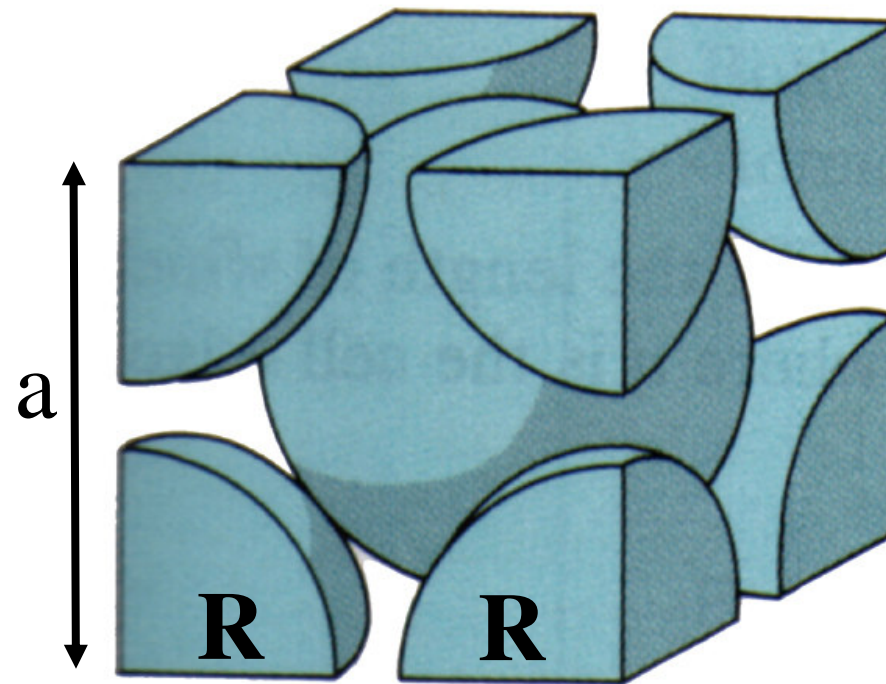
Close-packed directions:
length = $4R$
 $= \sqrt{3} a$

Unit cell contains:
 $1 + 8 \times 1/8$
 $= 2 \text{ atoms/unit cell}$

$$\text{APF} = \frac{\text{atoms/unit cell} \times \text{volume/atom}}{\text{volume/unit cell}}$$

$$\text{APF} = \frac{2 \times \frac{4}{3} \pi (\sqrt{3}a/4)^3}{a^3}$$

- Calcule a densidade linear de uma BCC na direcao [100]
- $a = 4R/\sqrt{3}$
- $LD = L_C/L_I = 2R/(4R/\sqrt{3}) = 0.866$



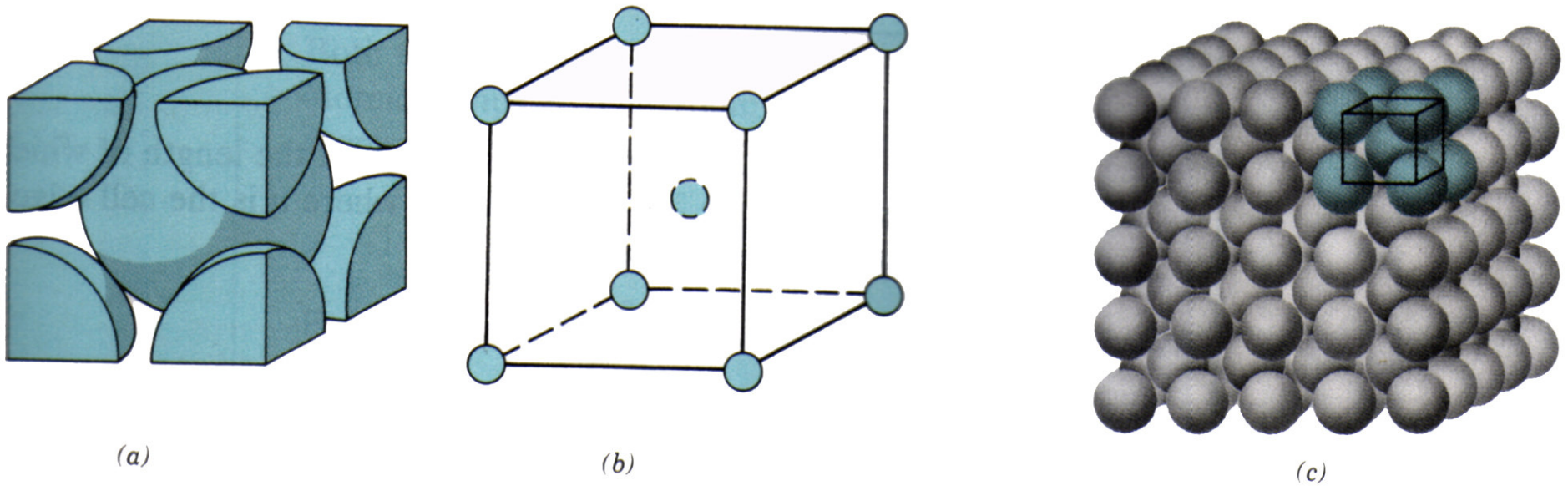


FIGURE 3.2 For the body-centered cubic crystal structure, (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. (William D. Callister, JR. *Materials Science and Engineering an Introduction*, John Wiley & Sons, Inc.)

Body-centered cubic Bravais lattice

Primitive vectors

$$\mathbf{a}_1 = a\hat{x}, \quad \mathbf{a}_2 = a\hat{y}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \quad (4.3)$$

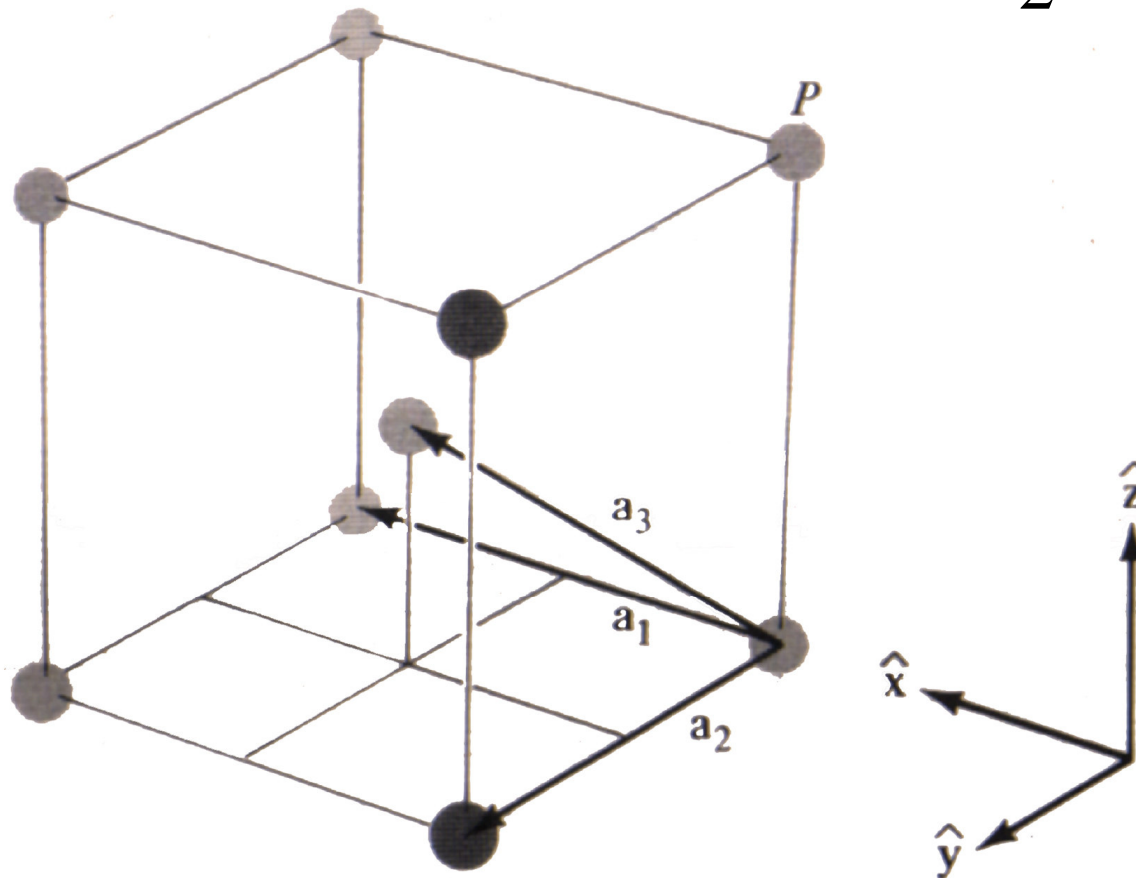


FIGURE Three primitive vectors, specified in Eq. (4.3), for the body-centered cubic Bravais lattice. The lattice is formed by taking all linear combinations of the primitive vectors with integral coefficients. The point P, for example, is $\mathbf{P} = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3$. (Ashcroft, Neil W. *Solid state physics*.)

Body-centered cubic Bravais lattice

Primitive vectors

$$\mathbf{a}_1 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \quad (4.4)$$

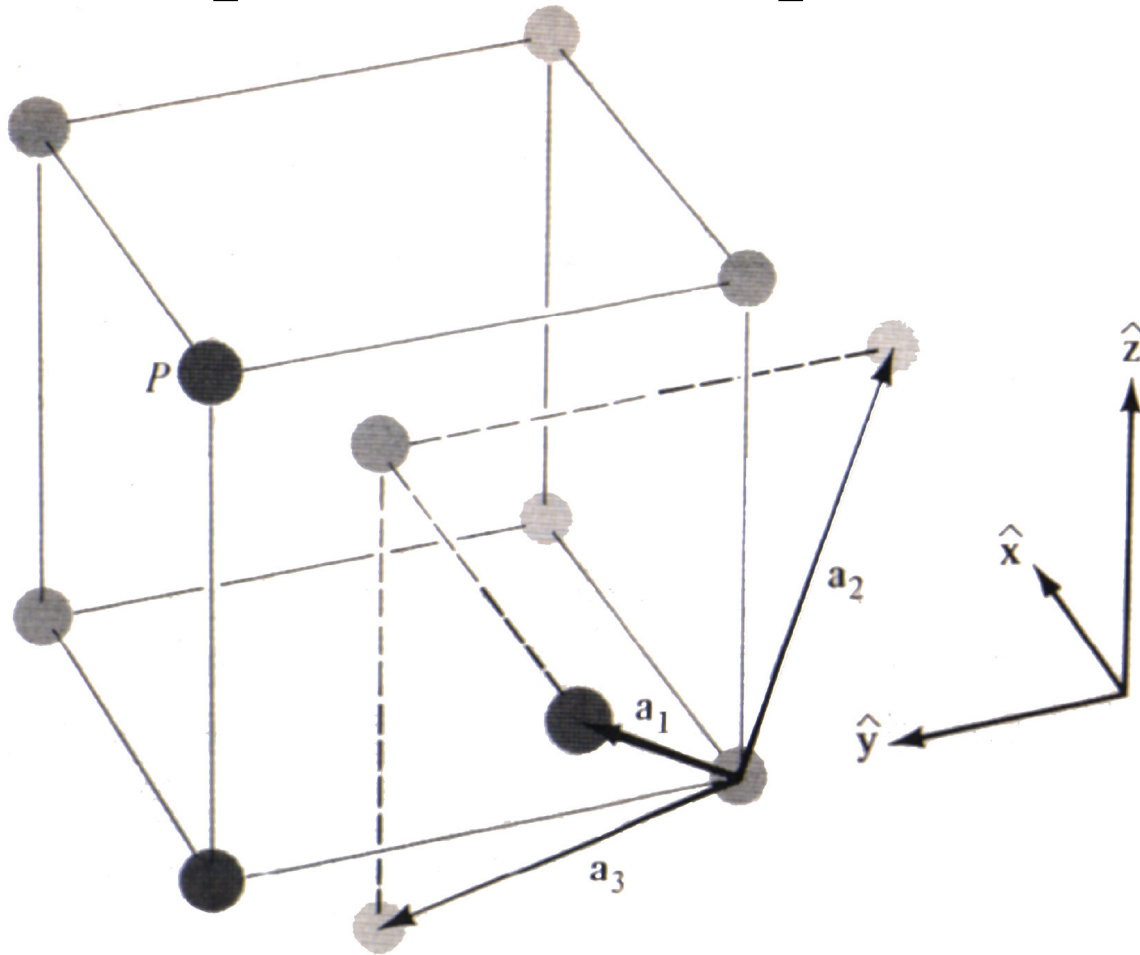
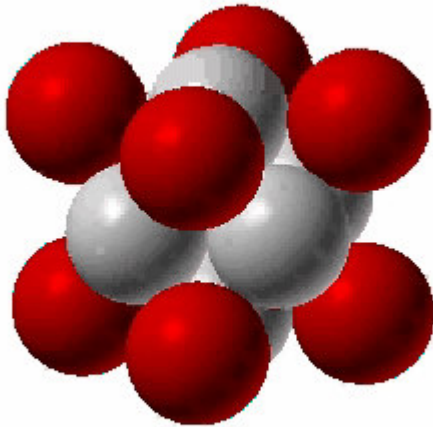


FIGURE A more symmetric set of primitive vectors, specified in Eq. (4.4), for the body-centered cubic Bravais lattice. The point P , for example, has the form $P = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$. (Ashcroft, Neil W. *Solid state physics*.)

