

Física dos Materiais – 4300502

1º Semestre de 2016

Instituto de Física
Universidade de São Paulo

Professor: **Luiz C. C. M. Nagamine**

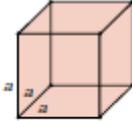
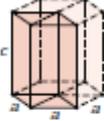
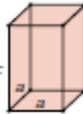
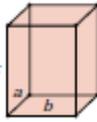
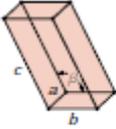
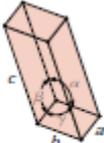
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Estrutura cristalina

Table 3.6 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	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

Tipos de redes cristalinas

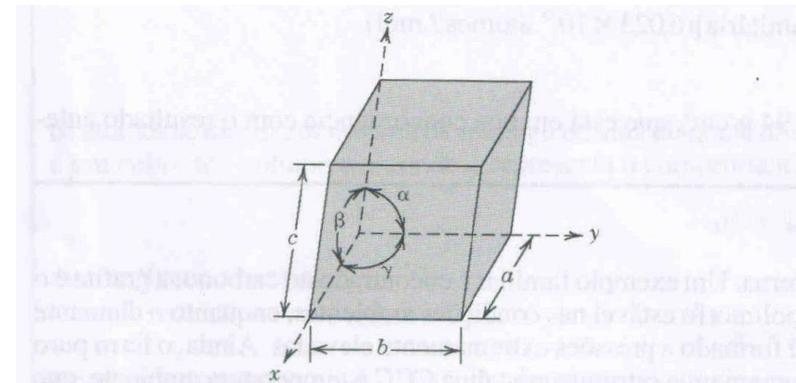


Fig. 3.4 Uma célula unitária com os eixos coordenados x , y e z , mostrando os comprimentos axiais (a , b e c) e os ângulos interaxiais (α , β e γ).

TABLE OF PERIODIC PROPERTIES OF THE ELEMENTS

Percent Ionic Character of a Single Chemical Bond

Difference in electronegativity	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2
Percent ionic character %	0.5	1	2	4	6	9	12	15	19	22	26	30	34	39	43	47	51	55	59	63	67	70	74	76	79	82	84	86	88	89	91	92

GROUP IA	GROUP IIA
H 0.32 2.20 0.99 0.4904 14.4 0.02848 13.599 14.304 0.001815	Li 1.23 0.98 2.05 145.720 13.10 3.00 5.292 1.06 3.6 0.847 Na 1.54 0.93 2.23 96.900 23.7 3.398 5.139 1.01 1.23 1.41
Be 1.40 1.57 9.00 293.40 5.0 12.30 1.052 1.05 1.82 2.00	Mg 1.31 1.21 1.72 127.40 8.954 1.72 1.36

DATA CONCERNING THE MORE STABLE ELEMENTARY (SUBATOMIC) PARTICLES				
Symbol	Neutron	Proton	Electron*	Photon
Rest mass (kg)	1.67495x10 ⁻²⁷	1.67265x10 ⁻²⁷	9.10959x10 ⁻³¹	0
Relative atomic mass (¹² C = 12)	1.008665	1.007276	5.48580x10 ⁻⁴	0
Charge (C)	0	1.60219x10 ⁻¹⁹	-1.60219x10 ⁻¹⁹	0
Radius (m)	8x10 ⁻¹⁶	8x10 ⁻¹⁶	<1x10 ⁻¹⁶	0
Spin quantum number	1/2	1/2	1/2	1
Magnetic Moment†	-1.913 μ _N	2.793 μ _N	1.001 μ _B	0

* The positron (e⁺) has properties similar to those of the (negative) electron or beta particle except that its charge has opposite sign (+). The antineutrino ($\bar{\nu}$) has properties similar to those of the neutrino except that its spin (or rotation) is opposite in relation to its direction of propagation.
† μ_B = Bohr magneton and μ_N = Nuclear magneton.

GROUP IIIB	GROUP IVB	GROUP VB	GROUP VIB	GROUP VIIB	GROUP VIII
B 0.82 2.04 1.17 489.70 4.4 30.20 0.299 1.06 1.03 0.270	C 0.77 1.53 0.91 355.80 4.58 11.260 1.000 0.71 1.29	N 0.75 3.04 0.729 0.65 14.324 1.04 0.002359	O 0.73 3.44 0.45 3.4099 14.0 0.22259 0.92 0.0002474	F 0.72 3.98 0.57 3.2698 17.1 0.2552 17.422	Ne 0.71 34.987 5.193 0.00152
Al 1.18 1.61 1.82 391.40 10.0 10.790 5.986 1.07 0.90 2.37	Si 1.31 1.90 1.46 344.220 12.1 50.550 1.81 151.775 0.151 150.0 0.71 1.48	P 1.06 2.19 1.29 344.0 15.1 17.175 10.486 9 0.77 0.00235	S 1.02 2.58 1.52 320.70 17.0 6.87 30.360 6.94 0.92 0.0002474	Cl 0.99 3.16 1.72 35.453 32.7 3.023 17.822	Ar 0.98 39.948 1.661 18.998 0.0001772

