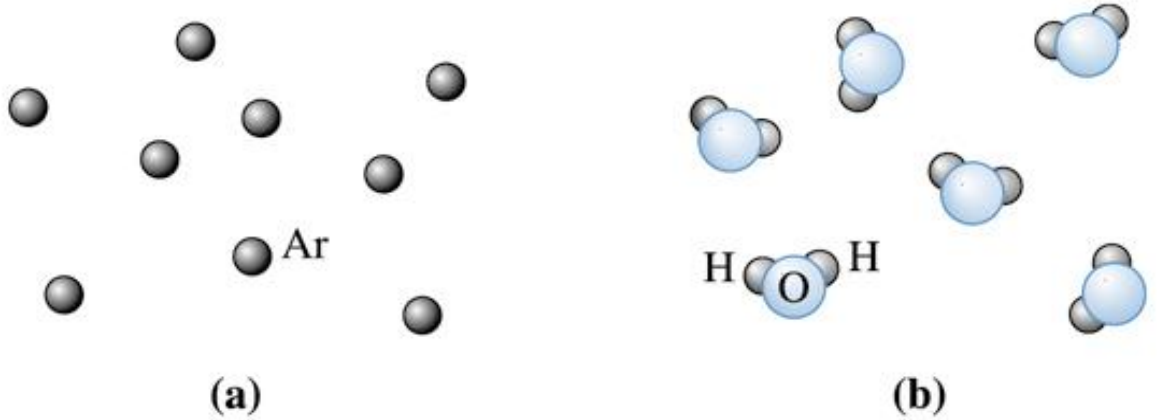
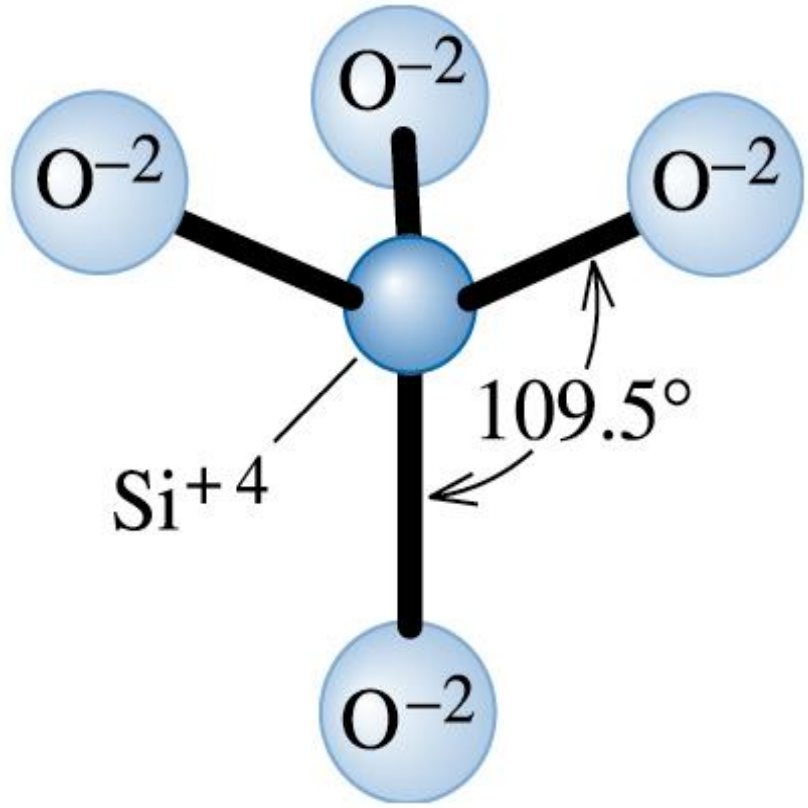
Estruturas Metálicas

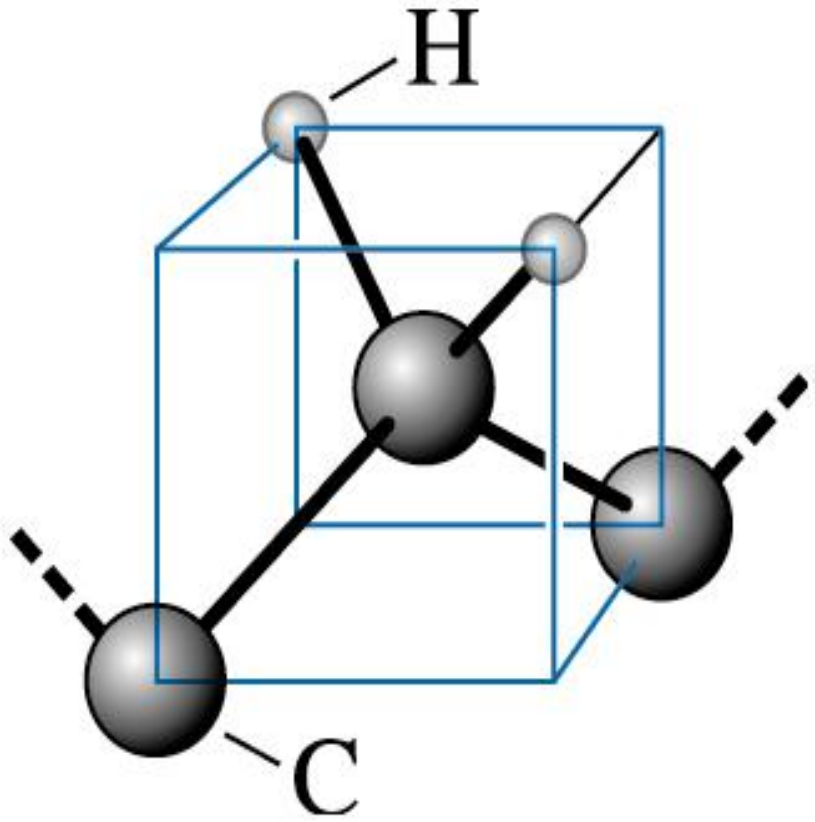
- Conceitos Gerais
- Cristais Metálicos

Níveis de organização

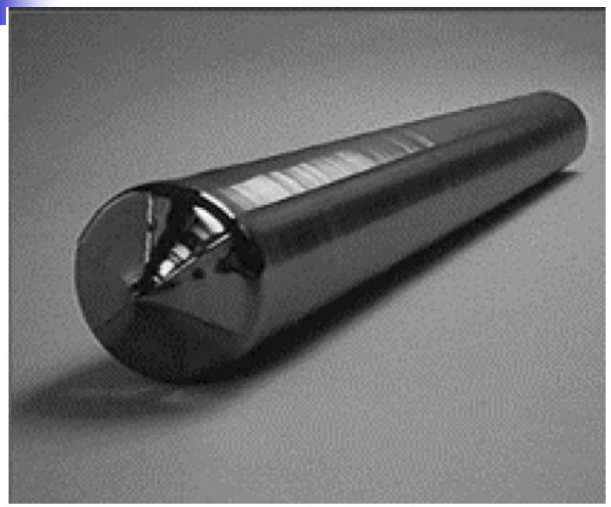


Curto Alcance



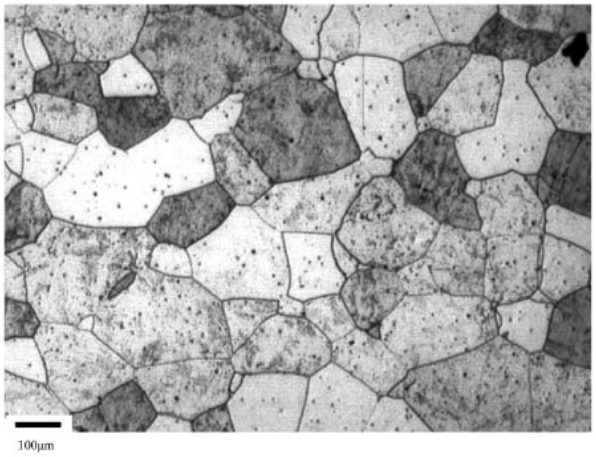


Longo Alcance (Cristais)



(a)

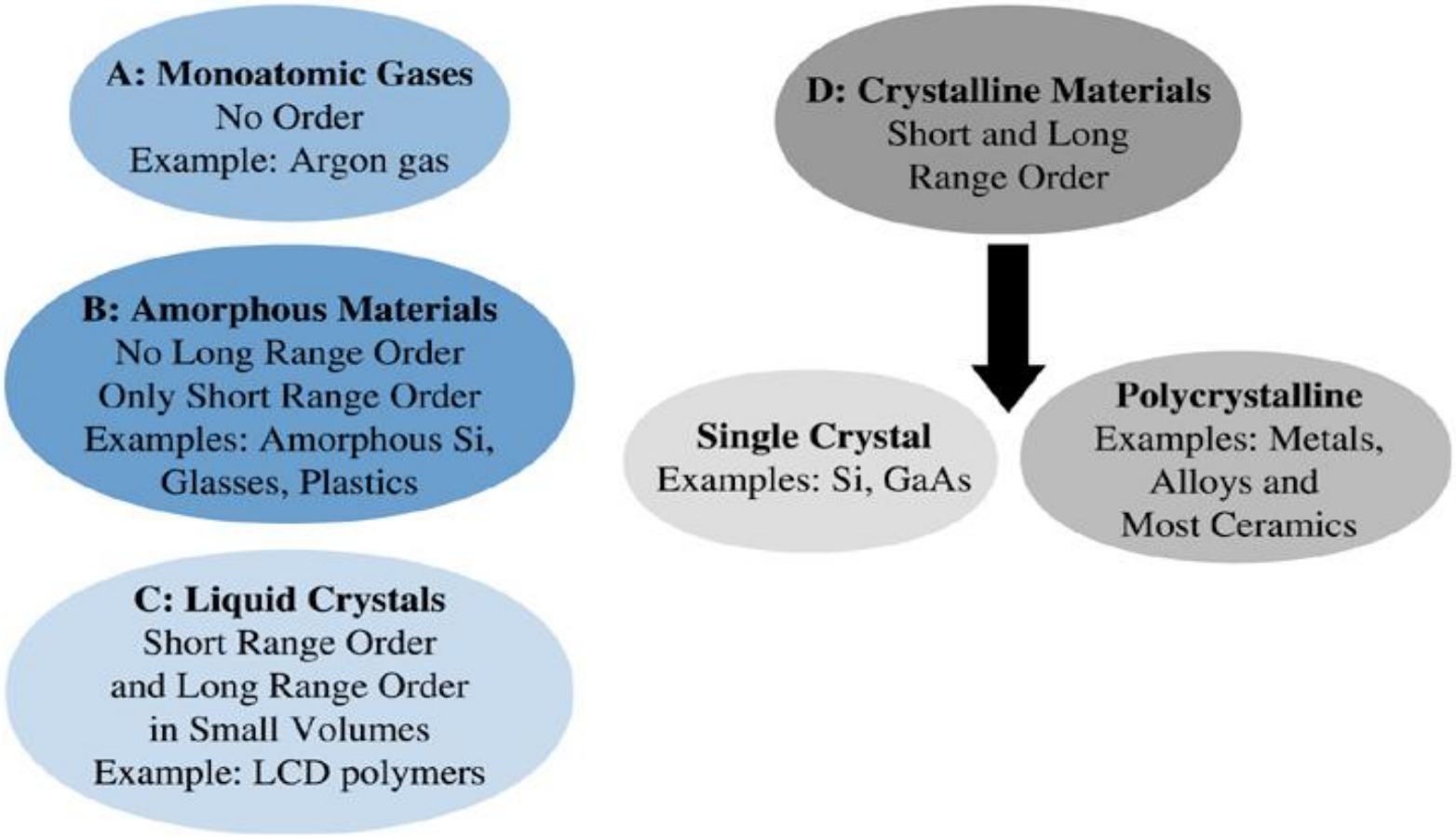
Monocrital (Si)