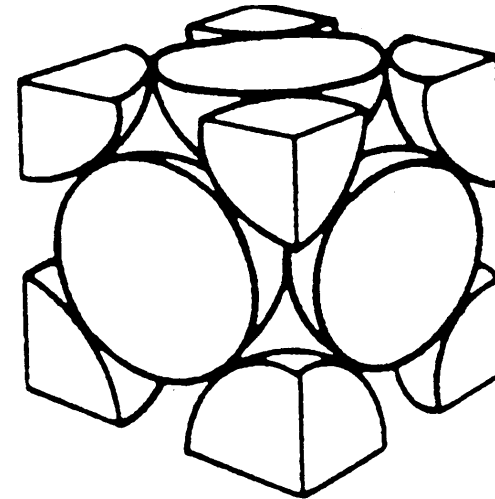
FACE CENTERED CUBIC STRUCTURE (FCC)

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

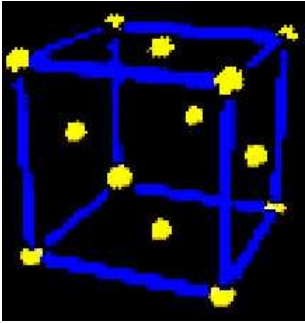
- **Coordination # = 12**



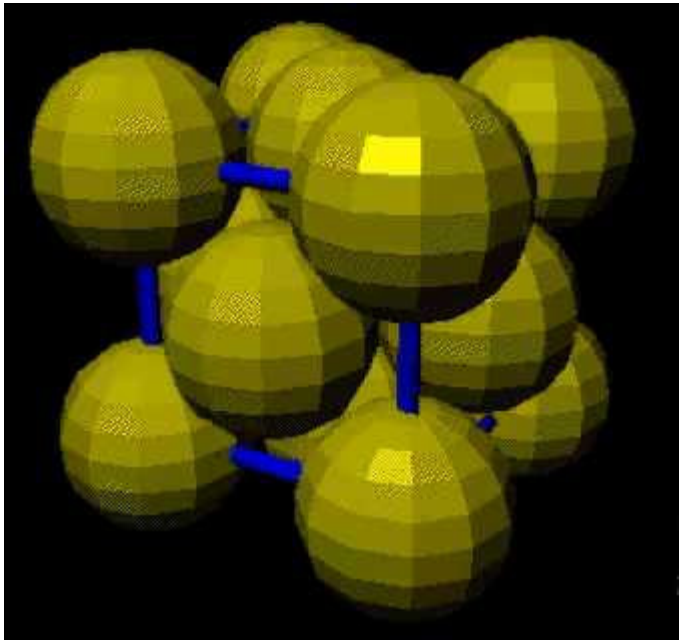
(Courtesy P.M. Anderson)



Adapted from Fig. 3.1(a),
Callister 6e.

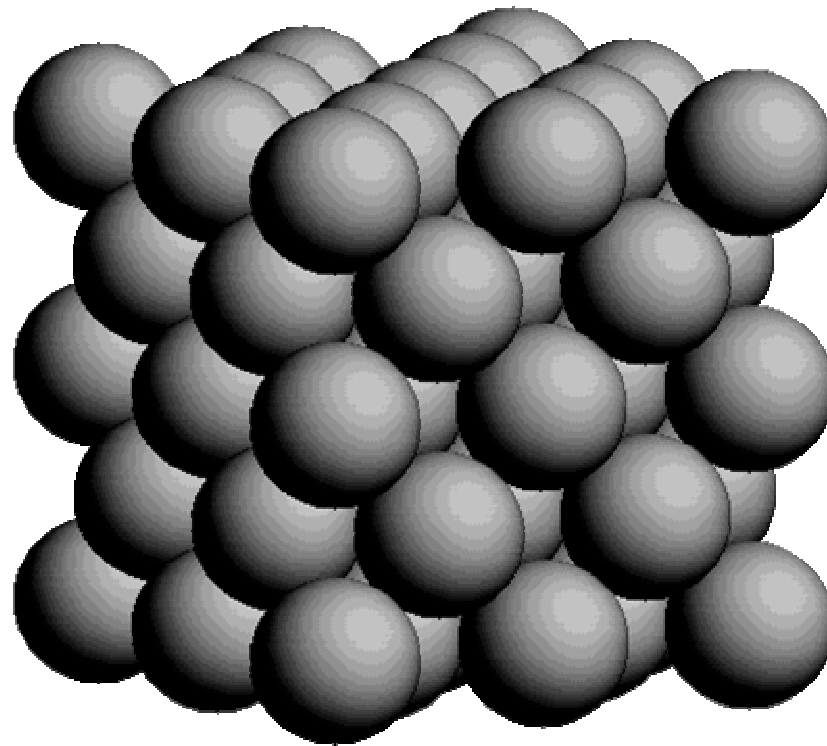


EST. CÚBICA DE FACE CENTRADA



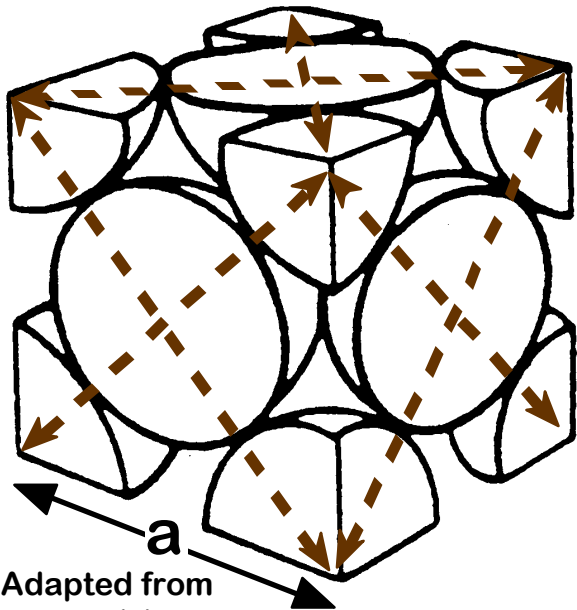
- Na est. cfc cada átomo dos vertices do cubo é dividido com 8 células unitárias
- Já os átomos das faces pertencem somente a duas células unitárias
- Há 4 átomos por célula unitária na estrutura cfc
- É o sistema mais comum encontrado nos metais (Al, Fe, Cu, Pb, Ag, Ni,...)

Face Centered Cubic Lattice (111) Hard Sphere Model



ATOMIC PACKING FACTOR: FCC

- APF for a body-centered cubic structure = 0.74

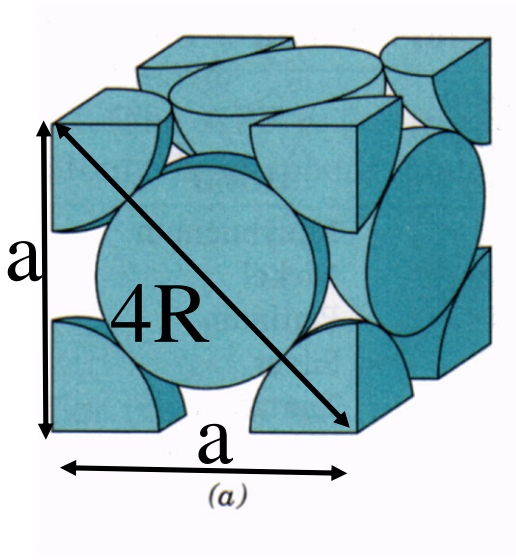


Adapted from
Fig. 3.1(a),
Callister 6e.

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

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

$$\text{APF} = \frac{\overbrace{4}^{\text{atoms}} \overbrace{\frac{4}{3} \pi (\sqrt{2}a/4)^3}^{\text{volume atom}}}{\underbrace{a^3}_{\text{volume unit cell}}}$$



$$APF = \frac{\text{Volume Total da Esfera } (V_s)}{\text{Volume Total da Celula Unitaria } (V_c)}$$

$$V_s = 4 \frac{4}{3} \pi R^3$$

$$V_c = 16R^3 \sqrt{2}$$

$$APF = 0.74$$

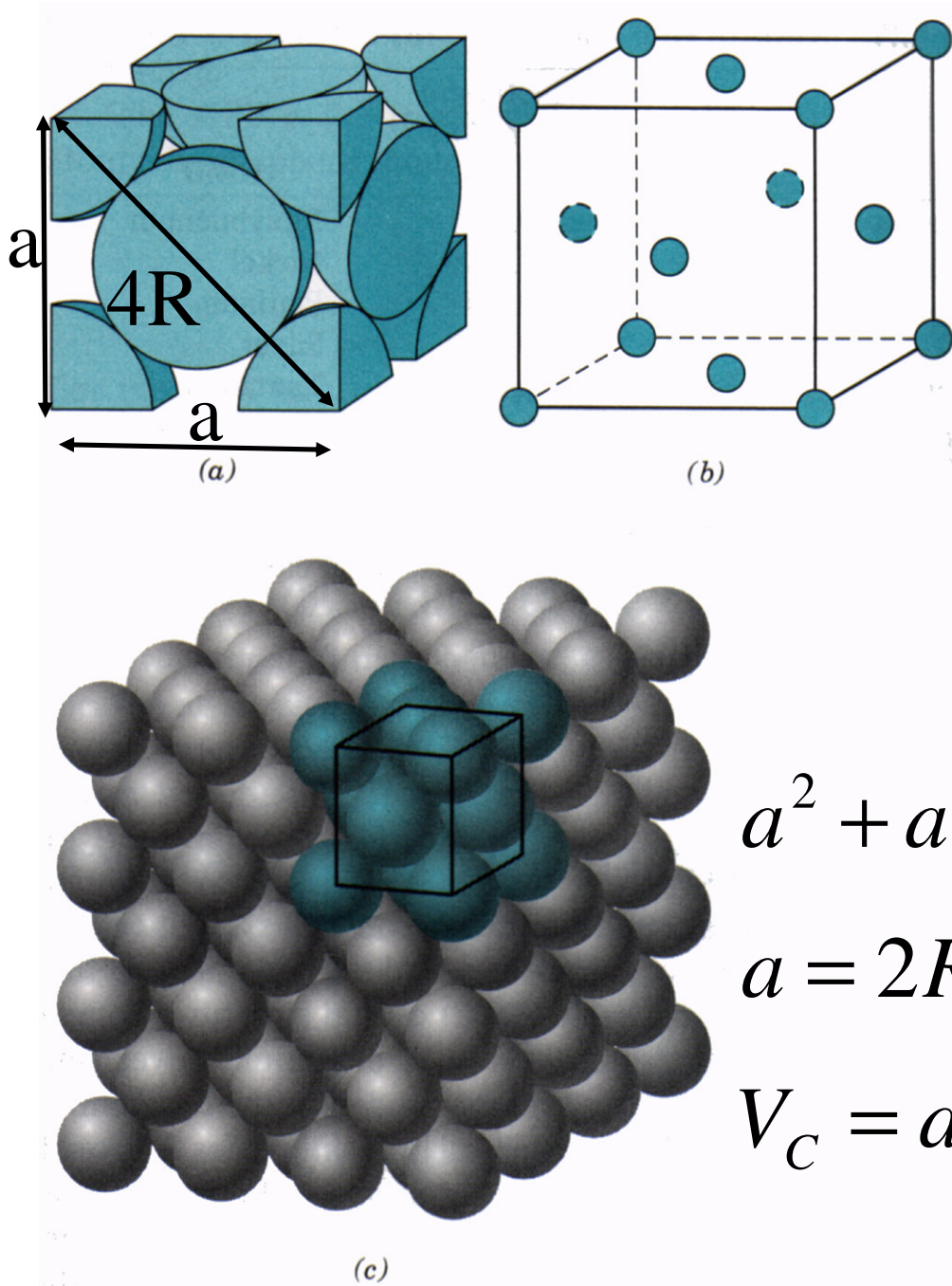


FIGURE 3.1 For the face-centered cubic crystal structure: (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. (William D. Callister, JR. *Materials Science and Engineering an Introduction*, John Wiley & Sons, Inc.)