GROUP IIIA	GROUP IVA	GROUP VA	GROUP VIA	GROUP VIIA	GROUP VIIIA	GROUP IB	GROUP IIB
K 0.82 1.74 1.00 2.07 79.870 43.41 2.334 4.40 1.36 0.75 1.024	Ca 1.23 1.36 2.00 421.00 15.0 14.10 6.54 0.000	Sc 1.44 1.36 2.09 214.20 15.0 14.10 6.54 0.000	Ti 1.32 1.54 2.00 421.00 15.0 14.10 6.54 0.000	V 1.32 1.63 1.89 364.30 15.0 14.10 6.54 0.000	Cr 1.18 1.66 1.89 364.30 15.0 14.10 6.54 0.000	Mn 1.17 1.55 1.79 324.60 15.0 14.10 6.54 0.000	Fe 1.16 1.88 1.67 376.30 15.0 14.10 6.54 0.000

The names and symbols of elements 104-110 are those recommended by IUPAC. No systematic alternatives to those originally by the present discoverers. Relative (IUPAC) molecular masses are given in parentheses. For the element 104 and relative (IUPAC) molecular masses are given in parentheses. For the element 105, relative (IUPAC) molecular masses are given in parentheses. For the element 106, relative (IUPAC) molecular masses are given in parentheses. For the element 107, relative (IUPAC) molecular masses are given in parentheses. For the element 108, relative (IUPAC) molecular masses are given in parentheses. For the element 109, relative (IUPAC) molecular masses are given in parentheses. For the element 110, relative (IUPAC) molecular masses are given in parentheses.

KEY

CRYSTAL STRUCTURE (2)

ACID-BASE PROPERTIES (1)

ELECTRONEGATIVITY (Pauling's)

HEAT OF VAPORIZATION, kJ/mol (4)

HEAT OF FUSION, kJ/mol (5)

ELECTRICAL CONDUCTIVITY, 10¹⁰ Ω⁻¹ cm⁻¹ (6)

THERMAL CONDUCTIVITY, W cm⁻¹ K⁻¹ (3)

COVALENT RADIUS, Å

ATOMIC RADIUS, Å (7)

ATOMIC VOLUME, cm³/mol (8)

FIRST IONIZATION POTENTIAL, V

SPECIFIC HEAT CAPACITY, J g⁻¹ K⁻¹ (3)

Zn

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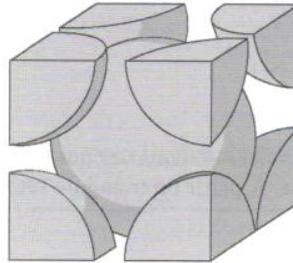
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
1.65 1.12 2.70 41.0 20.67 5.400 5.64 0.015 0.19 0.114	1.65 1.13 2.67 296.80 20.6 8.890 5.41 0.015 0.19 0.114	1.64 1.14 2.64 273.0 20.6 7.140 5.41 0.015 0.19 0.114	1.63 1.13 2.62 20.6 5.54 0.19 0.114	1.62 1.17 2.59 166.40 20.6 7.140 5.41 0.015 0.19 0.114	1.85 1.2 2.56 141.50 20.6 7.140 5.41 0.015 0.19 0.114	1.85 1.2 2.54 339.40 20.6 7.140 5.41 0.015 0.19 0.114	1.59 1.2 2.49 320.90 20.6 7.140 5.41 0.015 0.19 0.114	1.59 1.22 2.49 320.40 20.6 7.140 5.41 0.015 0.19 0.114	1.58 1.23 2.47 241.0 20.6 7.140 5.41 0.015 0.19 0.114	1.57 1.24 2.45 241.0 20.6 7.140 5.41 0.015 0.19 0.114	1.56 1.25 2.42 191.0 20.6 7.140 5.41 0.015 0.19 0.114	1.54 1.1 2.40 138.90 20.6 7.140 5.41 0.015 0.19 0.114	1.56 1.27 2.40 138.90 20.6 7.140 5.41 0.015 0.19 0.114

- NOTES: (1) For representative oxides (higher valence) of group. Oxide is acidic if color is red, basic if color is blue and amphoteric if both colors are shown. Intensity of color indicates relative strength.
- (2) Cubic, face centered; Cubic, body centered; Cubic;
- (3) At 300 K (27°C) (6) Generally at 293 K (20°C) (8) From density at 300 K (27°C) for liquid and solid elements; values for gaseous elements refer to liquid state at boiling point
- (4) At boiling point (7) Quantum mechanical value for free atom
- (5) At melting point
- NSRDS
SARGENT-WELCH SCIENTIFIC COMPANY
7300 LINDER AVENUE, SKOKIE, ILLINOIS 60077
Catalog Number S-18806