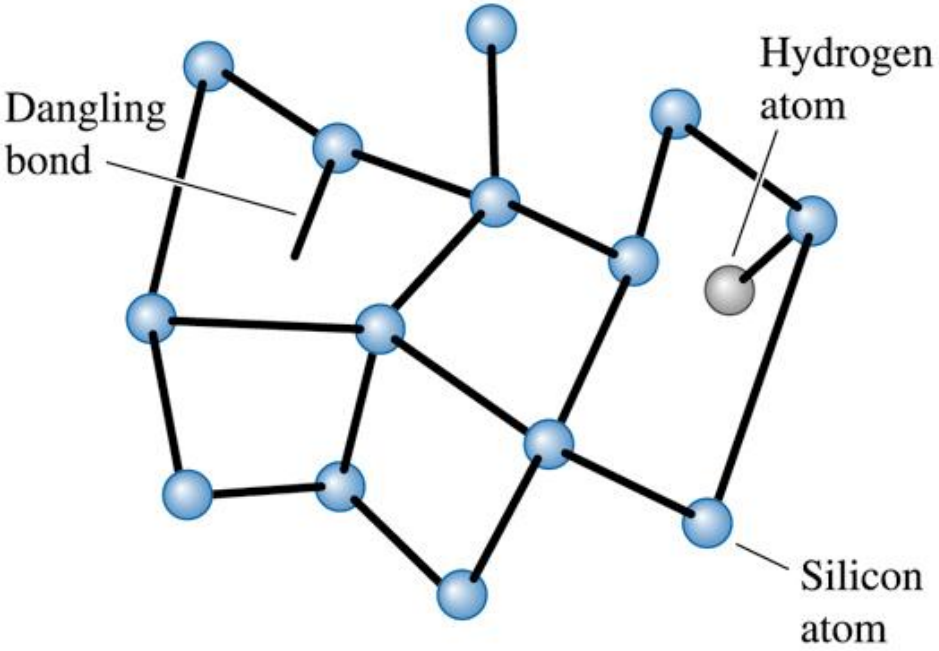
(b)

Material Policristalino (Aço)

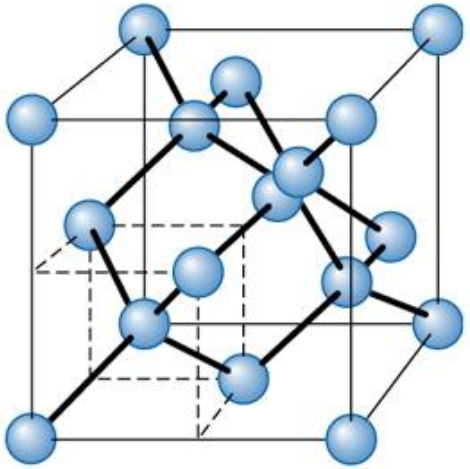
Resumo



Amorfo x Cristalino



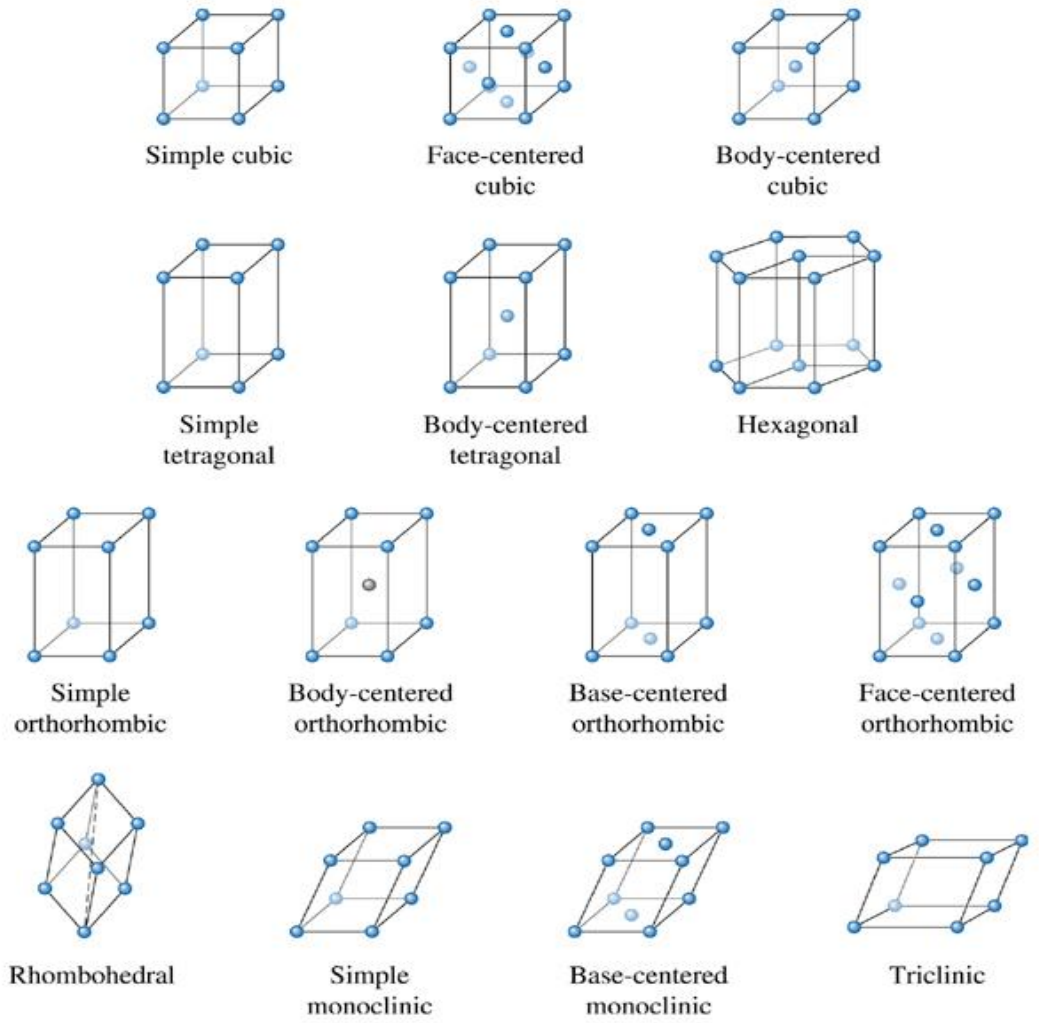
(a)



(b)

Redes de Bravais

14 Redes
7 Sistemas

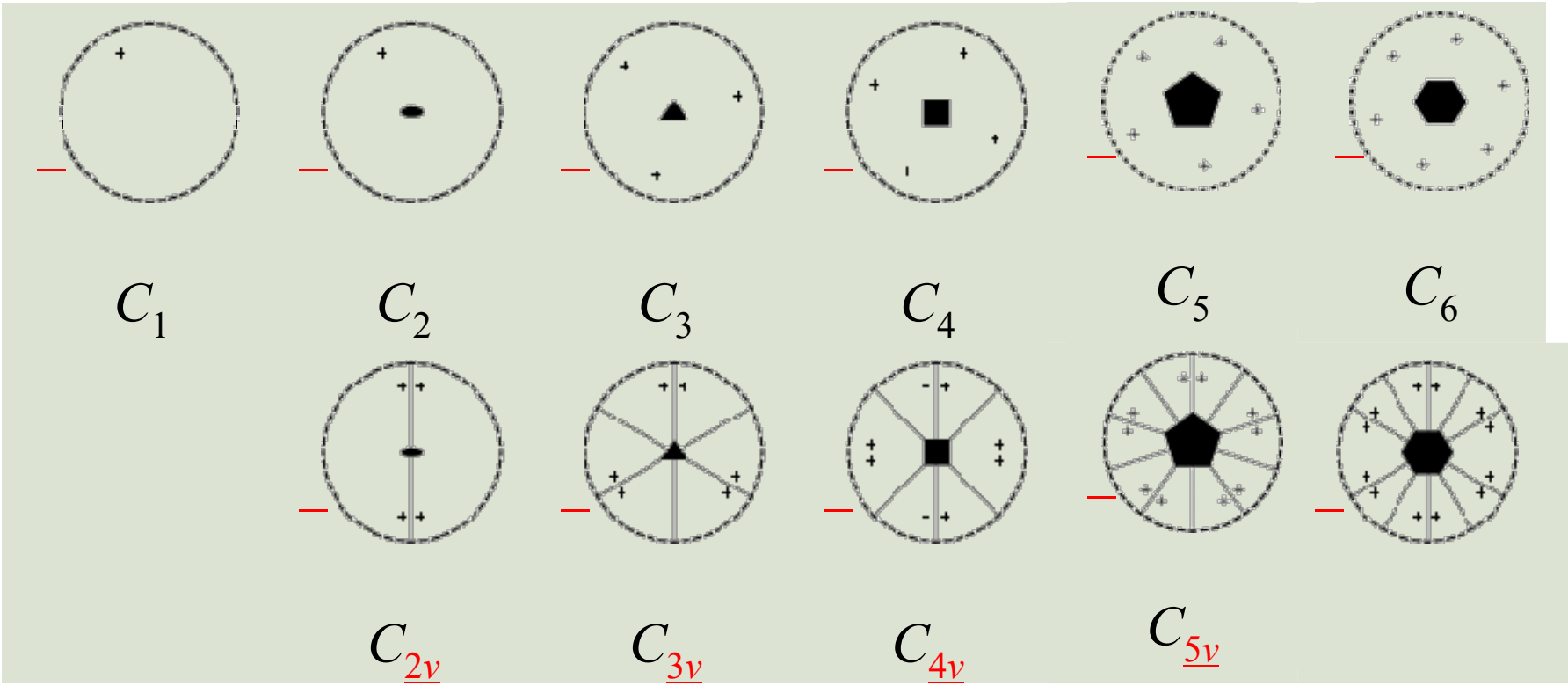


Características geométricas

TABLE 3-1 ■ ***Characteristics of the seven crystal systems***

Structure	Axes	Angles between Axes	Volume of the Unit Cell
Cubic	$a = b = c$	All angles equal 90°	a^3
Tetragonal	$a = b \neq c$	All angles equal 90°	a^2c
Orthorhombic	$a \neq b \neq c$	All angles equal 90°	abc
Hexagonal	$a = b \neq c$	Two angles equal 90°. One angle equals 120°.	$0.866a^2c$
Rhombohedral or trigonal	$a = b = c$	All angles are equal and none equals 90°	$a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$
Monoclinic	$a \neq b \neq c$	Two angles equal 90°. One angle (β) is not equal to 90°	$abc \sin\beta$
Triclinic	$a \neq b \neq c$	All angles are different and none equals 90°	$abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