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

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

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

Face-centered cubic Bravais lattice

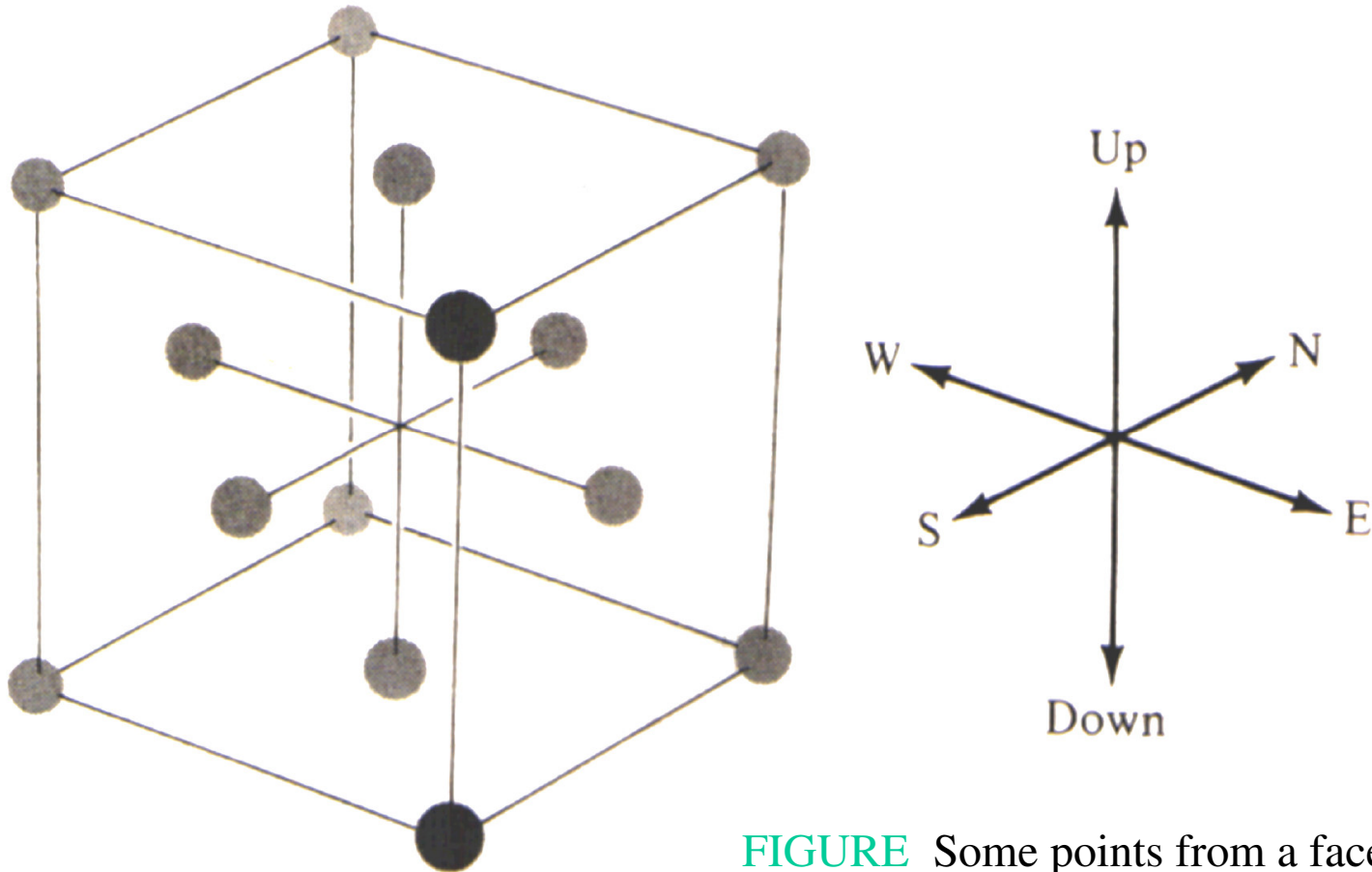


FIGURE Some points from a face-centered cubic Bravais lattice.
(Ashcroft, Neil W. *Solid state physics*.)

Face-centered cubic Bravais lattice

Primitive vectors

$$\mathbf{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{x} + \hat{z}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}). \quad (4.5)$$

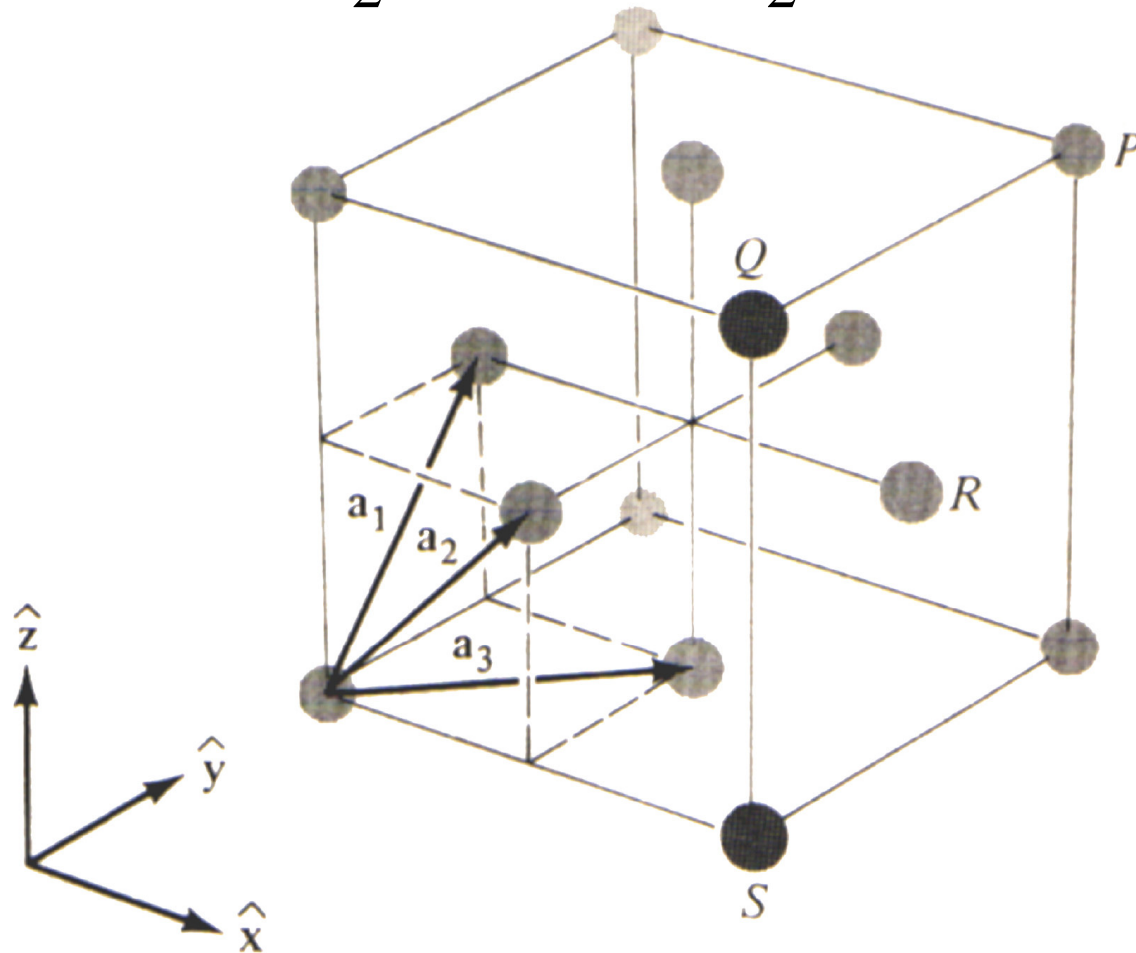


FIGURE A set of primitive vectors, as given in Eq. (4.5), for the face-centered cubic Bravais lattice. The labeled points are $\mathbf{P} = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$, $\mathbf{Q} = 2\mathbf{a}_2$, $\mathbf{R} = \mathbf{a}_2 + \mathbf{a}_3$, and $\mathbf{S} = -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$. (Ashcroft, Neil W. *Solid state physics*.)

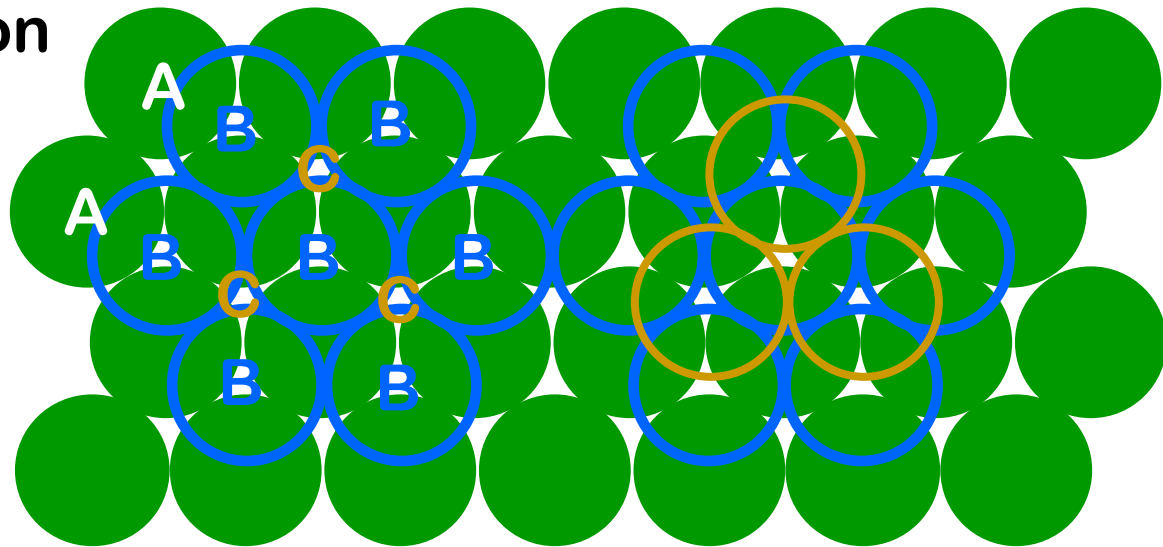
FCC STACKING SEQUENCE

- ABCABC... Stacking Sequence
- 2D Projection

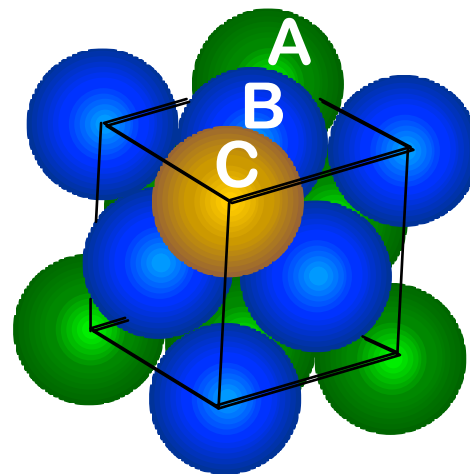
A sites

B sites

C sites

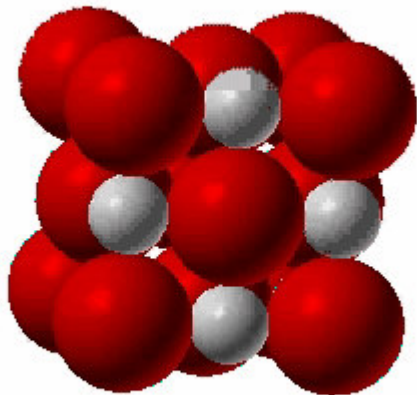


- FCC Unit Cell

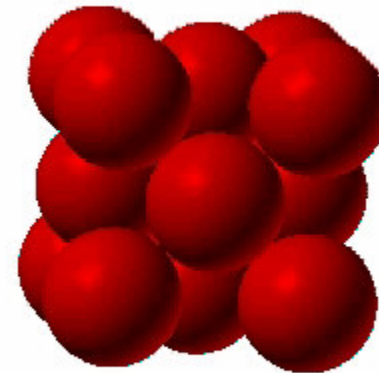


STRUCTURE OF COMPOUNDS: NaCl

- Compounds: Often have similar close-packed structures.
- Structure of NaCl
 - Close-packed directions
--along cube edges.