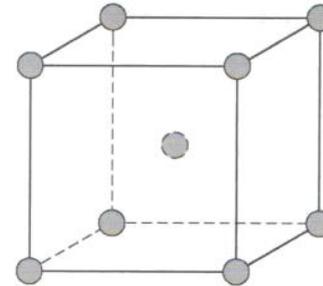
Estrutura cristalina

Rede cúbica de
corpo centrado

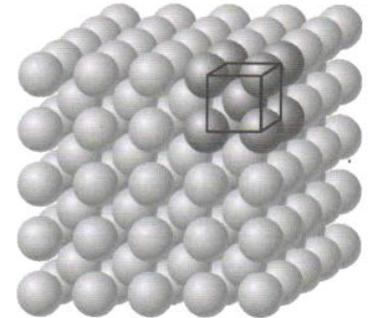
Célula unitária com
esferas rígidas



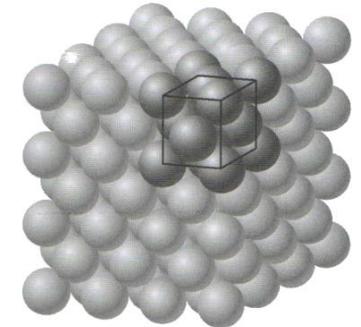
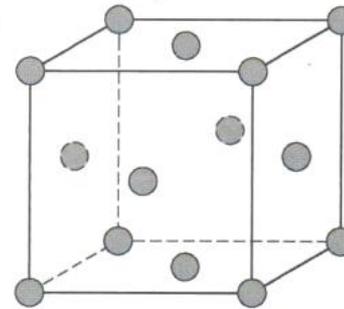
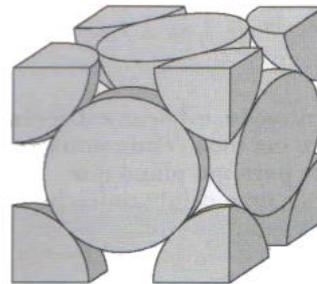
Célula unitária com
esferas reduzidas



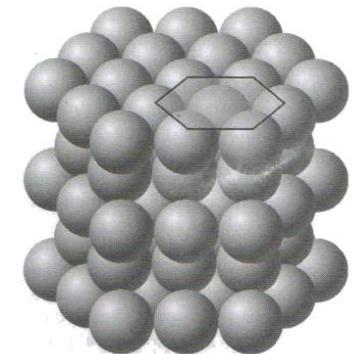
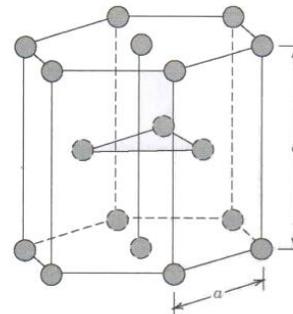
Agregado com
muitos átomos



Rede cúbica de
face centrada



Rede hexagonal
compacta

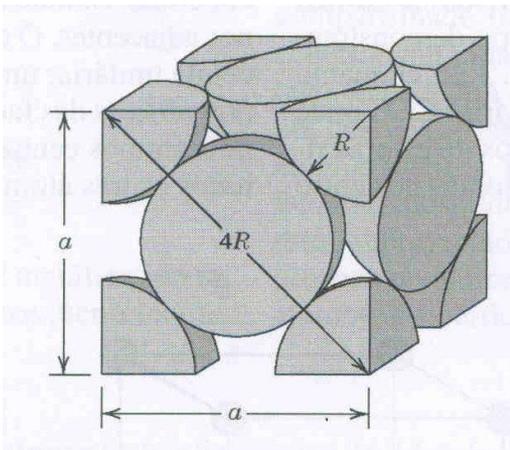


Estrutura cristalina

Alguns conceitos relacionados às redes cristalinas

Relação entre raio atômico (R), o parâmetro de rede (a) e o volume da célula unitária (V_c)

rede CFC (cúbica de face centrada)



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

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

Fator de empacotamento atômico (FEA)

(4 átomos por célula unitária)

$$FEA = \frac{V_E}{V_C} = \frac{4 \left(\frac{4}{3} \right) \pi R^3}{16R^3\sqrt{2}} = 0,74$$

Densidade (ρ)

(para o cobre: $A = 63,5$ g/mol e $R = 0,128$ nm)

$N_A = 6,023 \times 10^{23}$ at/mol

$$\rho = \frac{nm}{V_C} = \frac{nmN_A}{V_C N_A} = \frac{nA}{V_C N_A} = 8,89 \text{ g/cm}^3$$

Número de coordenação

p/ CFC é 12

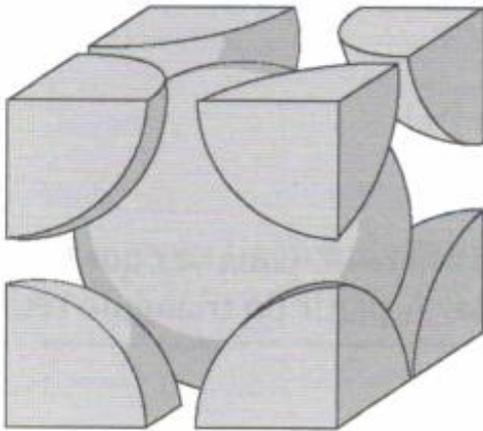
Estrutura cristalina

Alguns conceitos relacionados às redes cristalinas

Refazer os cálculos para Fe (CCC)

Relação entre raio atômico (R), o parâmetro de rede (a) e o volume da célula unitária (V_c)

rede CCC (cúbica de corpo centrado)



$$a = \frac{4R}{\sqrt{3}}$$

$$V_c = R^3 64\sqrt{3} / 9$$

Fator de empacotamento atômico (FEA)

(2 átomos por célula unitária)

$$FEA = \frac{V_E}{V_C} = \frac{2 \left(\frac{4}{3} \right) \pi R^3}{R^3 64\sqrt{3} / 9} = 0,68$$

Densidade (ρ)