Simetria (grupos de pontos)

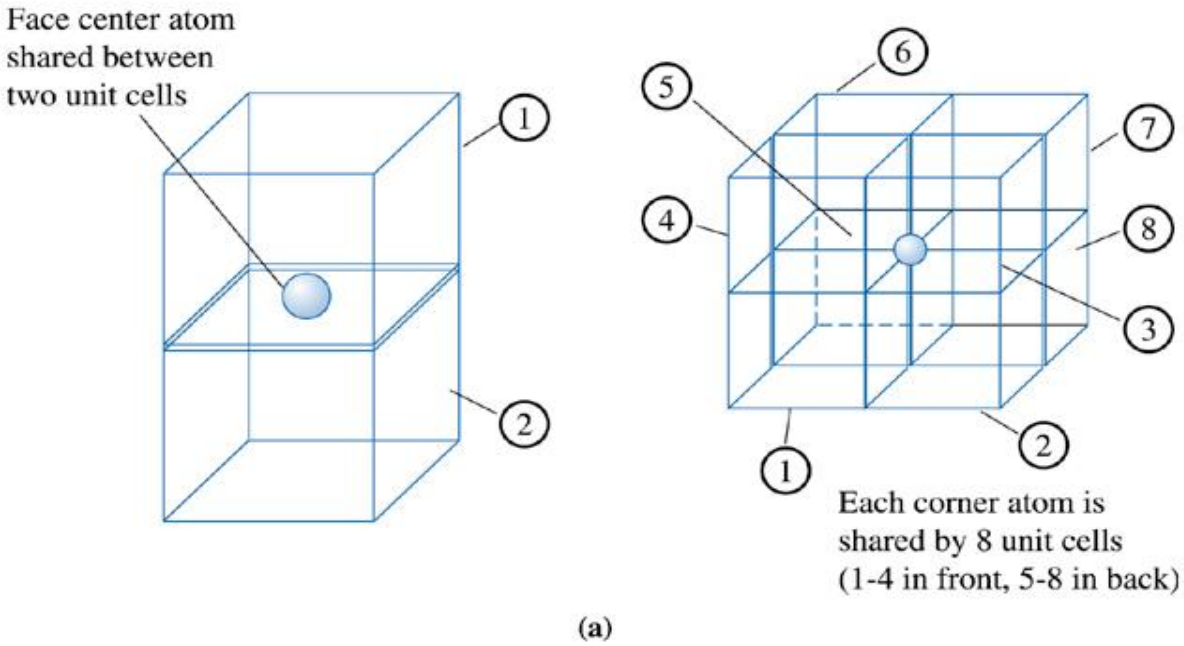


Grupos (pontos, espaciais)

Crystal system	No. of point groups	No. of bravais lattices	No. of space groups
Triclinic	2	1	2
Monoclinic	3	2	13
Orthorhombic	3	4	59
Tetragonal	7	2	68
Rhombohedral (Trigonal)	5	1	25
Hexagonal	7	1	27
Cubic	5	3	36
Total	32	14	230

Crystal system	Point group		#	Space groups (international short symbol)
	Hermann-Mauguin	Schönflies		
Triclinic (2)	1	C_1	1	P1
	$\bar{1}$	C_i	2	$P\bar{1}$
Monoclinic (13)	2	C_2	3-5	P2, $P2_1$, C2
	m	C_s	6-9	Pm, Pc, Cm, Cc
	2/m	C_{2h}	10-15	P2/m, $P2_1/m$, C2/m, P2/c, $P2_1/c$, C2/c
Orthorhombic (59)	222	D_2	16-24	P222, $P222_1$, $P2_12_12$, $P2_12_12_1$, $C222_1$, C222, F222, I222, $I2_12_12_1$
	mm2	C_{2v}	25-46	Pmm2, $Pmc2_1$, Pcc2, Pma2, $Pca2_1$, Pnc2, $Pmn2_1$, Pba2, $Pna2_1$, Pnn2, Cmm2, $Cmc2_1$, Ccc2, Amm2, Aem2, Ama2,Aea2, Fmm2, Fdd2, Imm2, Iba2, Ima2
	mmm	D_{2h}	47-74	Pmmm, Pnnn, Pccm, Pban, Pmma, Pnna, Pmna, Pcca, Pbam, Pccn, Pbcm, Pnnm, Pmmn, Pbcn, Pbca, Pnma, Cmcm, Cmce, Cmmm, Cccm, Cmme, Ccce, Fmmm, Fddd, Immm, Ibam, Ibca, Imma
Tetragonal (68)	4	C_4	75-80	P4, $P4_1$, $P4_2$, $P4_3$, I4, $I4_1$
	$\bar{4}$	S_4	81-82	$P\bar{4}$, $I\bar{4}$
	$\bar{4}$/m	C_{4h}	83-88	P4/m, $P4_2/m$, P4/n, $P4_2/n$, I4/m, $I4_1/a$
	422	D_4	89-98	P422, $P42_12$, $P4_122$, $P4_12_12$, $P4_222$, $P4_22_12$, $P4_322$, $P4_32_12$, I422, $I4_122$
	4mm	C_{4v}	99-110	P4mm, P4bm, $P4_2cm$, $P4_2nm$, P4cc, P4nc, $P4_2mc$, $P4_2bc$, I4mm, I4cm, $I4_1md$, $I4_1cd$
	$\bar{4}$2m	D_{2d}	111-122	$P\bar{4}2m$, $P\bar{4}2c$, $P\bar{4}2_1m$, $P\bar{4}2_1c$, $P\bar{4}m2$, $P\bar{4}c2$, $P\bar{4}b2$, $P\bar{4}n2$, $I\bar{4}m2$, $I\bar{4}c2$, $I\bar{4}2m$, $I\bar{4}2d$
	4/mmm	D_{4h}	123-142	P4/mmm, P4/mcc, P4/nbm, P4/nnc, P4/mbm, P4/mnc, P4/nmm, P4/ncc, $P4_2/mmc$, $P4_2/mcm$, $P4_2/nbc$, $P4_2/nnm$, $P4_2/mbc$, $P4_2/mnm$, $P4_2/nmc$, $P4_2/ncm$, I4/mmm, I4/mcm, $I4_1/amd$, $I4_1/acd$
Trigonal (25)	3	C_3	143-146	P3, $P3_1$, $P3_2$, R3
	$\bar{3}$	S_6	147-148	$P\bar{3}$, $R\bar{3}$
	32	D_3	149-155	P312, P321, $P3_112$, $P3_121$, $P3_212$, $P3_221$, R32
	3m	C_{3v}	156-161	P3m1, P31m, P3c1, P31c, R3m, R3c
	$\bar{3}$m	D_{3d}	162-167	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$,$R\bar{3}m$, $R\bar{3}c$,
Hexagonal (27)	6	C_6	168-173	P6, $P6_1$, $P6_5$, $P6_2$, $P6_4$, $P6_3$
	$\bar{6}$	C_{3h}	174	$P\bar{6}$
	6/m	C_{6h}	175-176	P6/m, $P6_3/m$
	622	D_6	177-182	P622, $P6_122$, $P6_522$, $P6_222$, $P6_422$, $P6_322$
	6mm	C_{6v}	183-186	P6mm, P6cc, $P6_3cm$, $P6_3mc$
	$\bar{6}$m2	D_{3h}	187-190	$P\bar{6}m2$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$
	6/mmm	D_{6h}	191-194	P6/mmm, P6/mcc, $P6_3/mcm$, $P6_3/mmc$
Cubic (36)	23	T	195-199	P23, F23, I23, $P2_13$, $I2_13$
	m$\bar{3}$	T_h	200-206	Pm$\bar{3}$, Pn$\bar{3}$, Fm$\bar{3}$, Fd$\bar{3}$, Im$\bar{3}$, Pa$\bar{3}$, Ia$\bar{3}$
	432	O	207-214	P432, $P4_232$, F432, $F4_132$, I432, $P4_332$, $P4_132$, $I4_132$
	$\bar{4}$3m	T_d	215-220	$P\bar{4}3m$, $F\bar{4}3m$, $I\bar{4}3m$, $P\bar{4}3n$, $F\bar{4}3c$, $I\bar{4}3d$
	m$\bar{3}$m	O_h	221-230	Pm$\bar{3}$m, Pn$\bar{3}$n, Pm$\bar{3}$n, Pn$\bar{3}$m, Fm$\bar{3}$m, Fm$\bar{3}$c, Fd$\bar{3}$m, Fd$\bar{3}$c, Im$\bar{3}$m, Ia$\bar{3}$d

Associando átomos a uma rede em estruturas metálicas



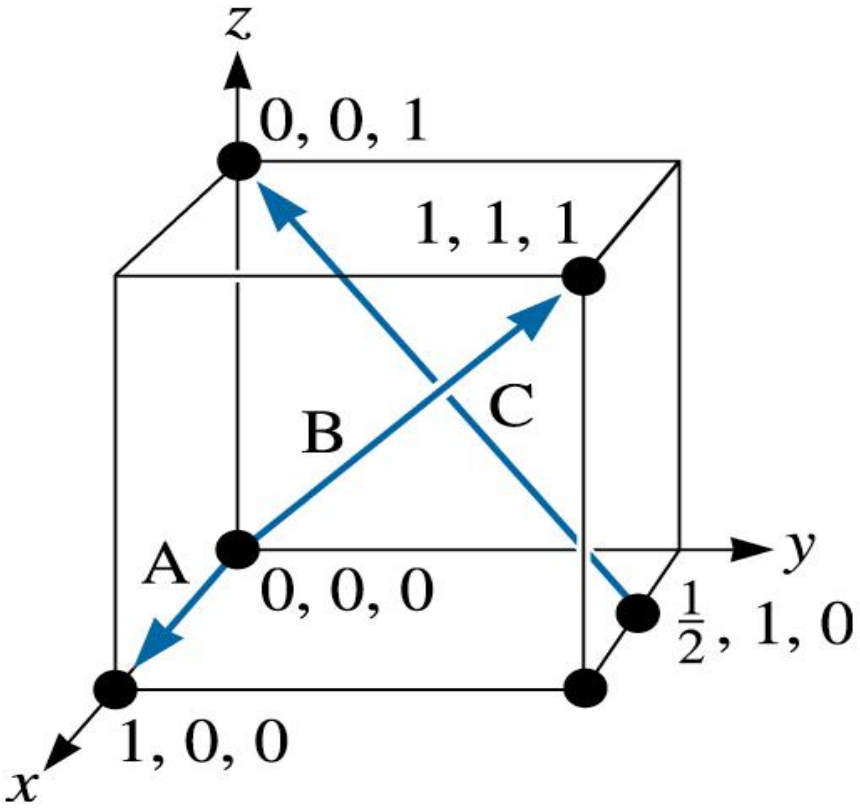
Fator de Empacotamento

TABLE 3-2 ■ *Crystal structure characteristics of some metals*

Structure	a_0 versus r	Atoms per Cell	Coordination Number	Packing Factor	Examples
Simple cubic (SC)	$a_0 = 2r$	1	6	0.52	Polonium (Po), α-Mn
Body-centered cubic	$a_0 = 4r/\sqrt{3}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
Face-centered cubic	$a_0 = 4r/\sqrt{2}$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
Hexagonal close-packed	$a_0 = 2r$ $c_0 \approx 1.633a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd

Demonstrar exemplo de cálculo

Direções



Notação empregada:
Índices de Miller
[hkl] e <hkl>

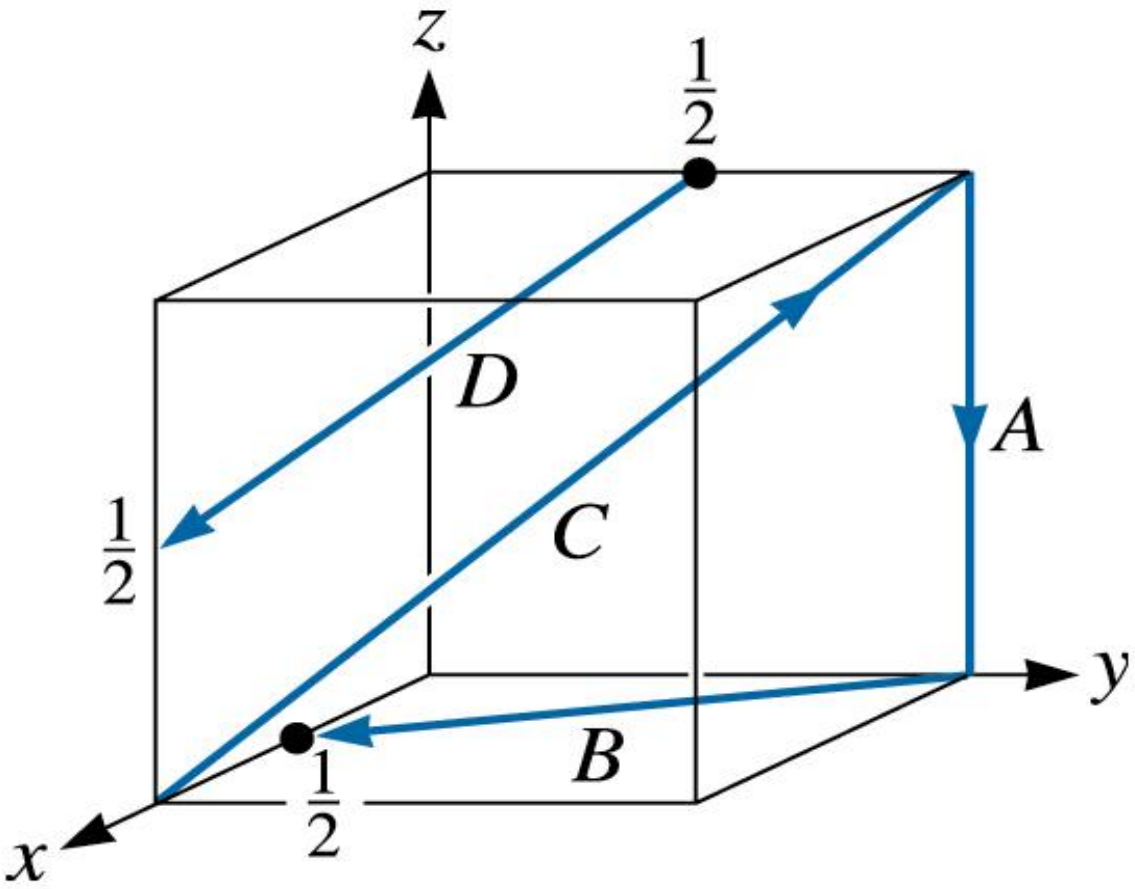


Figure 3.48 Directions in a cubic unit cell for Problem 3.51

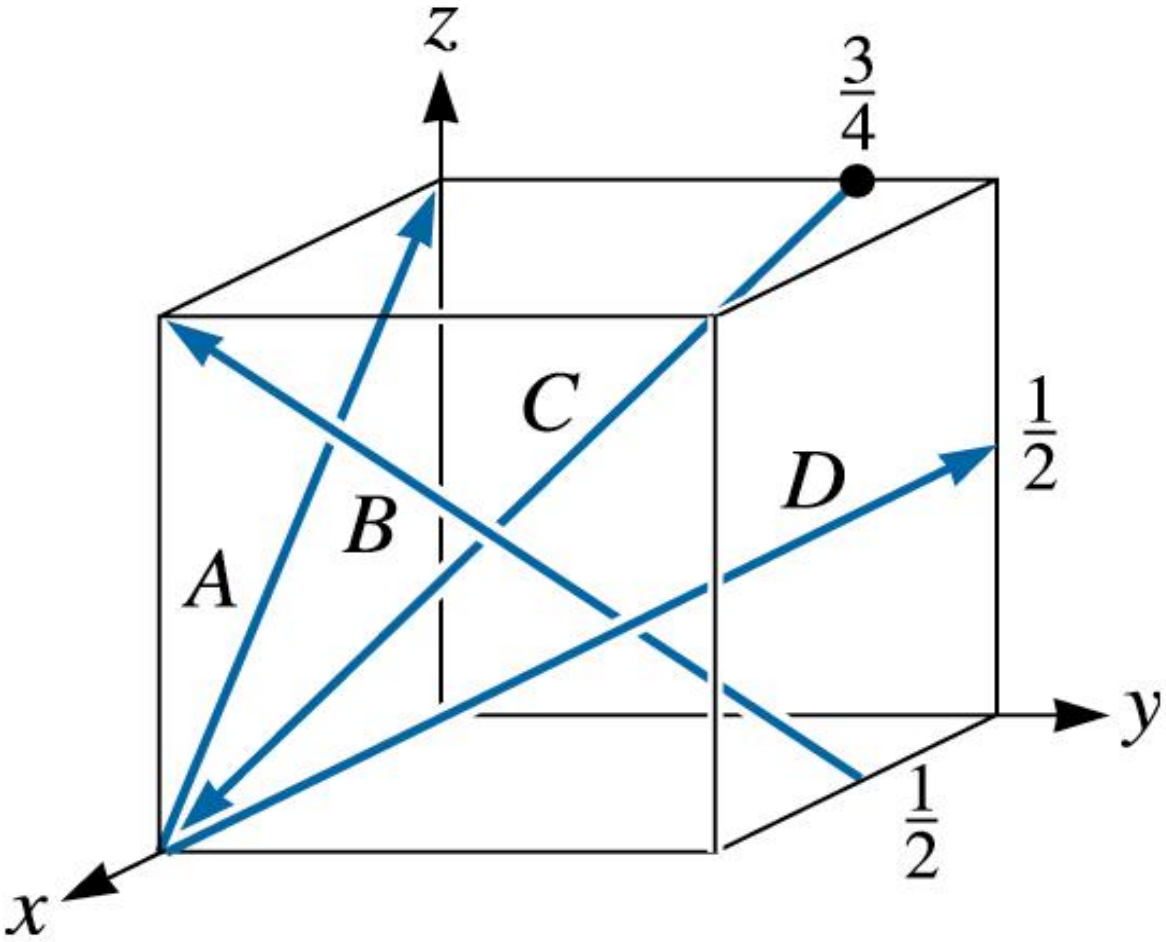
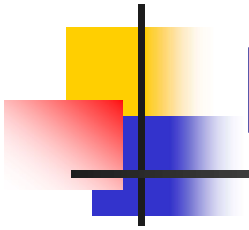


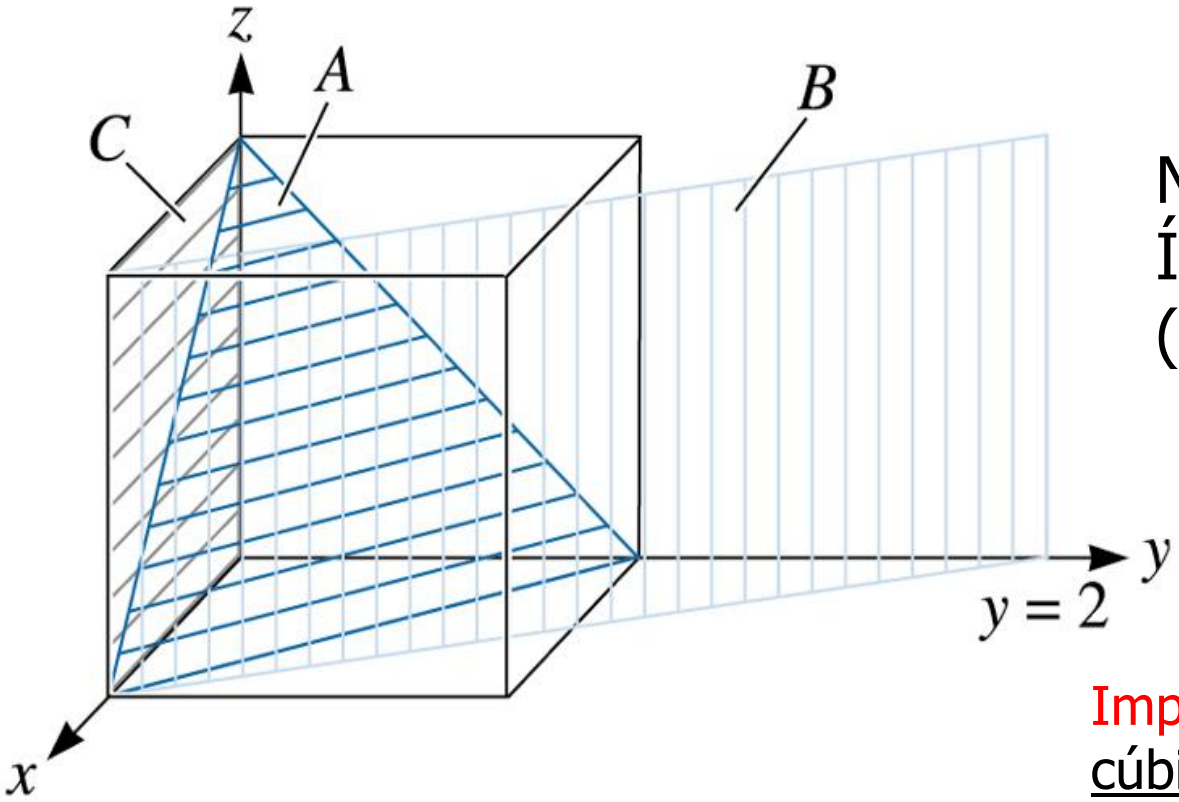
Figure 3.49 Directions in a cubic unit cell for Problem 3.52.