(Courtesy P.M. Anderson)



(Courtesy P.M. Anderson)

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

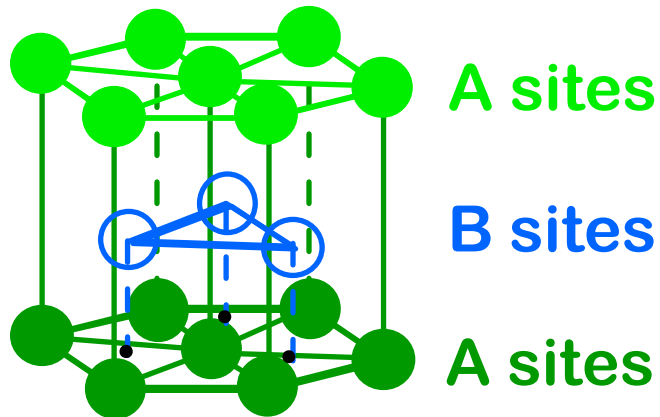
ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

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)		

- Materiais metálicos não cristalizam com a estrutura hexagonal simples!
- Eles preferem a hexagonal compacta (HCP). Nessa estrutura o cristal fica no estado de mais baixa energia.
- Fator de empacotamento da FCC = 0,74

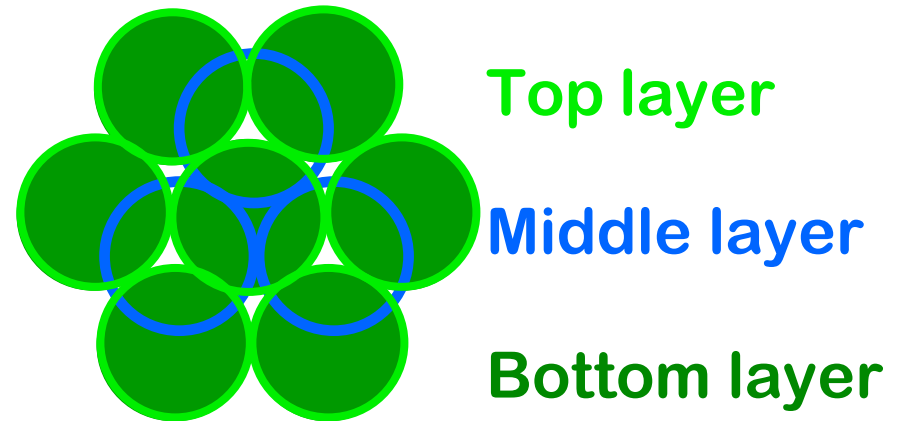
HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3,
Callister 6e.

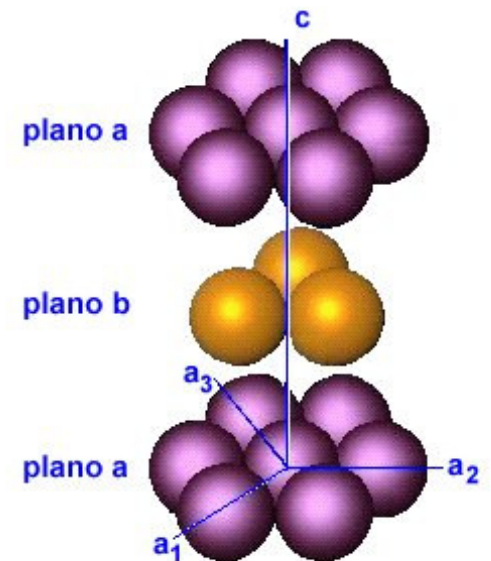
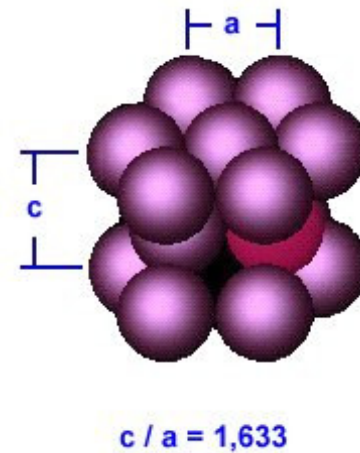
- 2D Projection



- Coordination # = 12
- APF = 0.74

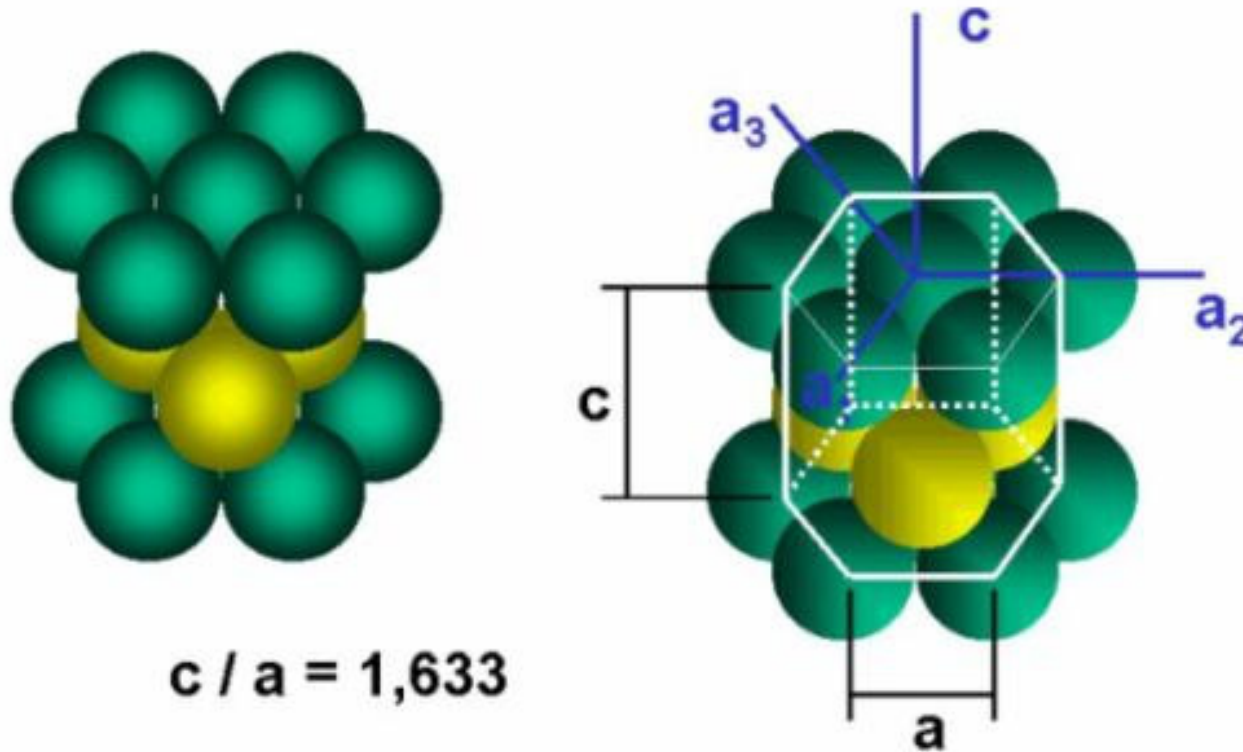
EST. HEXAGONAL COMPACTA

- Cada átomo tangencia 3 átomos da camada de cima, 6 átomos no seu próprio plano e 3 na camada de baixo do seu plano
- O número de coordenação para a estrutura HC é 12 e, portanto, o fator de empacotamento é o mesmo da cfc, ou seja, 0,74.



Relação entre R e a :
 $a = 2R$

EST. HEXAGONAL COMPACTA



Há 2 parâmetros de rede representando os parâmetros
Basais (a) e de altura (c)

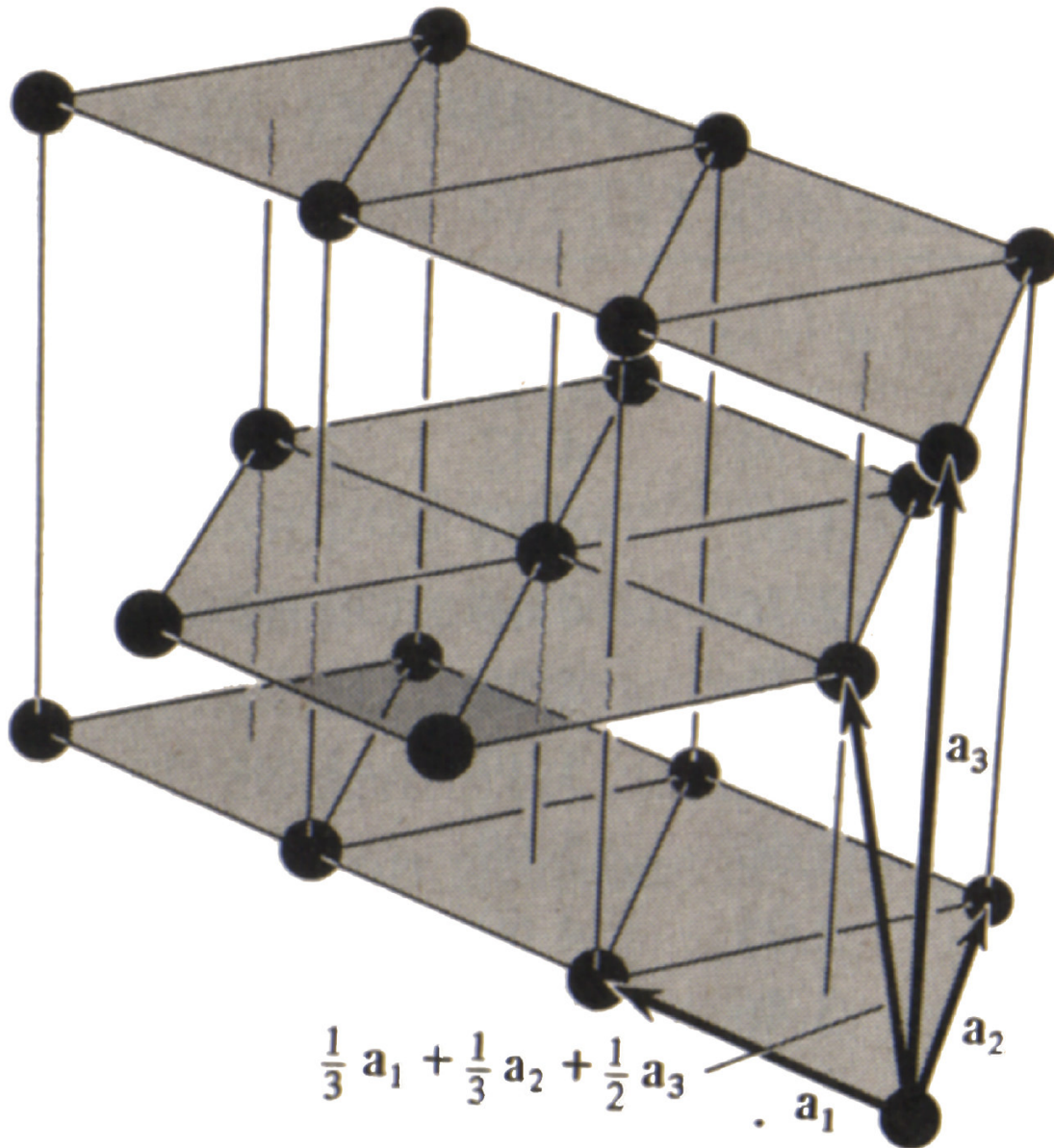
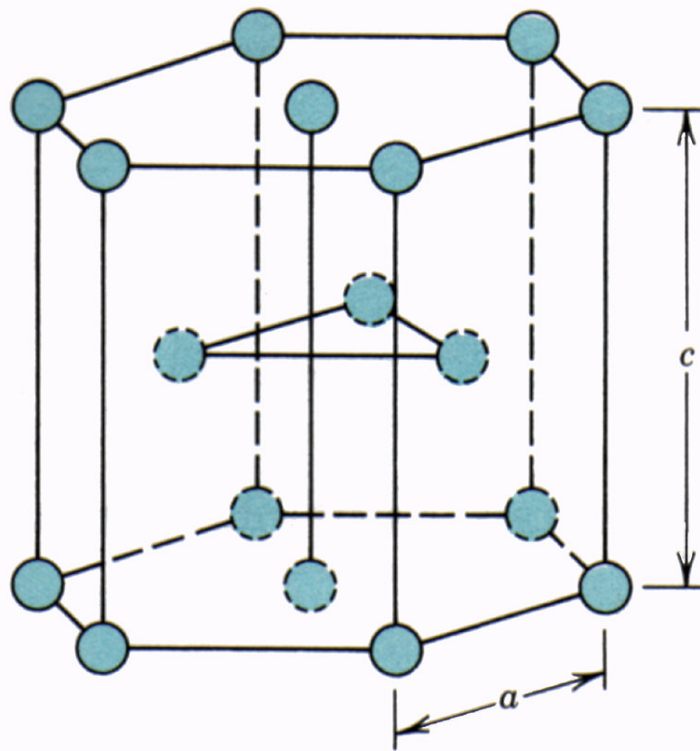
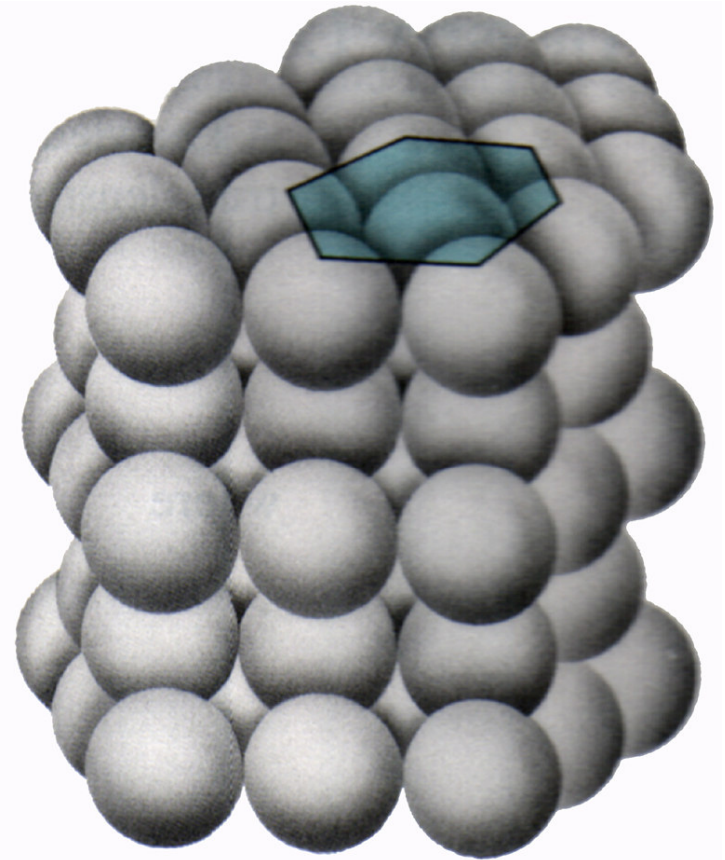