(para o ferro: $A = 55,847$ g/mol e $R = 0,126$ nm)

$$\rho = \frac{nA}{V_C N_A} = 7,53 \text{ g} / \text{cm}^3$$

Número de coordenação

p/ CCC é 8

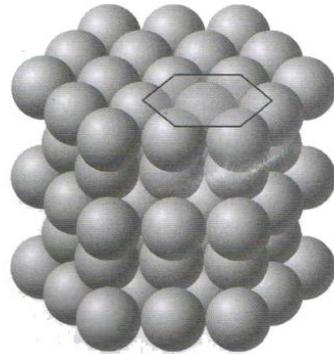
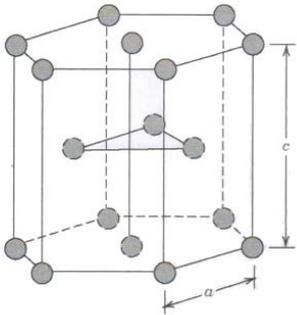
Estrutura cristalina

Alguns conceitos relacionados às redes cristalinas

Refazer os cálculos para Co (HCP razão $c/a= 1,633$)

Relação entre raio atômico (R), o parâmetro de rede (a) e o volume da célula unitária (V_c)

rede HC (hexagonal compacta)



$$a = 2R$$

$$c = \sqrt{\frac{8}{3}}a$$

$$V_c = R^3 24\sqrt{2}$$

Fator de empacotamento atômico (FEA)

(6 átomos por célula unitária)

$$FEA = \frac{V_E}{V_C} = \frac{6 \left(\frac{4}{3} \right) \pi R^3}{R^3 24\sqrt{2}} = 0,74$$

Densidade (ρ)

(para o cobalto: $A= 58,933$ g/mol e $R= 0,125$ nm)

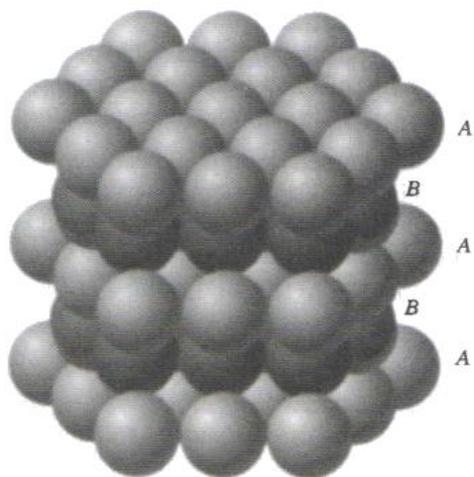
$$\rho = \frac{nA}{V_C N_A} = 8,86 \text{ g} / \text{cm}^3$$

Número de coordenação

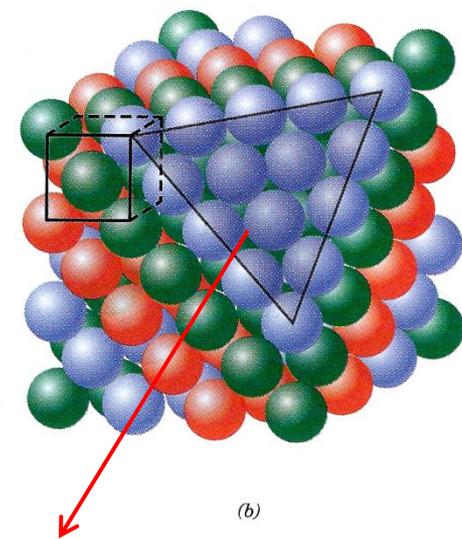
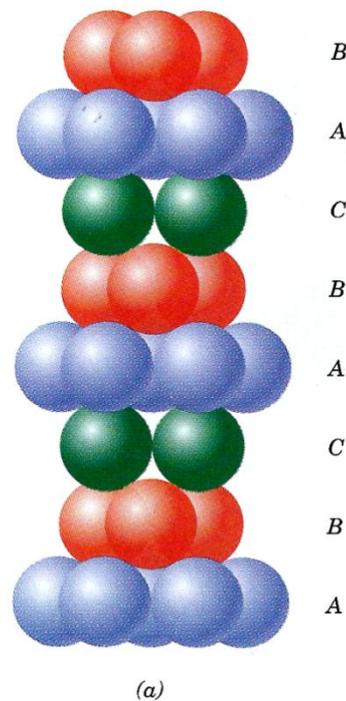
p/ HC é 12