Densidade Linear

- Exemplo

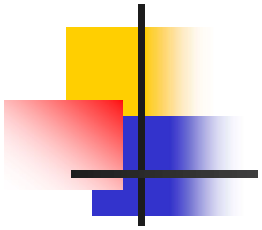
Planos

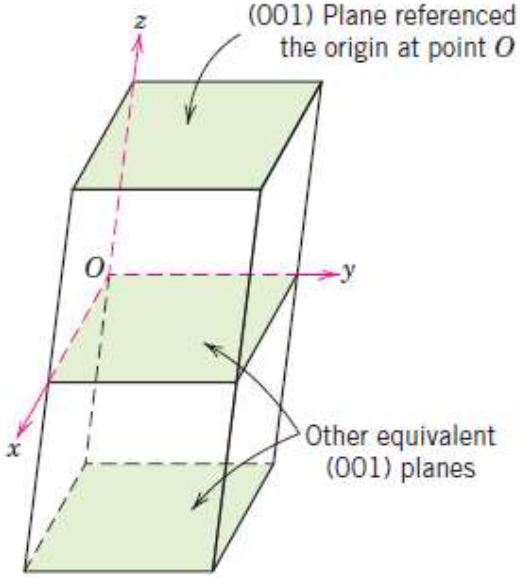


Notação empregada:
Índices de Miller
(hkl) e {hkl}

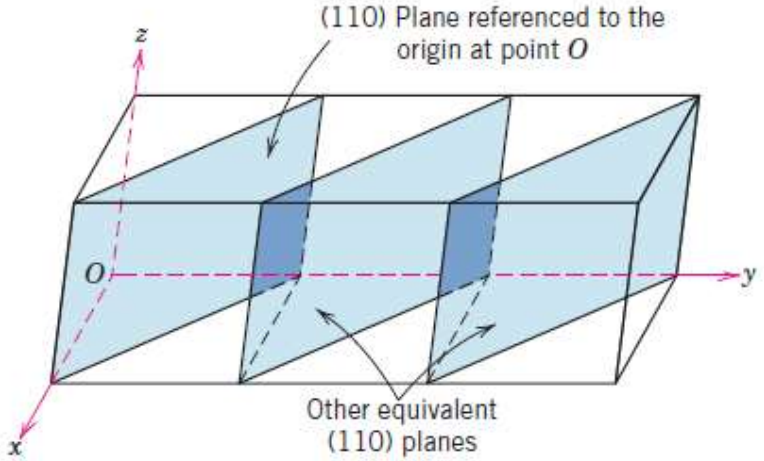
Exemplos: CCC e CFC

Importante: no sistema cúbico as direções [hkl] são perpendiculares aos planos (hkl)

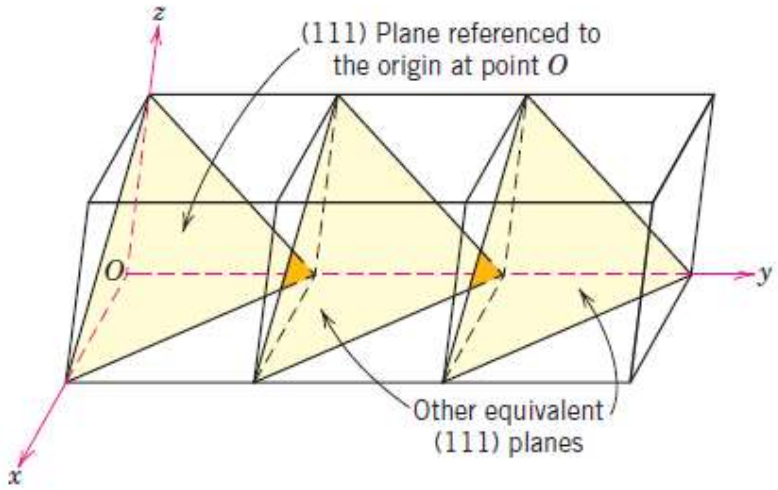



z
(001) Plane referenced to
the origin at point O
O
y
x
Other equivalent
(001) planes

(a)


z
(110) Plane referenced to the
origin at point O
O
y
x
Other equivalent
(110) planes

(b)


z
(111) Plane referenced to
the origin at point O
O
y
x
Other equivalent
(111) planes

(c)

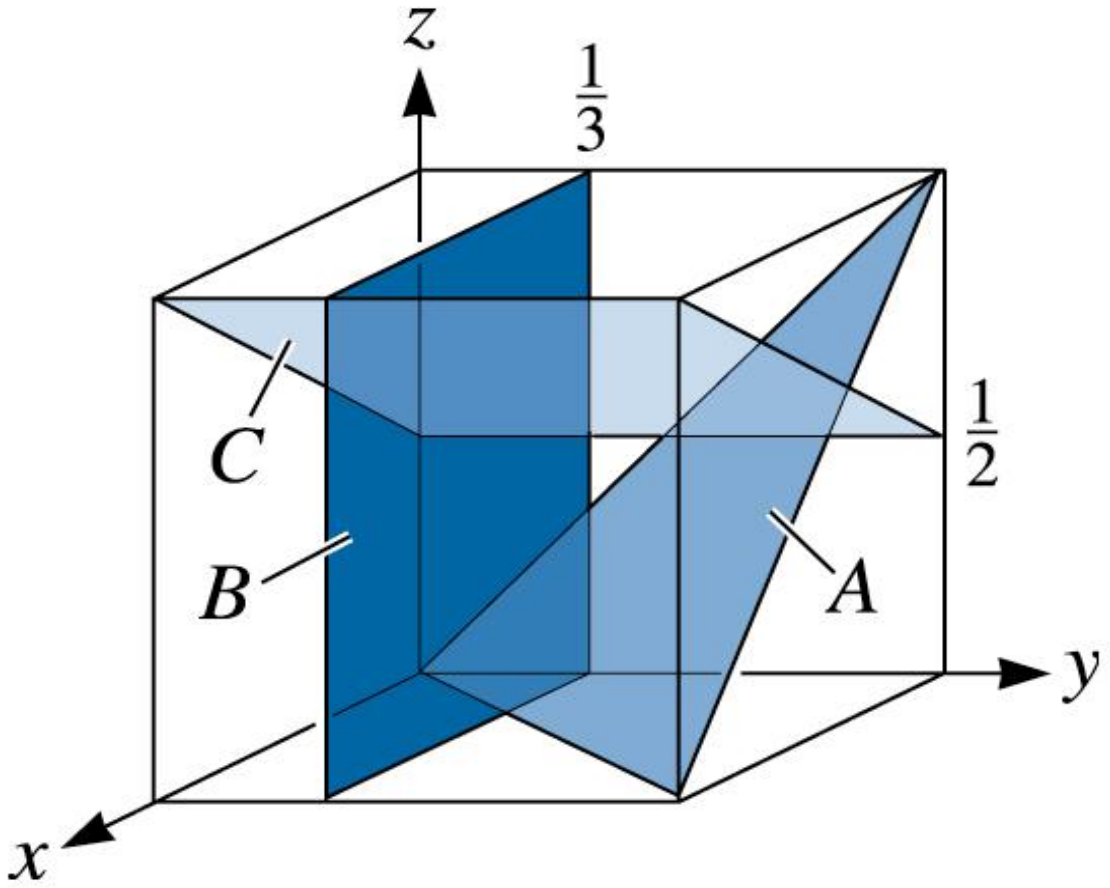


Figure 3.50 Planes in a cubic unit cell for Problem 3.53.