FIGURE The hexagonal close-packed crystal structure. It can be viewed as two interpenetrating simple hexagonal Bravais lattices, displaced vertically by a distance $c/2$ along the common c -axis, and displaced horizontally so that the points of one lie directly above the centers of the triangles formed by the points of the others. (Ashcroft, Neil W. *Solid state physics*.)



(a)



(b)

FIGURE 3.3 For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell (a and c represent the short and long edge lengths, respectively) and (b) an aggregate of many atoms. (William D. Callister, JR. *Materials Science and Engineering an Introduction*, John Wiley & Sons, Inc.)

OS 7 SISTEMAS CRISTALINOS

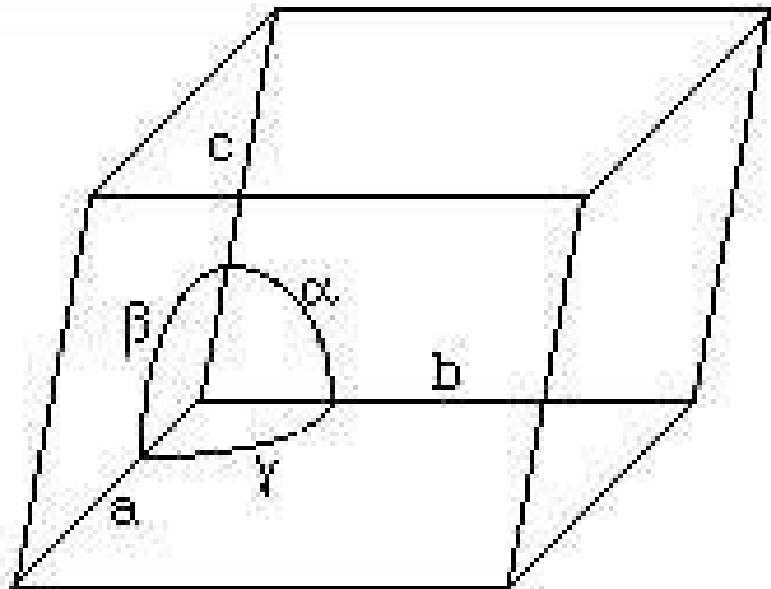
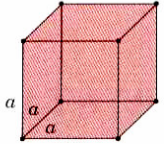
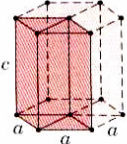
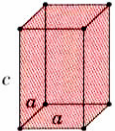
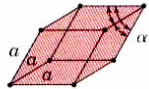
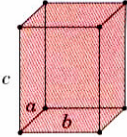
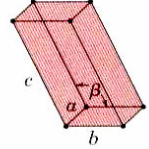
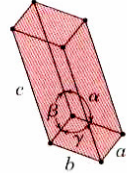
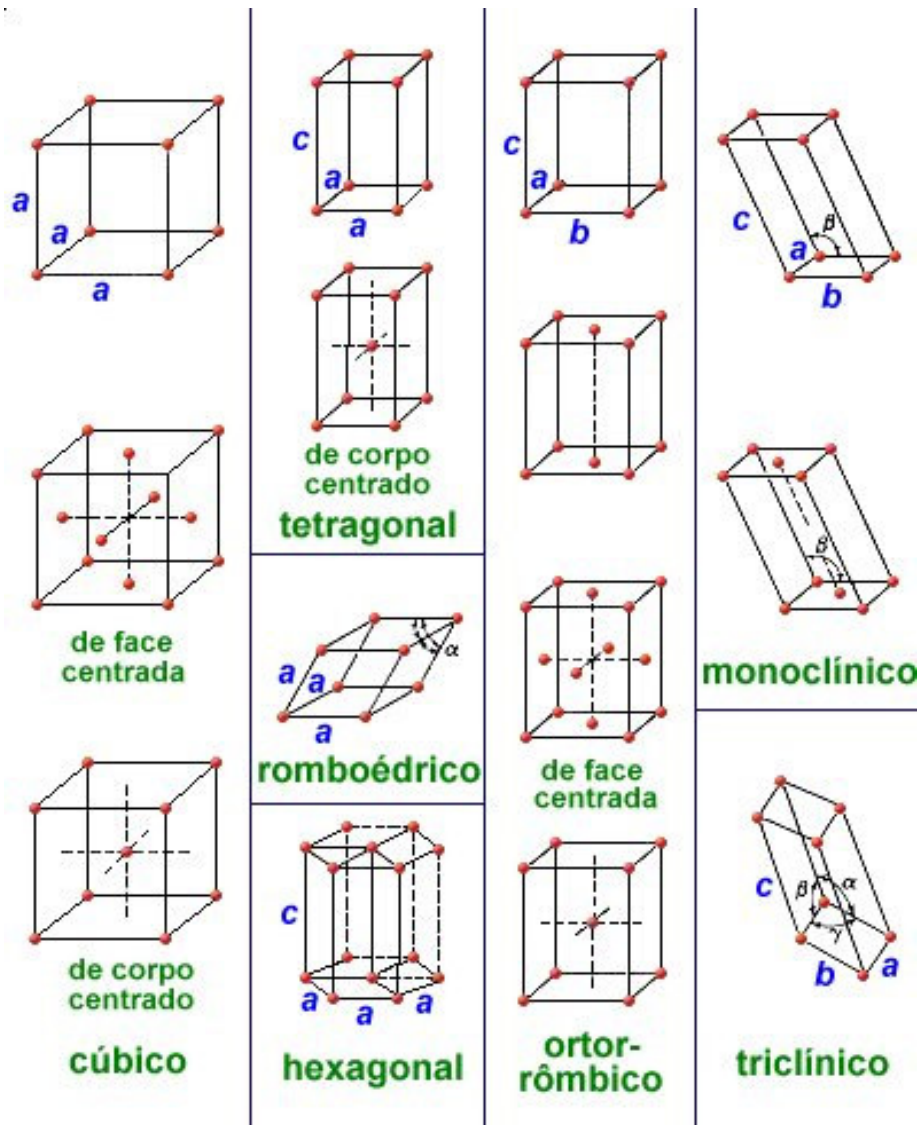


Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

<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	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

AS 14 REDES DE BRAVAIS



Dos 7 sistemas cristalinos podemos identificar 14 tipos diferentes de células unitárias, conhecidas com redes de Bravais. Cada uma destas células unitárias tem certas características que ajudam a diferenciá-las das outras células unitárias. Além do mais, estas características também auxiliam na definição das propriedades de um material particular.

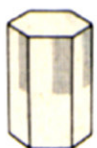
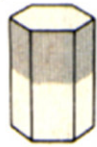
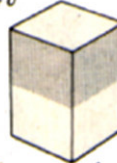
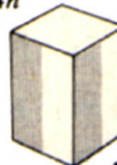
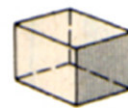
Characteristics of Selected Elements at 20C

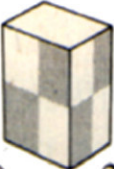
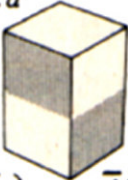
Element	Symbol	At. Weight (amu)	Density (g/cm ³)	Crystal Structure	Atomic radius (nm)	Adapted from Table, "Charac- teristics of Selected Elements", inside front cover, <i>Callister 6e.</i>
Aluminum	Al	26.98	2.71	FCC	0.143	
Argon	Ar	39.95	-----	-----	-----	
Barium	Ba	137.33	3.5	BCC	0.217	
Beryllium	Be	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	-----	-----	-----	

POINT AND SPACE GROUPS OF BRAVAIS LATTICES AND CRYSTAL STRUCTURES

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

THE NONCUBIC CRYSTALLOGRAPHIC POINT GROUPS^a

SCHOENFLIES	HEXAGONAL	TETRAGONAL	TRIGONAL	ORTHO-RHOMBIC	MONOCLINIC	TRICLINIC	INTER-NATIONAL
C_n	C_6  6	C_4  4	C_3  3		C_2  2	C_1  1	n
C_{nv}	C_{6v}  $6mm$	C_{4v}  $4mm$	C_{3v}  $3m$	C_{2v}  $2mm$			nm (n even) nm (n odd)
C_{nh}	C_{6h}  $6/m$	C_{4h}  $4/m$			C_{2h}  $2/m$		n/m
	C_{3h}  $\bar{6}$				C_{1h} ($\bar{2}$)  m		$\bar{n}$
S_n		S_4  $\bar{4}$	S_6  (C_{3i}) $\bar{3}$			S_2  (C_i) $\bar{1}$	

D_n	D_6  622	D_4  422	D_3  32	D_2  (V) 222			$n2\mathcal{C}$ (n even) $n2$ (n odd)
D_{nh}	D_{6h}  6/mmm	D_{4h}  4/mmm		D_{2h} (mmm)  (V _h) 2/mmm			$\frac{n}{m} \frac{2}{m} \frac{2}{m}$ (n/mmm)
	D_{3h}  $\bar{6}2m$						$\bar{n}2m$ (n even) $\bar{n} \frac{2}{m}$ (n odd)
D_{nd}		D_{2d}  (V _d) $\bar{4}2m$	D_{3d} ($\bar{3}m$)  $\bar{3} \frac{2}{m}$				

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

ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

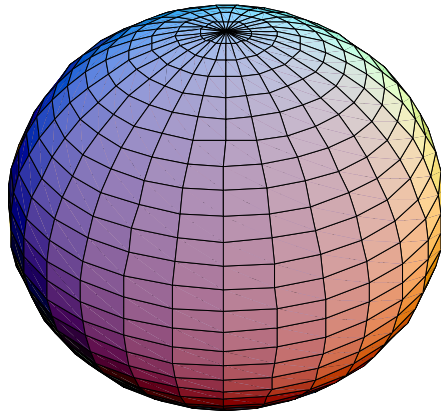
ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

SOME COMPOUNDS WITH THE ZINCBLLENDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
CuF	4.26	ZnS	5.41	AlSb	6.13
CuCl	5.41	ZnSe	5.67	GaP	5.45
CuBr	5.69	ZnTe	6.09	GaAs	5.65
CuI	6.04	CdS	5.82	GaSb	6.12
AgI	6.47	CdTe	6.48	InP	5.87
BeS	4.85	HgS	5.85	InAs	6.04
BeSe	5.07	HgSe	6.08	InSb	6.48
BeTe	5.54	HgTe	6.43	SiC	4.35
MnS (red)	5.60	AlP	5.45		
MnSe	5.82	AlAs	5.62		

Dream: Atom by Atom Engineering

H																			He					
Li	Be																		B	C	N	O	F	Ne
Na	Mg																		Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr							
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe							
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn							
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub													
		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								



$$V = \frac{4\pi}{3} R^3$$

$$S = 4\pi R^2$$

$$\frac{S}{V} = \frac{3}{R}$$

Há muito espaço lá embaixo

- Uma esfera de ferro, de um kilograma de massa, possui um raio de cerca de 31 milímetros.
- A mesma massa de Fe pode ser distribuída em trinta mil esferas de 1 mm de raio, com uma superfície total de 0,38 m².
- Ou ainda, em trinta mil bilhões de esferas de 1 μm de raio, com uma superfície total de 380 m².
- Ou ainda, em trinta mil bilhões de bilhões de esferas de 1 nm de raio, com uma superfície total de 380.000

THEORETICAL DENSITY, ρ

$$\rho = \frac{n A}{V_c N_A}$$

atoms/unit cell $\rightarrow$ n Atomic weight (g/mol) $\rightarrow$ A

Volume/unit cell
(cm³/unit cell) $\rightarrow$ V_c Avogadro's number
(6.023 x 10²³ atoms/mol) $\rightarrow$ N_A

Example: Copper

Data from Table inside front cover of Callister (see next slide):

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius $R = 0.128$ nm (1 nm = 10⁻⁷cm)

$$V_c = a^3; \text{ For FCC, } a = 4R/\sqrt{2}; V_c = 4.75 \times 10^{-23} \text{ cm}^3$$

Result: theoretical $\rho_{\text{Cu}} = 8.89 \text{ g/cm}^3$

Compare to actual: $\rho_{\text{Cu}} = 8.94 \text{ g/cm}^3$

DENSITIES OF MATERIAL CLASSES

ρ_{metals} ρ_{ceramics} ρ_{polymers}

Metals/
Alloys

Graphite/
Ceramics/
Semicond

Polymers

Composites/
fibers

Why?