Estrutura cristalina

Sequência de empilhamento de planos para a rede hexagonal compacta



Sequência de empilhamento de planos para a rede cúbica de face centrada

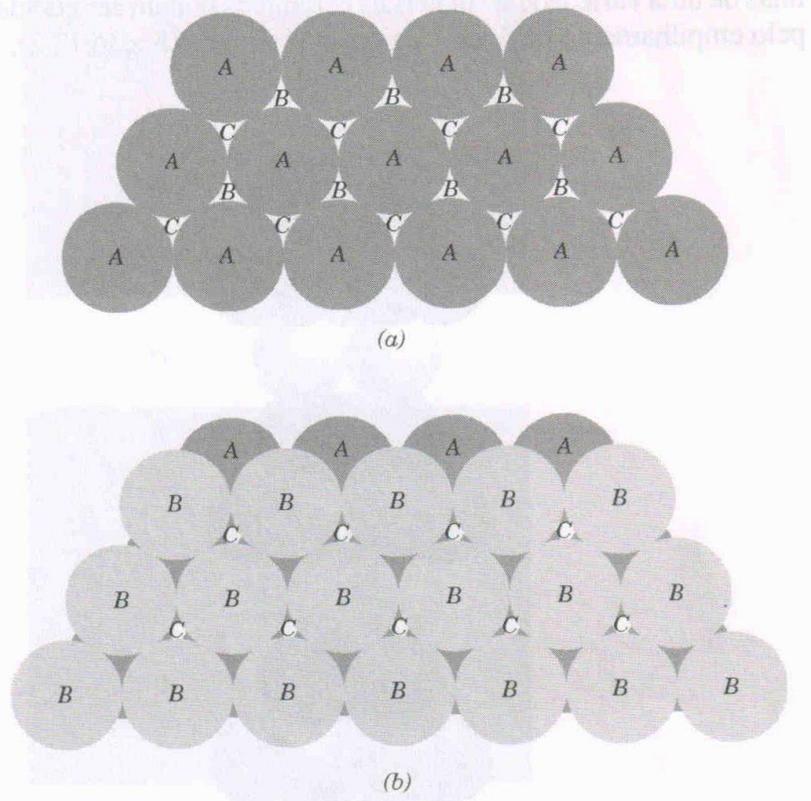
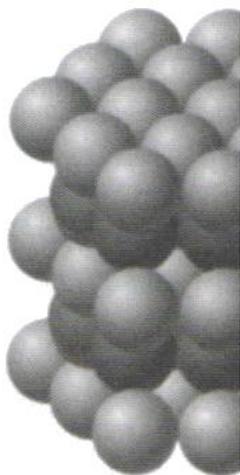


Plano (111)

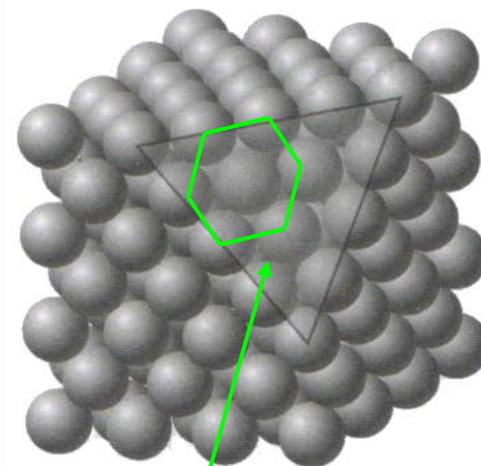
Diagonal do cubo

Estrutura cristalina

Sequência de en-
para a rede I



empilhamento de planos
de cúbica de face centrada



Plano (111)

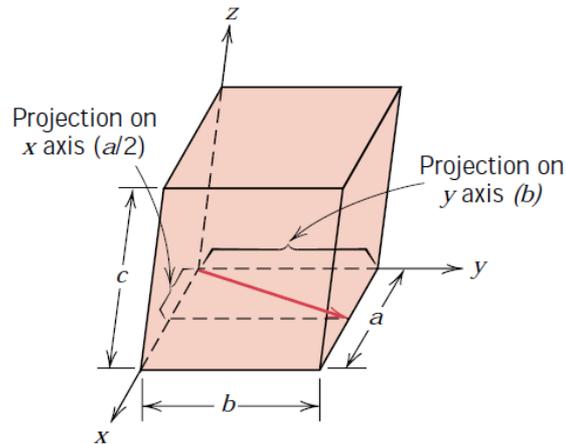
Diagonal do cubo

Fig. 3.12 (a) Uma fração de um plano compacto de átomos; as posições *A*, *B* e *C* estão indicadas. (b) A seqüência de empilhamento *AB* para planos atômicos compactos. (Adaptado de W. G. Moffatt, G. W. Pearsall e J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 50. Copyright © 1964 de John Wiley & Sons, New York. Reimpresso sob permissão de John Wiley & Sons, Inc.)

Direções cristalinas

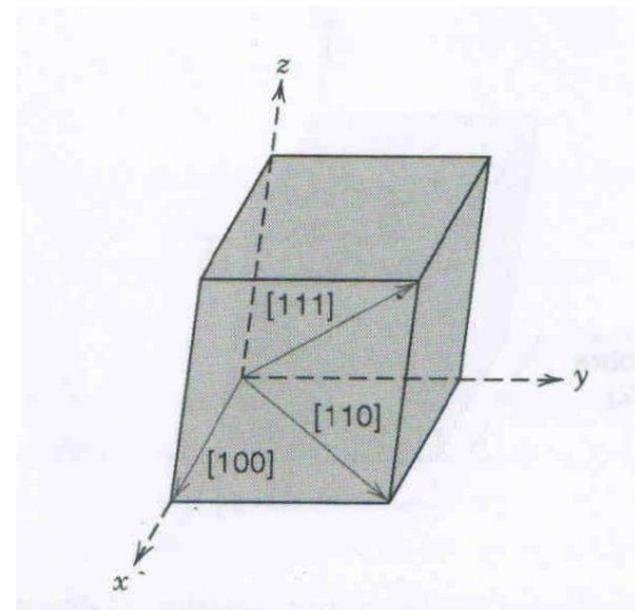
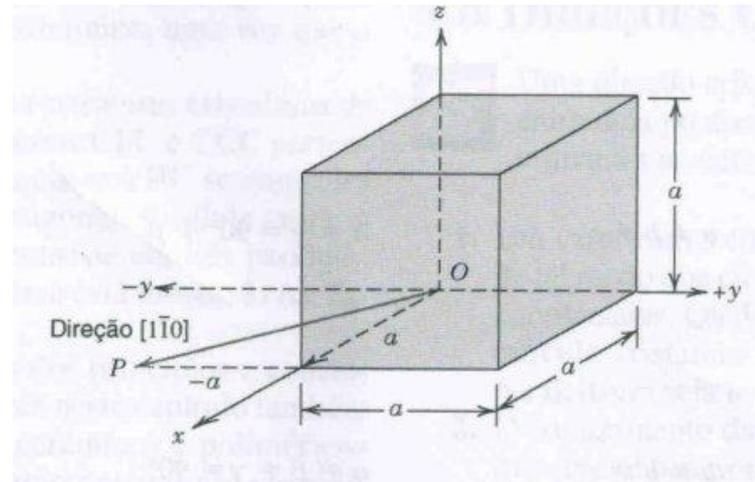
Uma direção cristalográfica é definida por um vetor