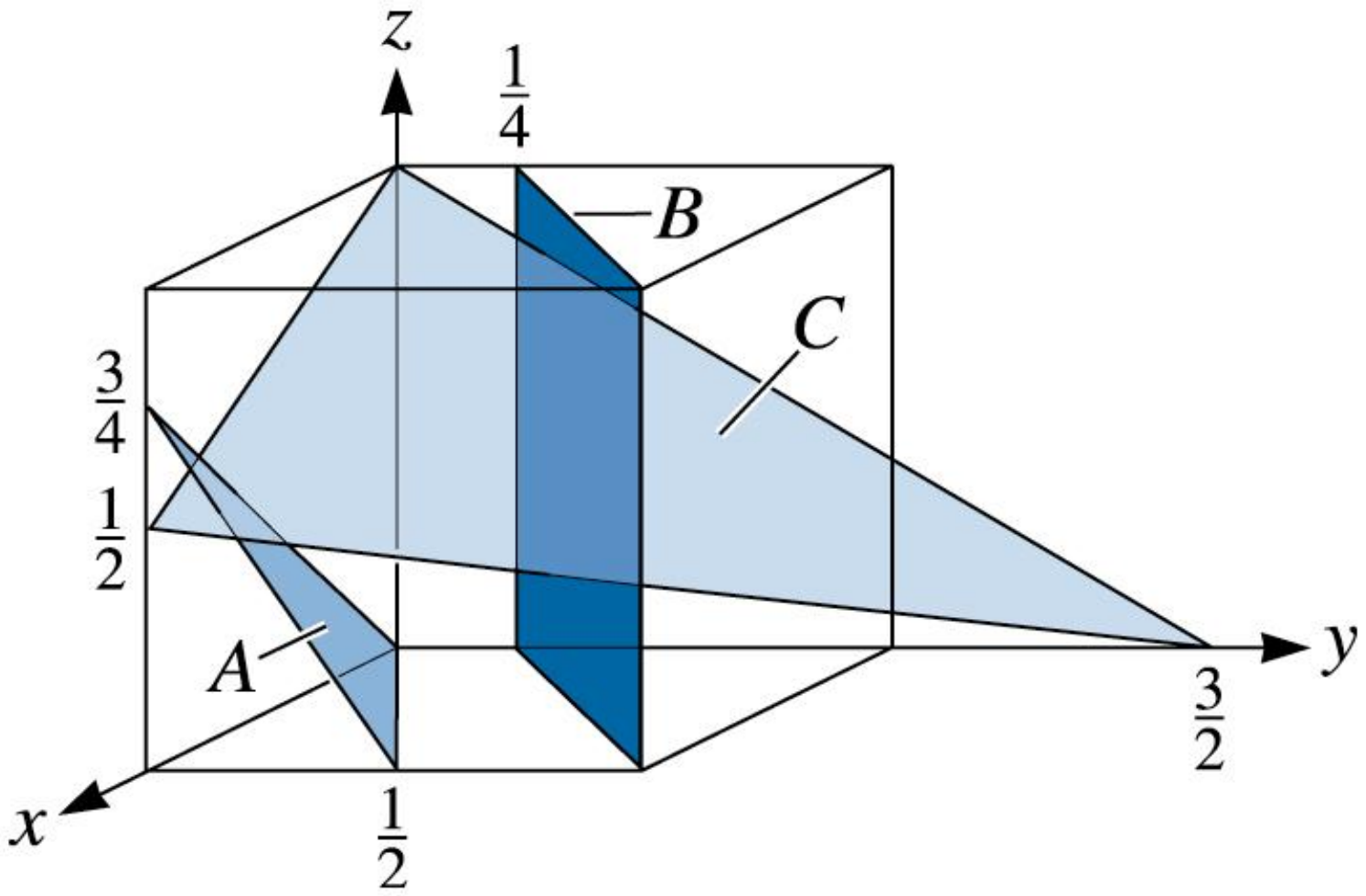
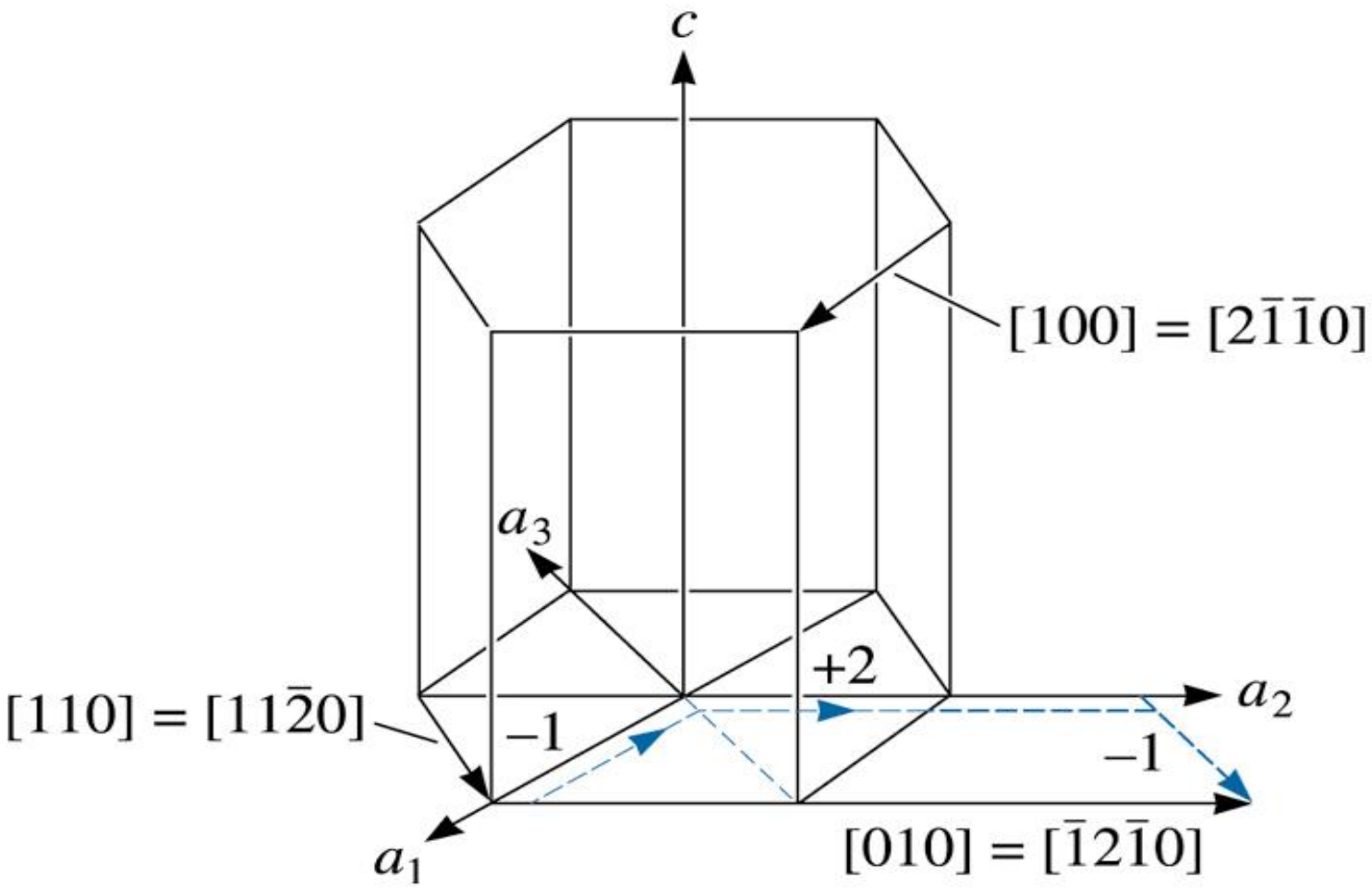


Figure 3.51 Planes in a cubic unit cell for Problem 3.54.

Direções (sist. hexagonal)



Índices no sistema hexagonal

- Por que usar a notação de Miller-Bravais de 4 índices?
  - Para que as direções [hkil] e planos (hkil) equivalentes tenham um conjunto similar de índices.

Conversões de índices

- Miller-Bravais para Miller
  - Direções: [uvtw] para [u'v'w']
    - u'=u-t, v'=v-t e w'=w
  - Planos: (hkil) para (h'k'l')
    - h'=h, k'=k e l'=l
- Miller para Miller-Bravais
  - Direções: [uvw] para [u'v't'w']
    - u'=(2u-v)/3, v'=(2v-u)/3, t'=-(u+v)/3=-(u'+v') e w'=w
  - Planos: (hkl) para (h'k'i'l')
    - h'=h, k'=k, i'=-(h+k) e l'=l

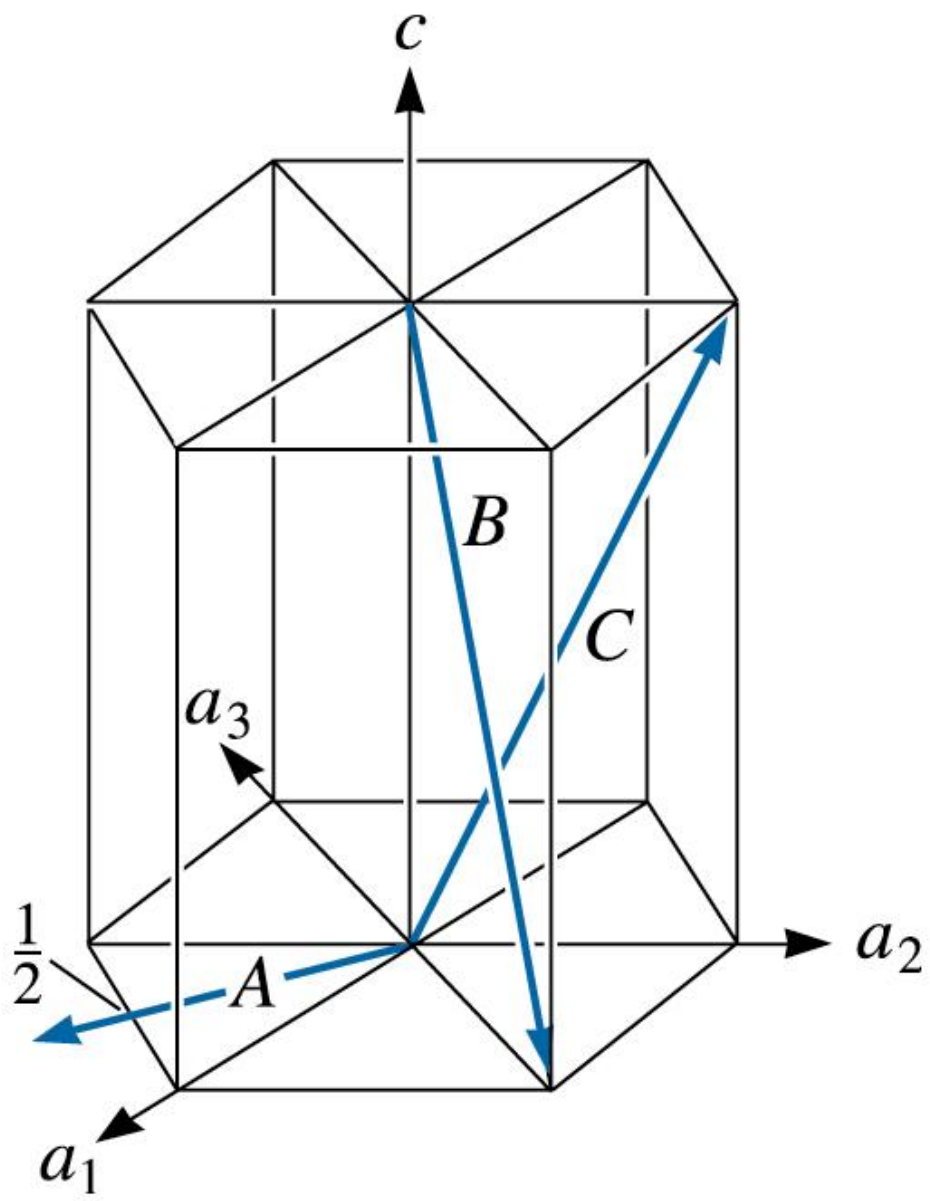


Figure 3.52
Directions in a hexagonal lattice for Problem 3.55.