Metals have...

- close-packing
(metallic bonding)
- large atomic mass

Ceramics have...

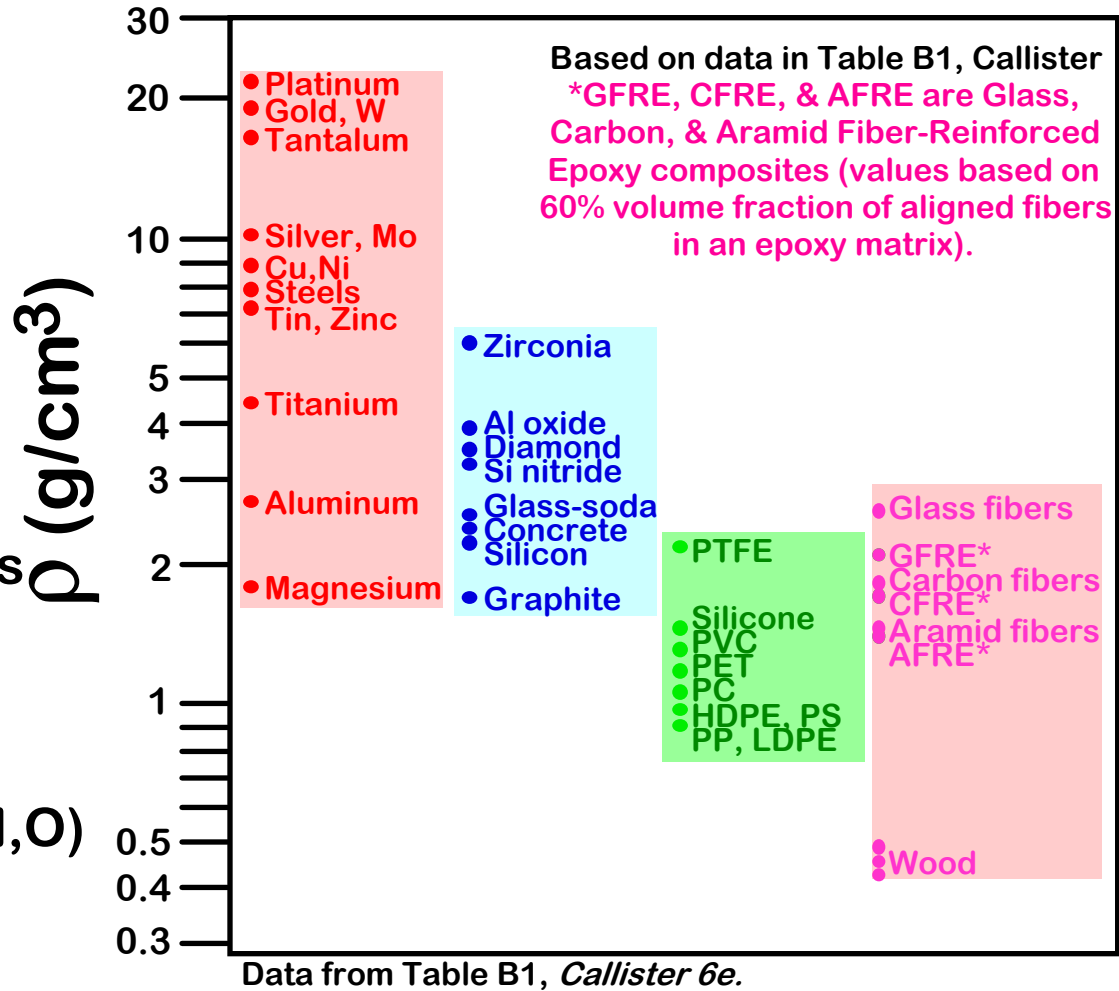
- less dense packing
(covalent bonding)
- often lighter elements

Polymers have...

- poor packing
(often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values



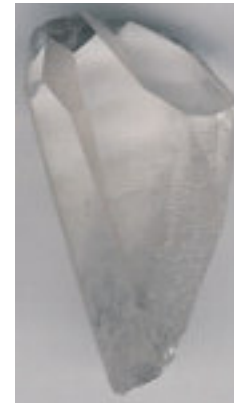
CRYSTALS AS BUILDING BLOCKS

- ***Some* engineering applications require single crystals:**
 - diamond single crystals for abrasives
 - turbine blades



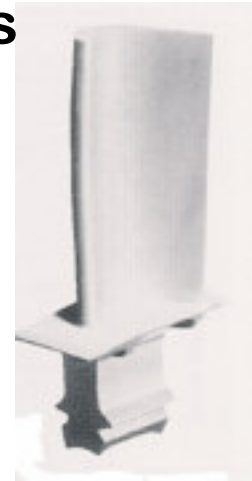
(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

- **Crystal properties reveal features of atomic structure.**
 - Ex: Certain crystal planes in quartz fracture more easily than others.



(Courtesy P.M. Anderson)

Fig. 8.30(c), *Callister 6e*.
(Fig. 8.30(c) courtesy of Pratt and Whitney).



POLYCRYSTALS

- *Most* engineering materials are **polycrystals**.



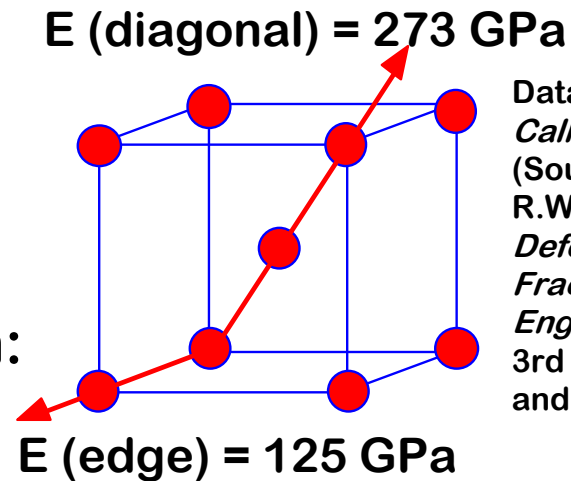
Adapted from Fig. K,
color inset pages of
Callister 6e.
(Fig. K is courtesy of
Paul E. Danielson,
Teledyne Wah Chang
Albany)

- Nb-Hf-W plate with an electron beam weld.
- Each "grain" is a single crystal.
- If crystals are randomly oriented,
overall component properties are not directional.
- Crystal sizes typ. range from 1 nm to 2 cm
(i.e., from a few to millions of atomic layers).

SINGLE VS POLYCRYSTALS

- Single Crystals

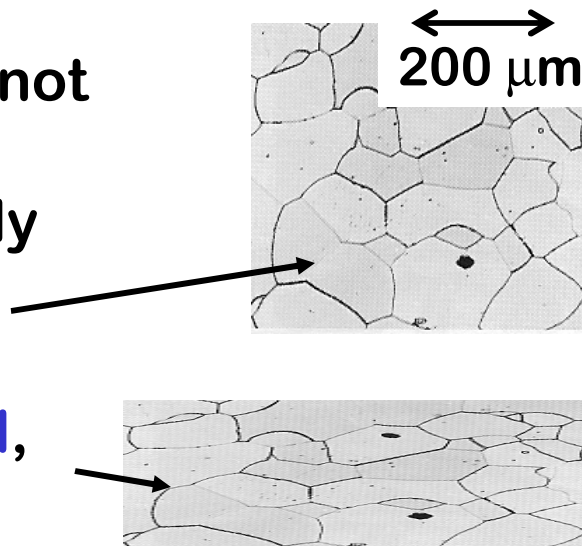
- Properties vary with direction: **anisotropic**.
- Example: the modulus of elasticity (E) in BCC iron:



Data from Table 3.3, *Callister 6e*.
(Source of data is R.W. Hertzberg, *Deformation and Fracture Mechanics of Engineering Materials*, 3rd ed., John Wiley and Sons, 1989.)

- Polycrystals

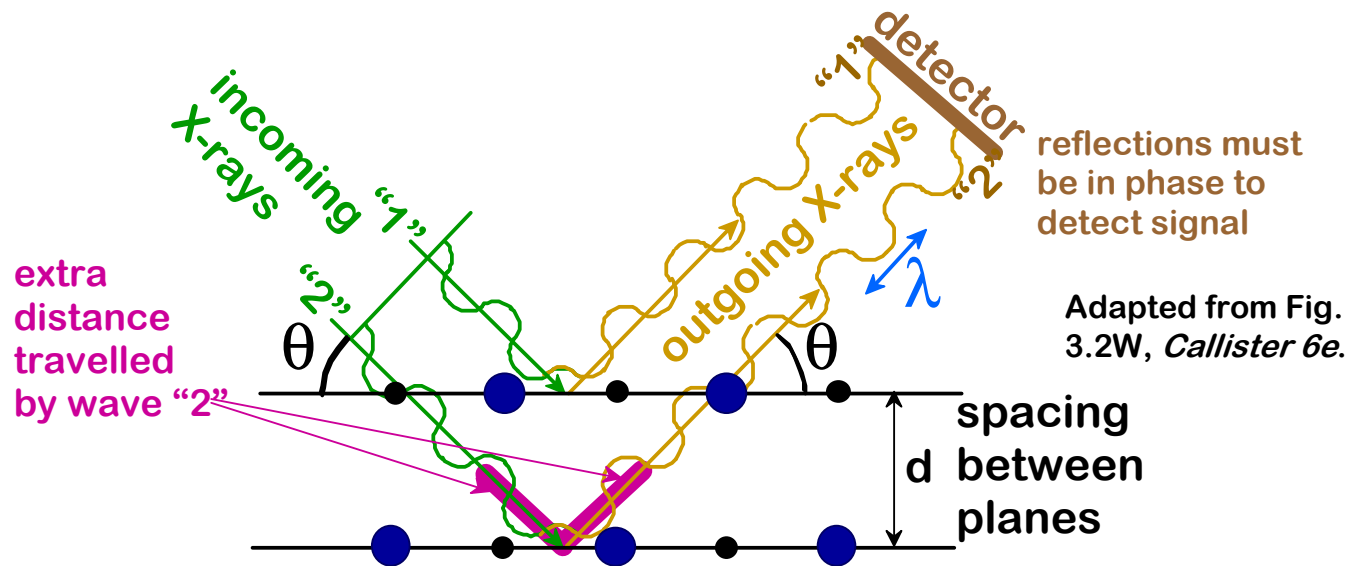
- Properties may/may not vary with direction.
- If grains are randomly oriented: **isotropic**.
($E_{\text{poly iron}} = 210$ GPa)
- If grains are **textured**, anisotropic.