1. Um vetor com o comprimento conveniente é posicionado de tal modo que ele passa através da origem do sistema de coordenadas. Qualquer vetor pode ser movido através do retículo cristalino sem sofrer alterações, desde que seu paralelismo seja mantido.
2. O comprimento da projeção do vetor sobre cada um dos três eixos é determinado; *estes são medidos em termos das dimensões da célula unitária, a , b e c .*
3. Estes três números são multiplicados ou divididos por um fator comum, a fim de reduzi-los aos menores valores inteiros.
4. Os três índices, não separados por vírgulas, são colocados entre colchetes: $[uvw]$. Os inteiros u , v , e w correspondem às projeções reduzidas ao longo dos eixos x , y e z , respectivamente.



x	y	z
$a/2$	b	$0c$
$\frac{1}{2}$	1	0
1	2	0
$[120]$		

Direção $[1\bar{1}0]$



Direções cristalinias

Para redes hexagonais existe uma definição alternativa [uvw]

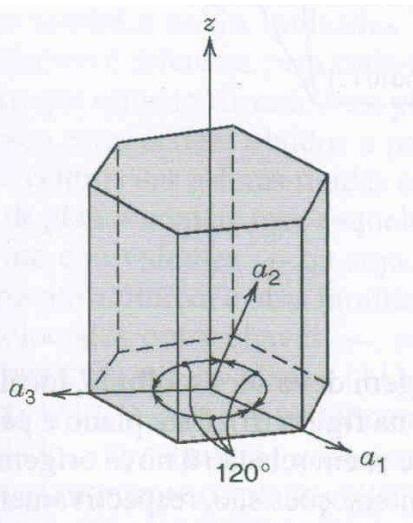
$$[u'v'w'] \rightarrow [uvw]$$

$$u = \frac{n}{3}(2u' - v')$$

$$v = \frac{n}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = nw'$$



$$[010] \rightarrow \left[\frac{-n}{3} \quad \frac{2n}{3} - \frac{n}{3} \quad 0 \right] \rightarrow [\bar{1}2\bar{1}0]$$

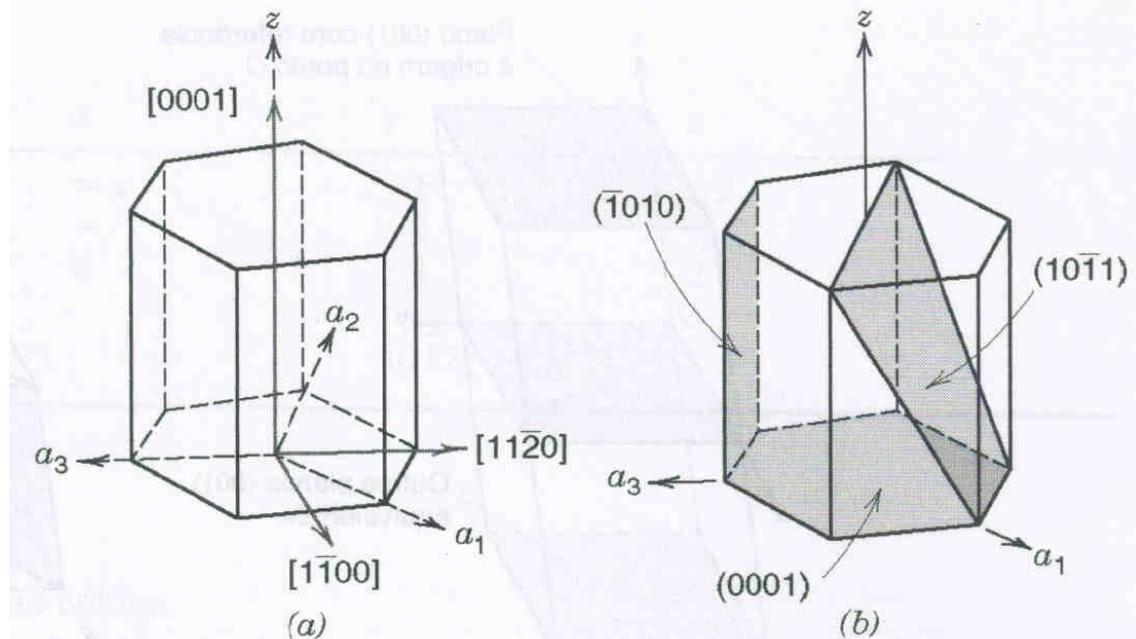
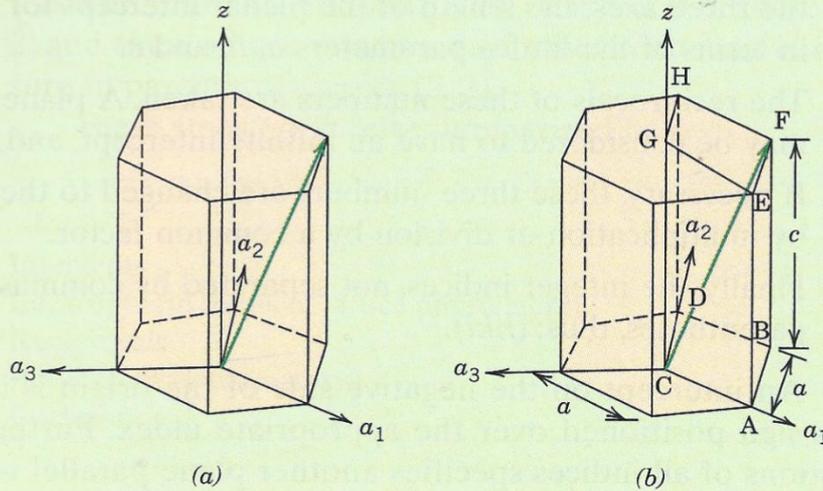