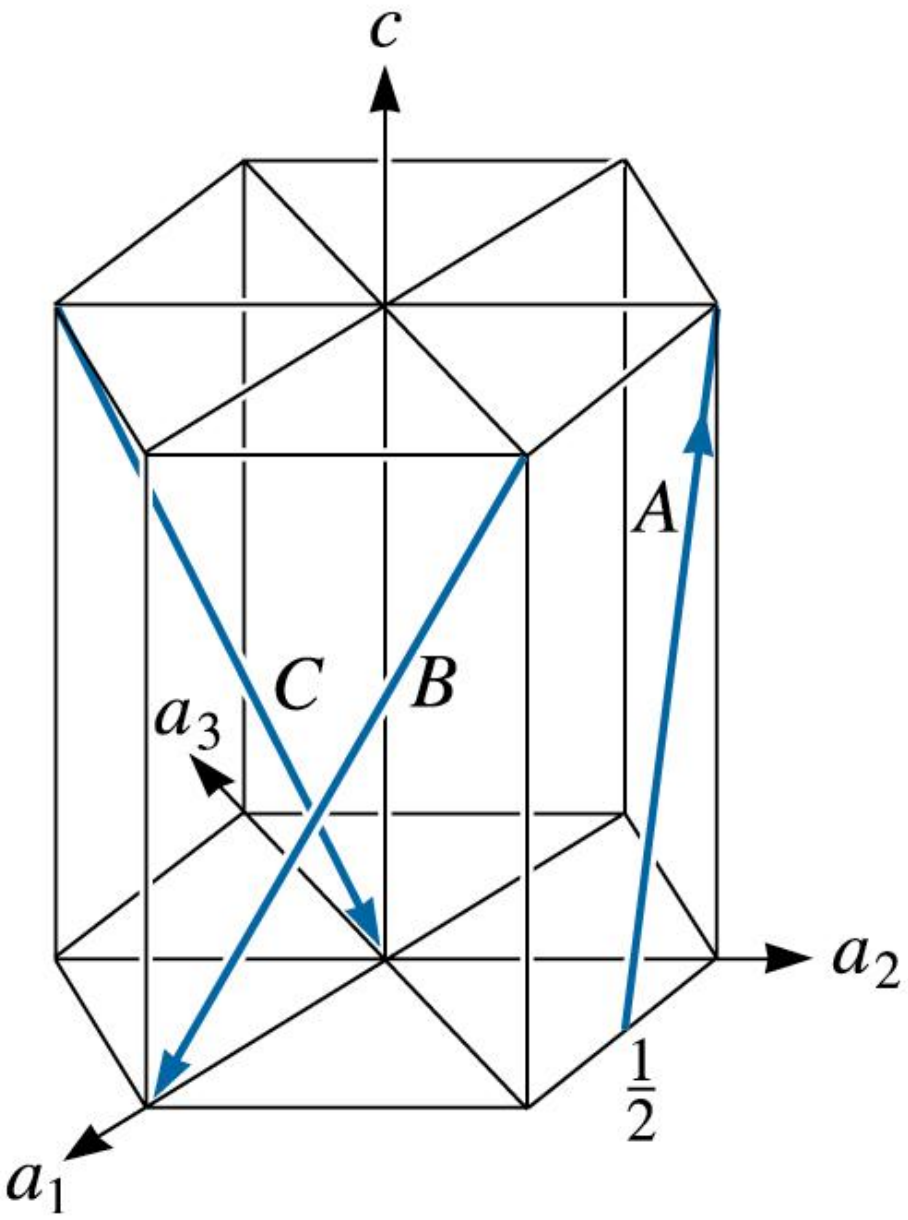
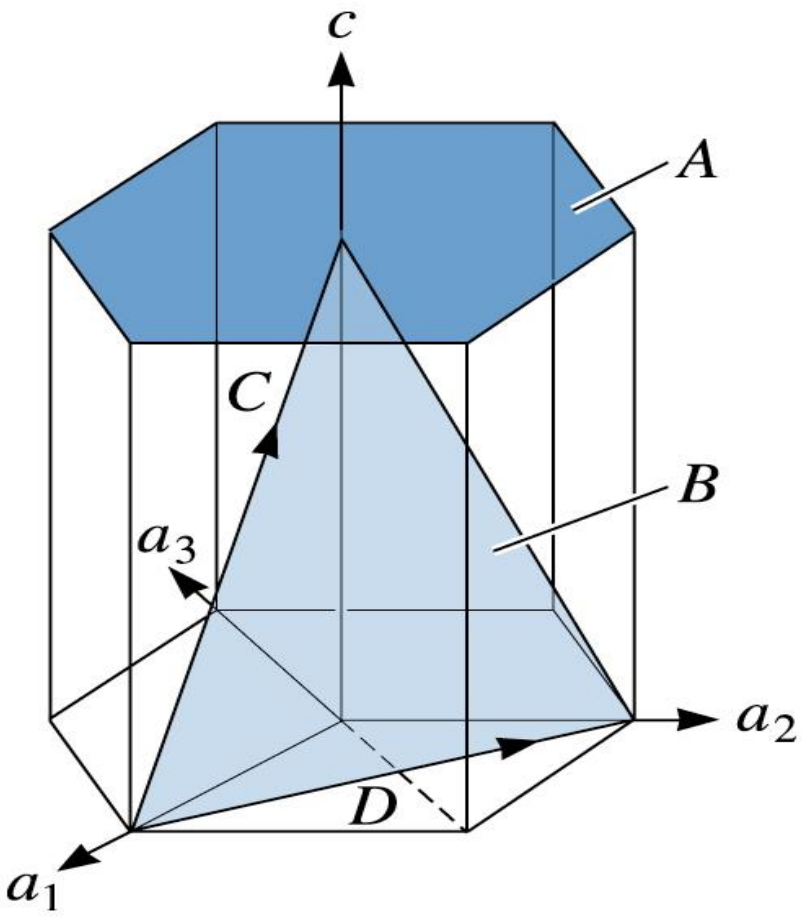


Figure 3.53 Directions in a hexagonal lattice for Problem 3.56.

Planos (sist. Hexagonal)



Exemplos

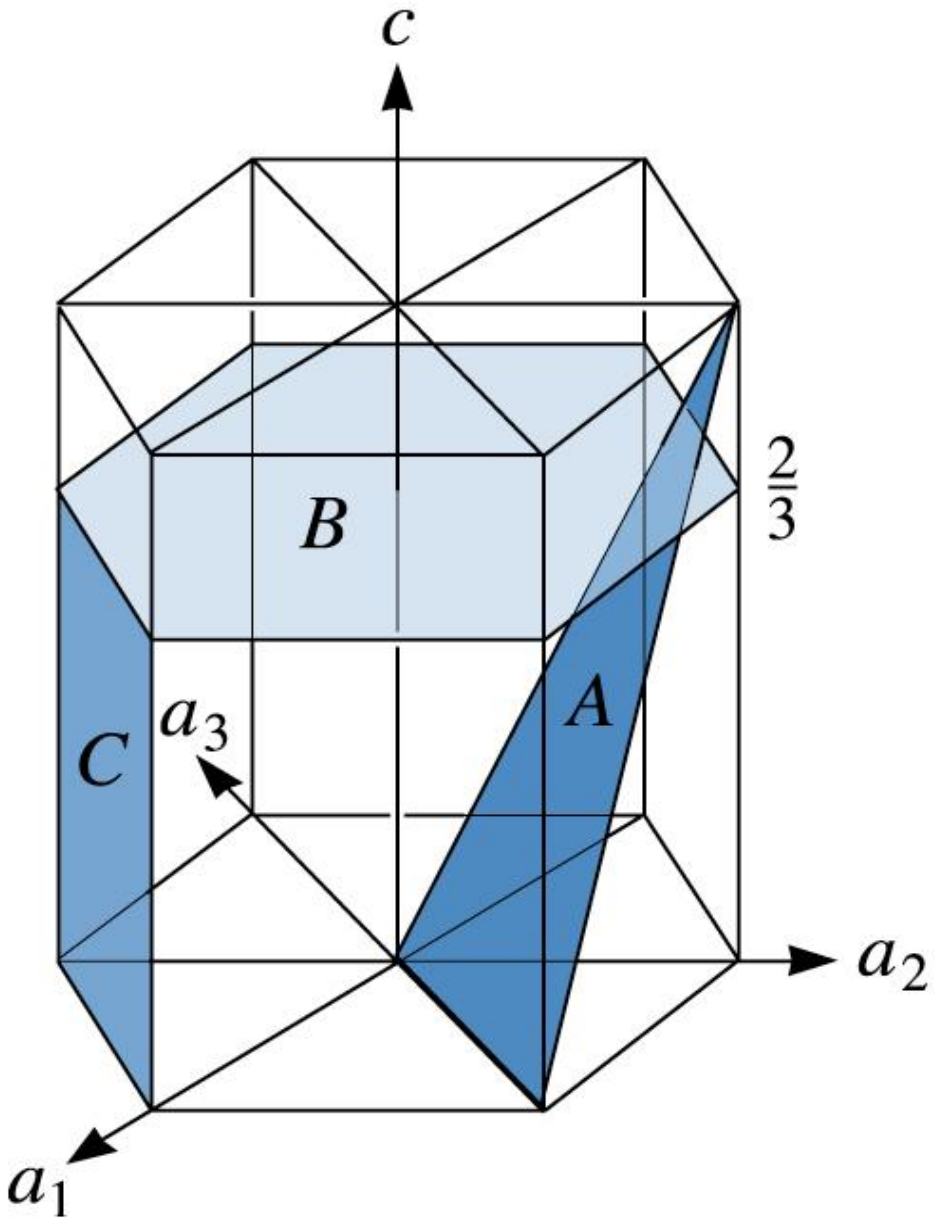


Figure 3.54 Planes in a hexagonal lattice for Problem 3.57.