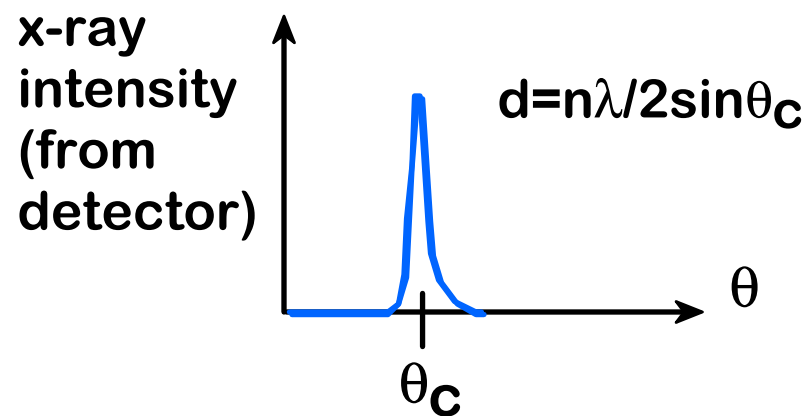
Adapted from Fig. 4.12(b), *Callister 6e*.
(Fig. 4.12(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

X-RAYS TO CONFIRM CRYSTAL STRUCTURE

- Incoming X-rays **diffract** from crystal planes.

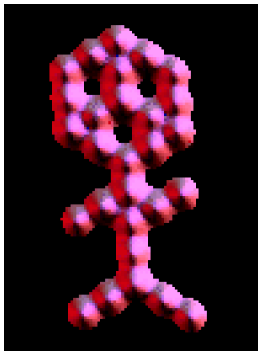


- Measurement of:
Critical angles, θ_c ,
for X-rays provide
atomic spacing, d .

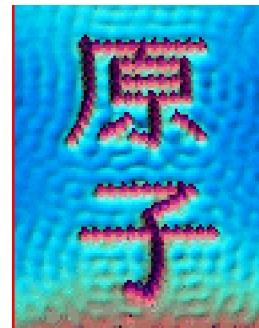


SCANNING TUNNELING MICROSCOPY

- Atoms can be arranged and imaged!



Carbon monoxide
molecules arranged
on a platinum (111)
surface.

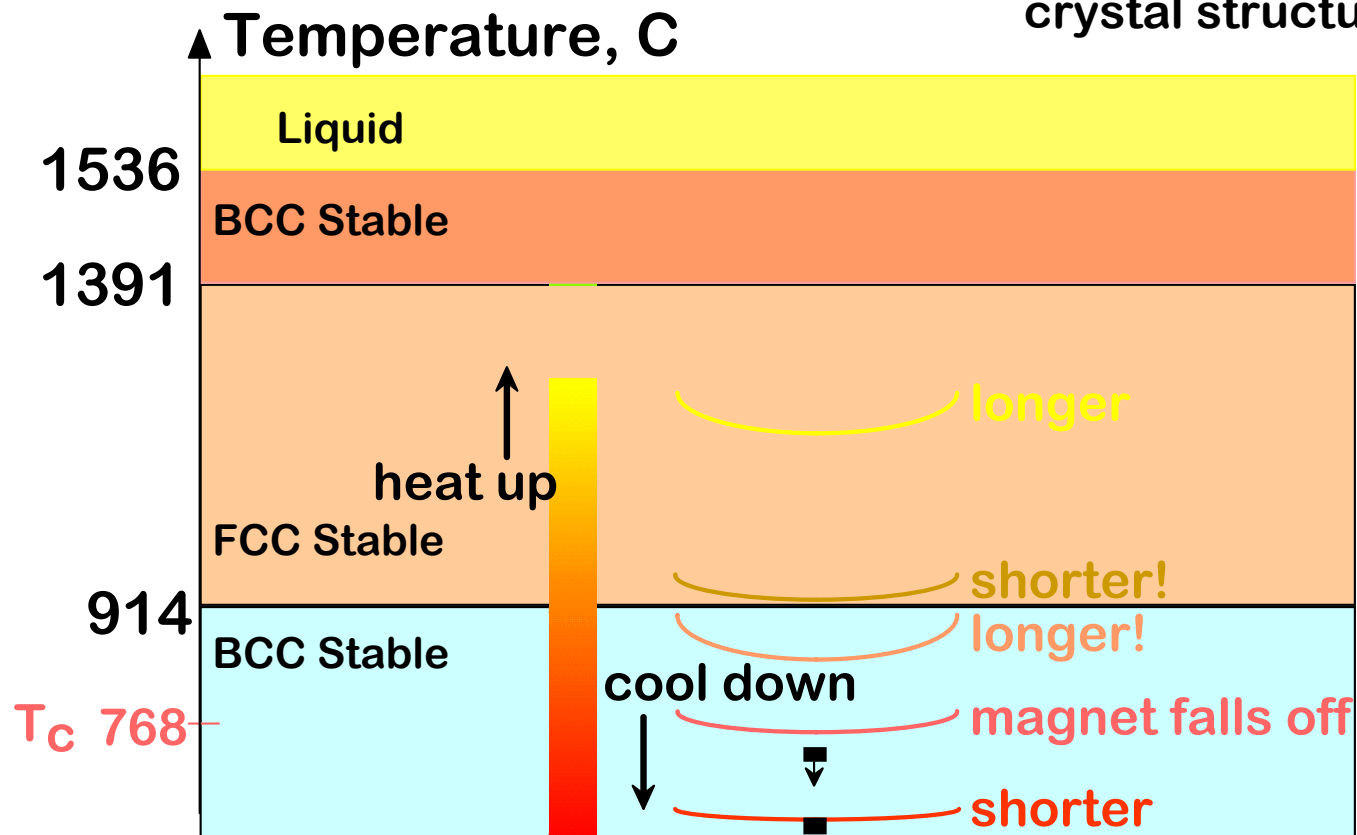


Iron atoms
arranged on a
copper (111)
surface. These
Kanji characters
represent the word
“atom”.

Photos produced from
the work of C.P. Lutz,
Zeppenfeld, and D.M.
Eigler. Reprinted with
permission from
International Business
Machines
Corporation,
copyright 1995.

DEMO: HEATING AND COOLING OF AN IRON WIRE

- Demonstrates "**polymorphism**" ← The same atoms can have more than one crystal structure.



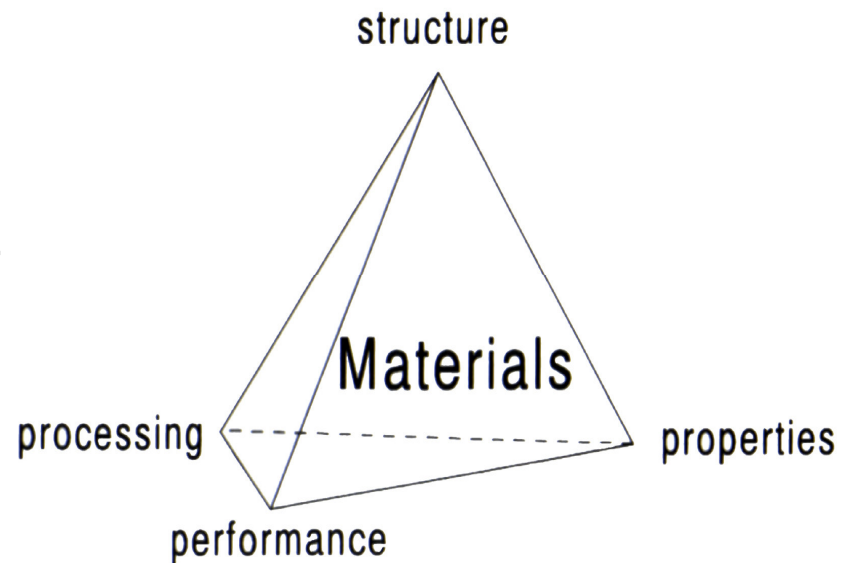
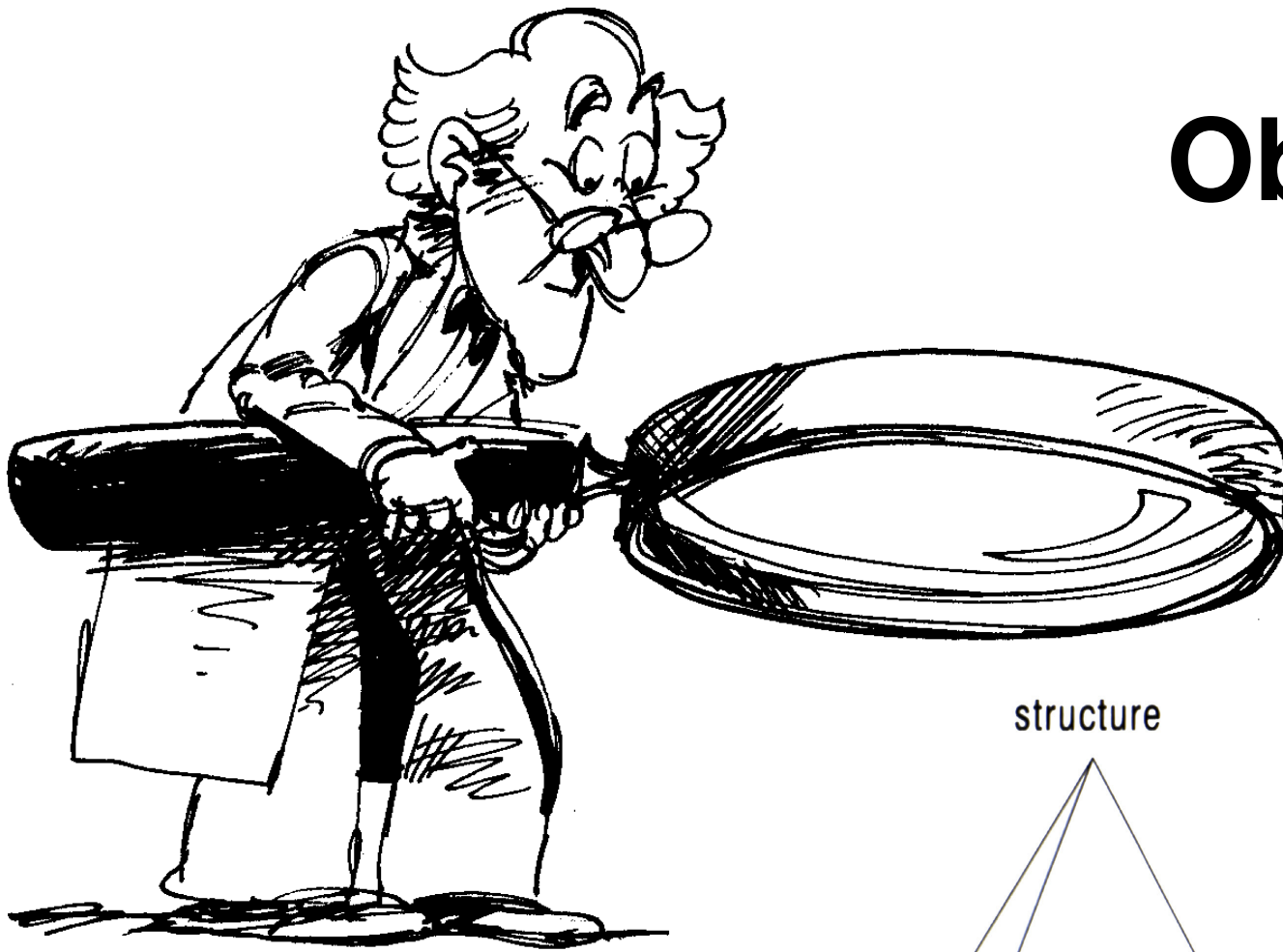
SUMMARY

- Atoms may assemble into **crystalline** or **amorphous** structures.
- We can predict the **density** of a material, provided we know the **atomic weight**, **atomic radius**, and **crystal geometry** (e.g., FCC, BCC, HCP).
- Material properties generally vary with single crystal orientation (i.e., they are **anisotropic**), but properties are generally non-directional (i.e., they are **isotropic**) in polycrystals with randomly oriented grains.

Até aqui, tudo bem

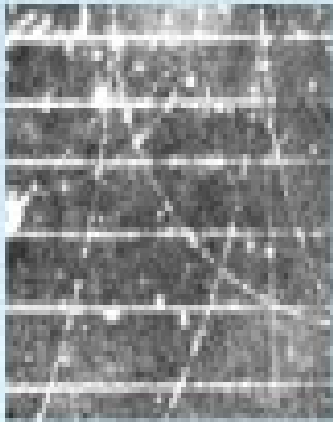


Obrigado !