Fig. 3.7 Para o sistema cristalino hexagonal, (a) as direções [0001], [1100] e [1120] e (b) os planos (0001), (1011) e (1010).

EXAMPLE PROBLEM 3.8

Determination of Directional Indices for a Hexagonal Unit Cell

Determine the indices for the direction shown in the hexagonal unit cell of sketch (a) below.



$$u' = 1 \quad v' = 1 \quad w' = 1$$

Also, from Equations 3.6a, 3.6b, 3.6c, and 3.6d

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(1) - 1] = \frac{1}{3}$$

$$t = -(u + v) = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3}$$

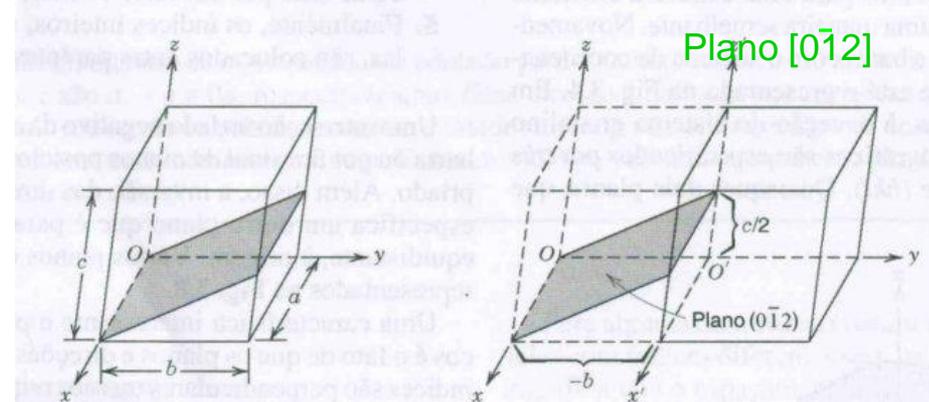
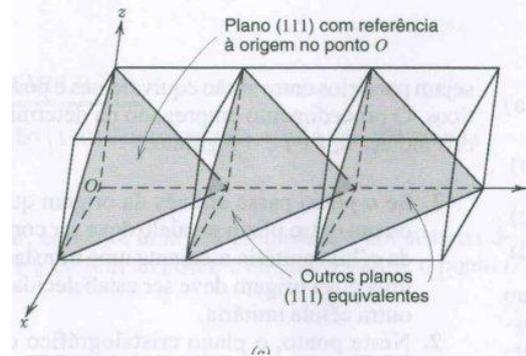
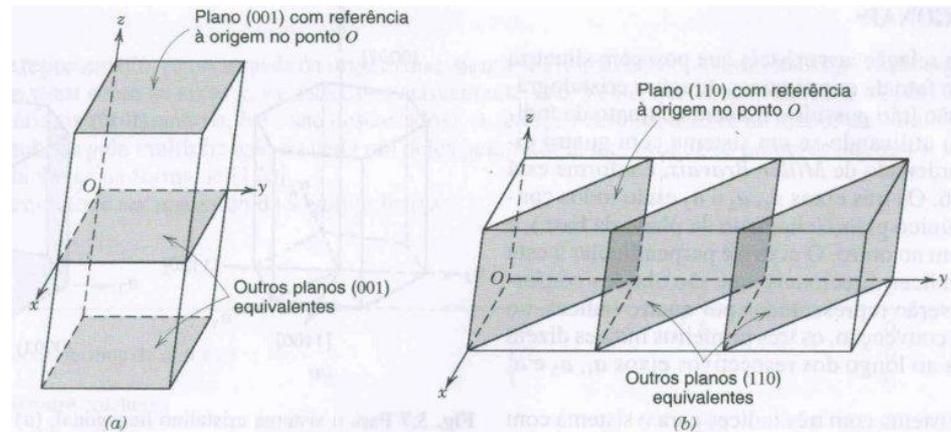
$$w = w' = 1$$

$$[11\bar{2}3]$$

Planos cristalinos

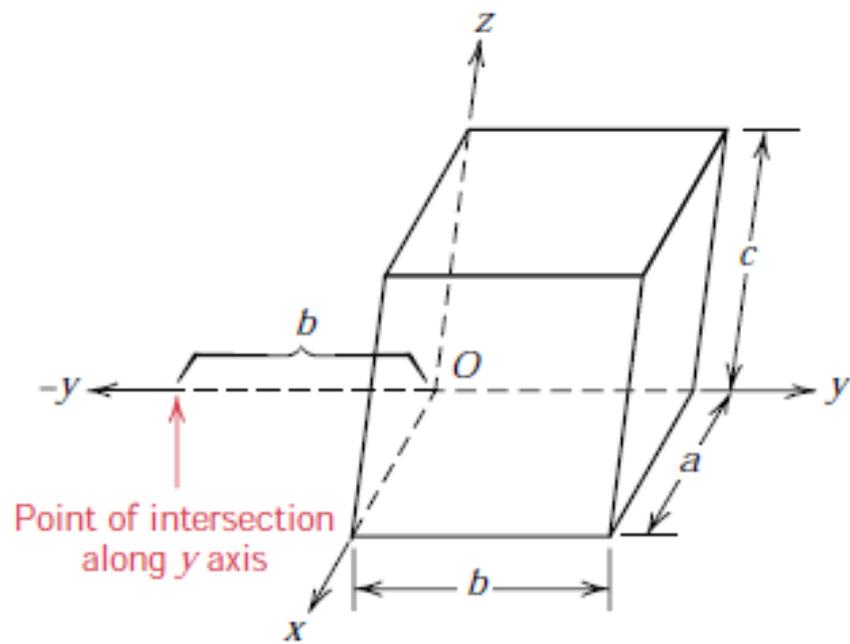
Uma plano cristalográfico é definido pelos índices de Miller (hkl)

1. Se o plano passa através da origem que foi selecionada, ou um outro plano paralelo deve ser construído no interior da célula unitária mediante uma translação apropriada, ou uma nova origem deve ser estabelecida no vértice de uma outra célula unitária.
2. Neste ponto, o plano cristalográfico ou intercepta ou é paralelo a cada um dos três eixos; o comprimento da interseção planar para cada eixo é determinado em termos dos parâmetros de rede a , b , e c .
3. Os valores inversos desses números são calculados e tomados. Um plano que é paralelo a um eixo pode ser considerado como tendo uma interseção no infinito e, portanto, um índice igual a zero.
4. Se necessário, estes três números são modificados para o conjunto de menores números inteiros pela multiplicação ou divisão por um fator comum.¹
5. Finalmente, os índices inteiros, não separados por vírgulas, são colocados entre parênteses, assim: (hkl) .

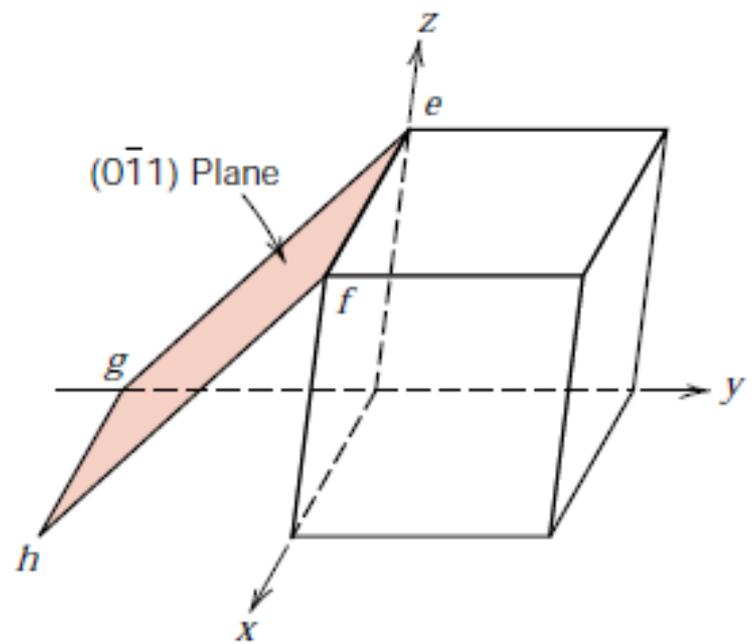


EXAMPLE PROBLEM 3.10

Construct a $(0\bar{1}1)$ plane within a cubic unit cell.



(a)

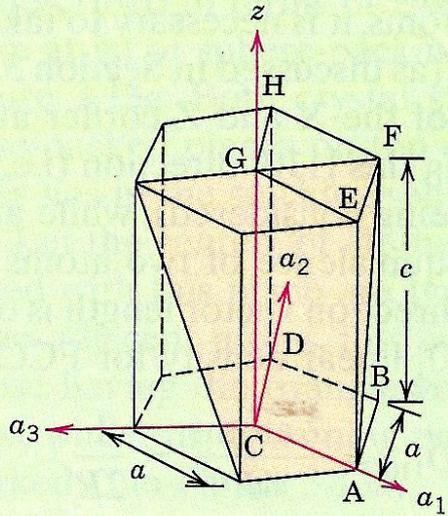


(b)

EXAMPLE PROBLEM 3.11

Determination of Miller–Bravais Indices for a Plane Within a Hexagonal Unit Cell

Determine the Miller–Bravais indices for the plane shown in the hexagonal unit cell.



$$(hkil)$$

$$(1\bar{1}01)$$

$$h=1$$

$$k=-1$$

$$l=1$$

$$i=-(h+k)=0$$