Prof. Aguinaldo M Severino

Physics

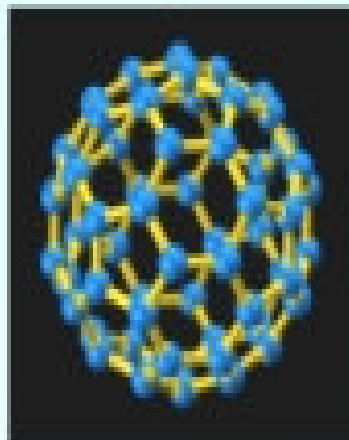


Engineering



Materials Science

Chemistry

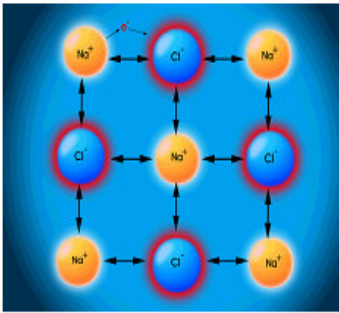


Mathematics

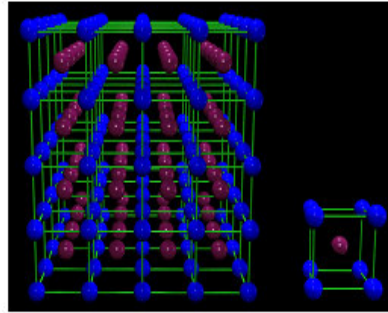
$$\frac{\partial C}{\partial t} = D \cdot \left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right]$$

Materials Science $\Rightarrow$ Bridge between Natural Science and Engineering Sciences

Atomic bonding



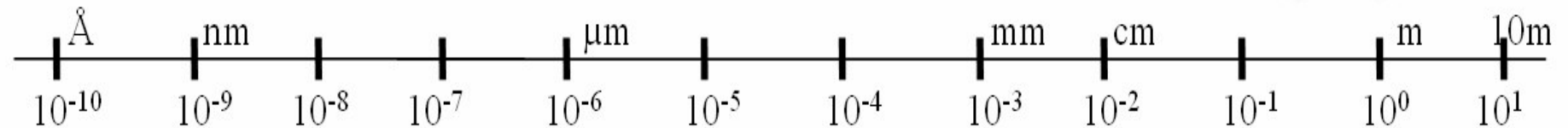
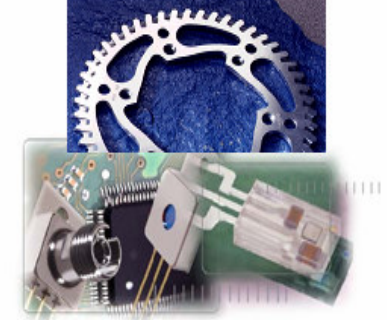
Crystal structure



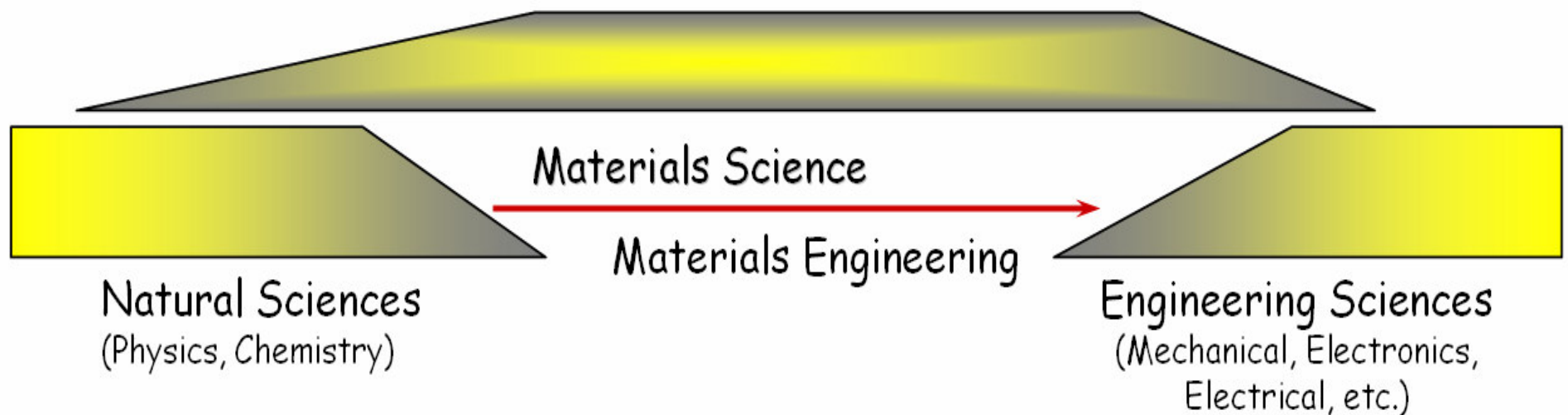
Microstructure



Construction Part



Atom Molecule Protein Light wave Hair thickness Nerve tissue Handy Auto Airplane
Crystal structure Virus Cell Blood vessel



PERIODIC TABLE

Atomic Properties of the Elements

NIST

National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Frequently used fundamental physical constants			
For the most accurate values of these and other constants, visit physics.nist.gov/constants			
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs			
speed of light in vacuum	c	$299\,792\,458\text{ m s}^{-1}$	(exact)
Planck constant	h	$6.6261 \times 10^{-34}\text{ J s}$	($h = h/2\pi$)
elementary charge	e	$1.6022 \times 10^{-19}\text{ C}$	
electron mass	m_e	$9.1094 \times 10^{-31}\text{ kg}$	
	$m_e c^2$	0.5110 MeV	
proton mass	m_p	$1.6726 \times 10^{-27}\text{ kg}$	
fine-structure constant	α	$1/137.036$	
Rydberg constant	R_∞	$10\,973\,732\text{ m}^{-1}$	
	$R_\infty c$	$3.289\,84 \times 10^{15}\text{ Hz}$	
	$R_\infty hc$	13.6057 eV	
Boltzmann constant	k	$1.3807 \times 10^{-23}\text{ J K}^{-1}$	

■ Solids
■ Liquids
■ Gases
■ Artificially Prepared

Physics Laboratory
physics.nist.gov

Standard Reference Data Program
www.nist.gov/srd

Frequently used fundamental physical constants										Physics Laboratory physics.nist.gov		Standard Reference Data Program www.nist.gov/srd		
For the most accurate values of these and other constants, visit physics.nist.gov/constants														
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³ Cs														
speed of light in vacuum										c	299 792 458	m s ⁻¹	(exact)	
Planck constant										h	6.6261 × 10 ⁻³⁴	J s	(h = h/2π)	
elementary charge										e	1.6022 × 10 ⁻¹⁹	C		
electron mass										m _e	9.1094 × 10 ⁻³¹	kg		
										m _e c ²	0.5110	MeV		
proton mass										m _p	1.6726 × 10 ⁻²⁷	kg		
fine-structure constant										α	1/137.036			
Rydberg constant										R _∞	10 973 732	m ⁻¹		
										R _∞ c	3.289 84 × 10 ¹⁵	Hz		
										R _∞ hc	13.6057	eV		
Boltzmann constant										k	1.3807 × 10 ⁻²³	J K ⁻¹		

Atomic Number
 Ground-state Level
 Symbol
 Name
 Atomic Weight
 Ground-state Configuration
 Ionization Energy (eV)

[†]Based upon ^{12}C . () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

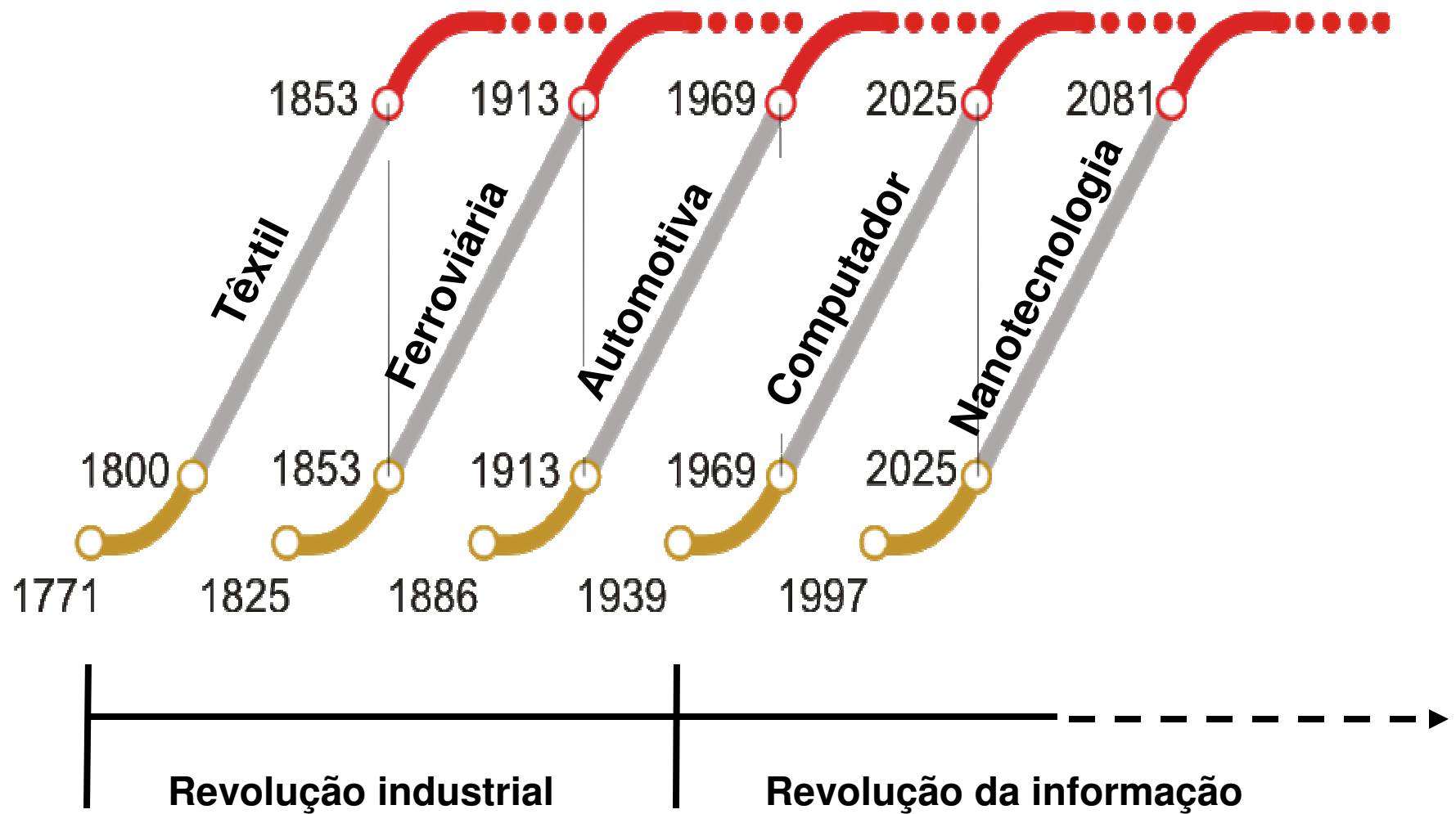
NIST SP 966 (March 2001)



MATERIALS

- **Metals:** Materials that are normally combinations of "metallic elements". These elements, when combined, usually have electrons that are non localized and as a consequence have generic types of properties. Metals usually are good conductors of heat and electricity. Also, they are quite strong but malleable and tend to have a lustrous look when polished.
- **Ceramics:** Ceramics are generally compounds between metallic and nonmetallic elements and include such compounds as oxides, nitrides, and carbides. Typically they are insulating and resistant to high temperatures and harsh environments.
- **Plastics:** Plastics (or polymers) are generally organic compounds based upon carbon and hydrogen. They are very large molecular structures. Usually they are low density and are not stable at high temperatures.
- **Semiconductors:** Semiconductors have electrical properties intermediate between metallic conductors and ceramic insulators. Also, the electrical properties are strongly dependent upon small amounts of impurities.
- **Composites:** Composites consist of more than one material type. Fiberglass, a combination of glass and a polymer, is an example. Concrete and plywood are other familiar composites. Many new combinations include ceramic fibers in metal or polymer matrix.

FORÇAS TÉCNOLÓGICAS REVOLUCIONÁRIAS



- Introdução da tecnologia
- Ampla utilização
- Final do crescimento rápido

© SIEMENS AG, CT, Manfred Weick Montag 1, Marz 2004
Grundlagen und State of he Art der Nanotehnologie.ppt

Ref: Milunovich S. and Roy J.M.A.:
The Next Small Thing RC 30224705
Merril Lynch, 4 September, 2001

Aula 02

SOME COMPOUNDS WITH THE ZINCBLLENDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
CuF	4.26	ZnS	5.41	AlSb	6.13
CuCl	5.41	ZnSe	5.67	GaP	5.45
CuBr	5.69	ZnTe	6.09	GaAs	5.65
CuI	6.04	CdS	5.82	GaSb	6.12
AgI	6.47	CdTe	6.48	InP	5.87
BeS	4.85	HgS	5.85	InAs	6.04
BeSe	5.07	HgSe	6.08	InSb	6.48
BeTe	5.54	HgTe	6.43	SiC	4.35
MnS (red)	5.60	AlP	5.45		
MnSe	5.82	AlAs	5.62		