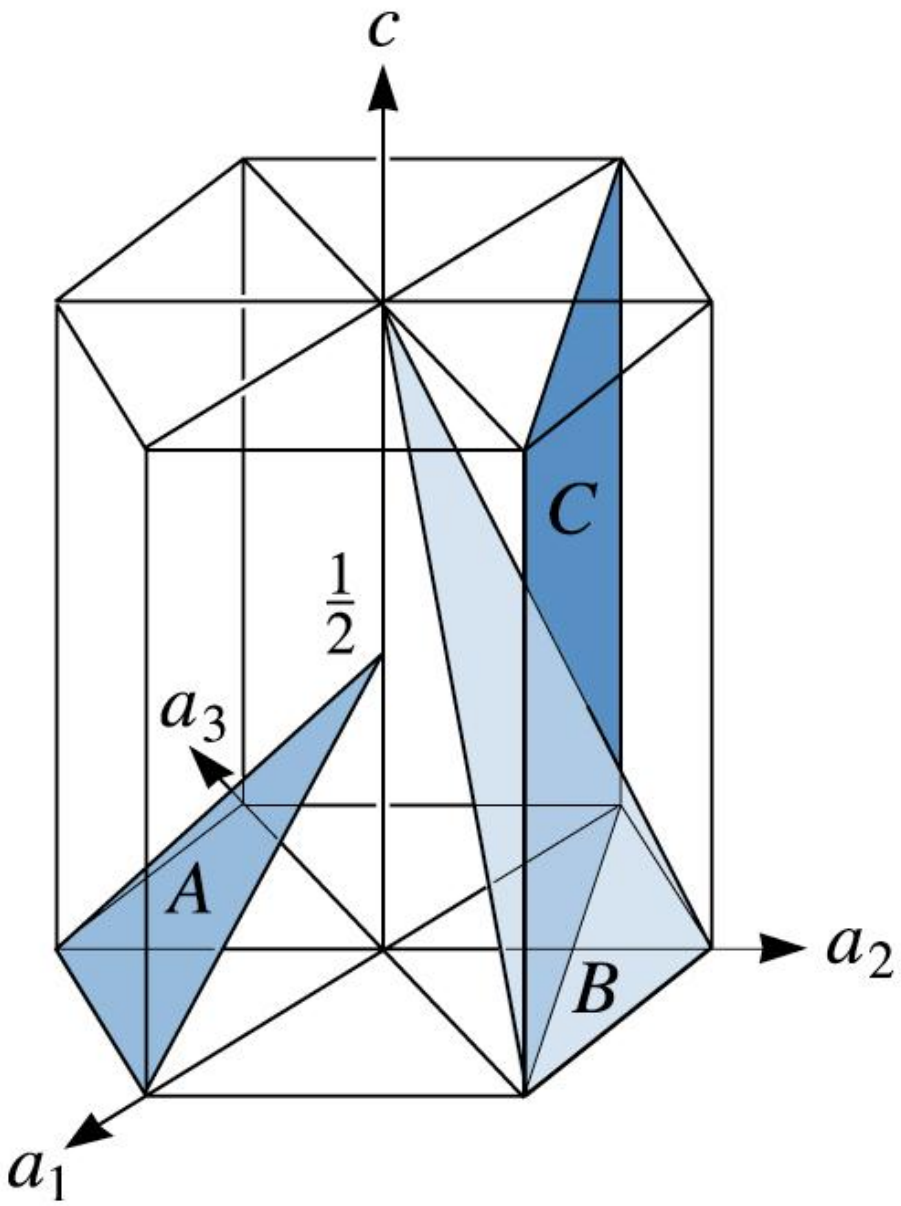
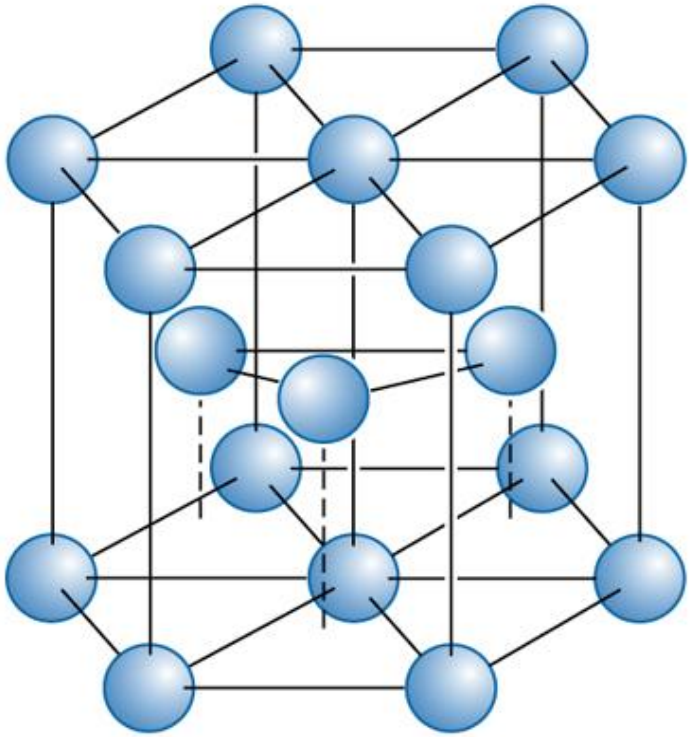
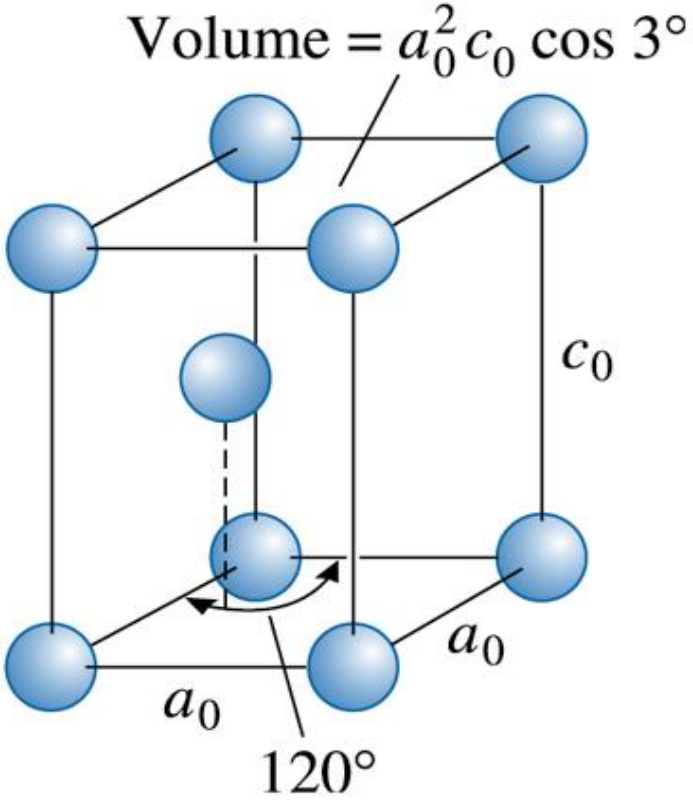


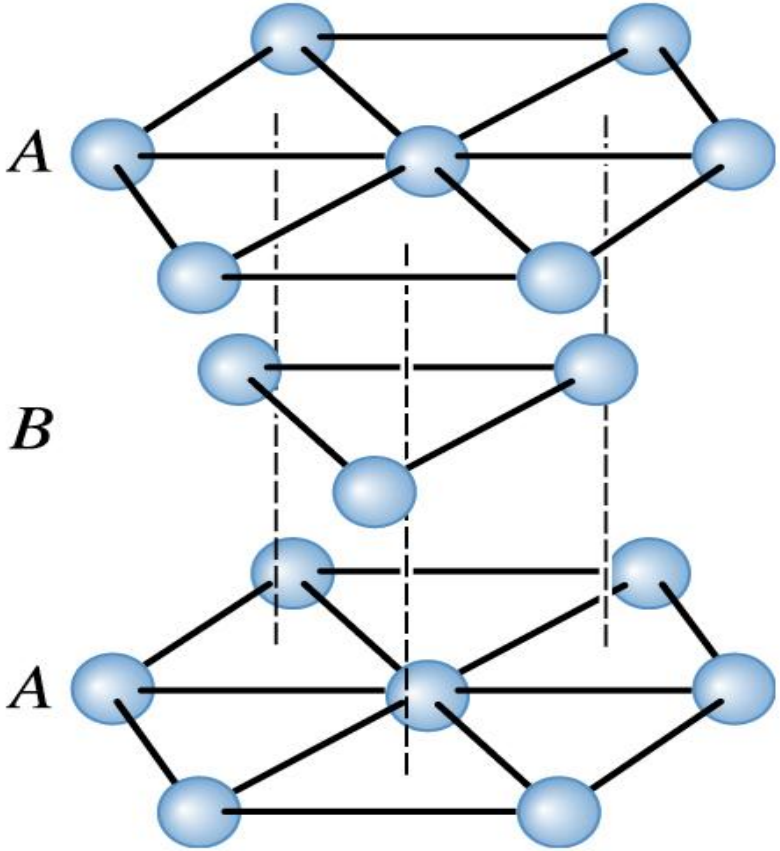
Figure 3.55 Planes in a hexagonal lattice for Problem 3.58.

Estrutura hexagonal compacta (HCP)

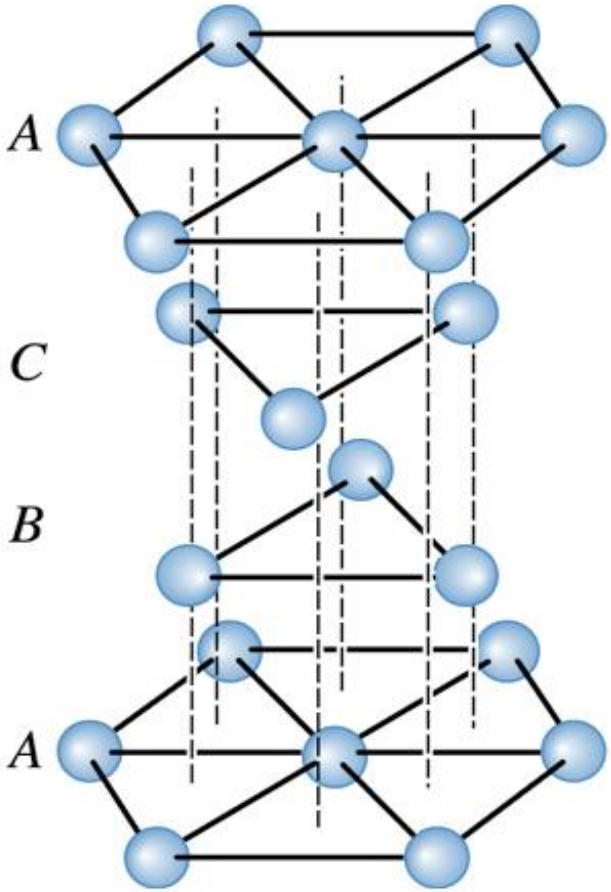


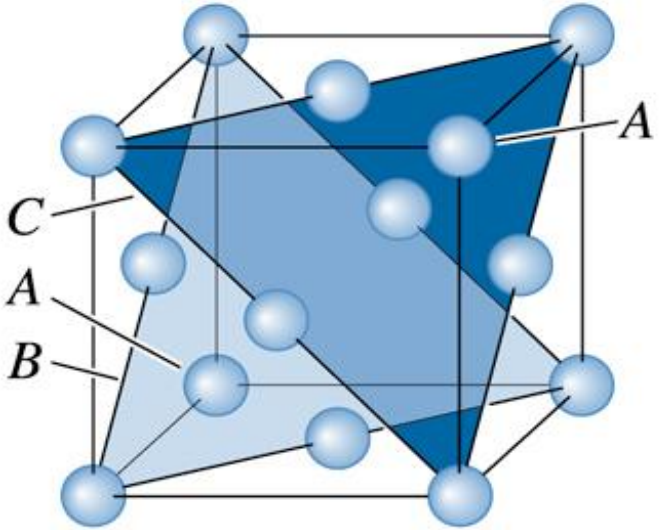


HCP (empilhamento de planos)

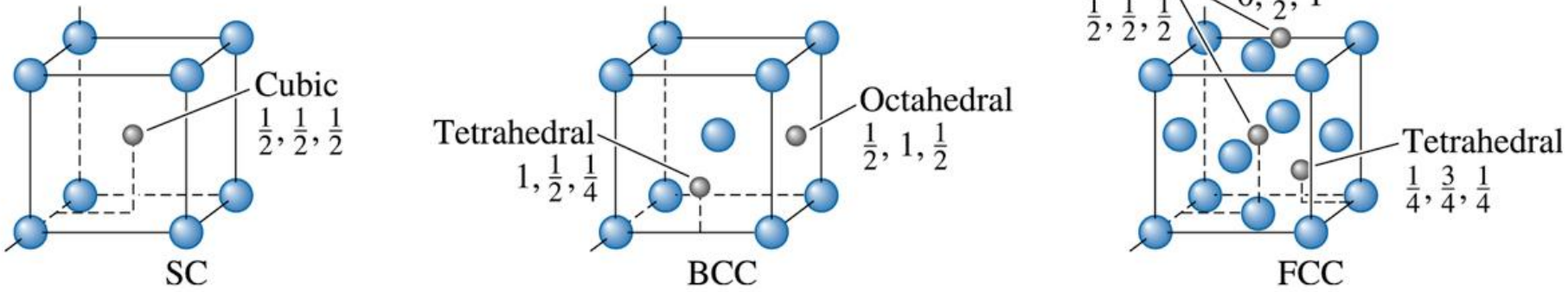


CFC (empilhamento de planos)

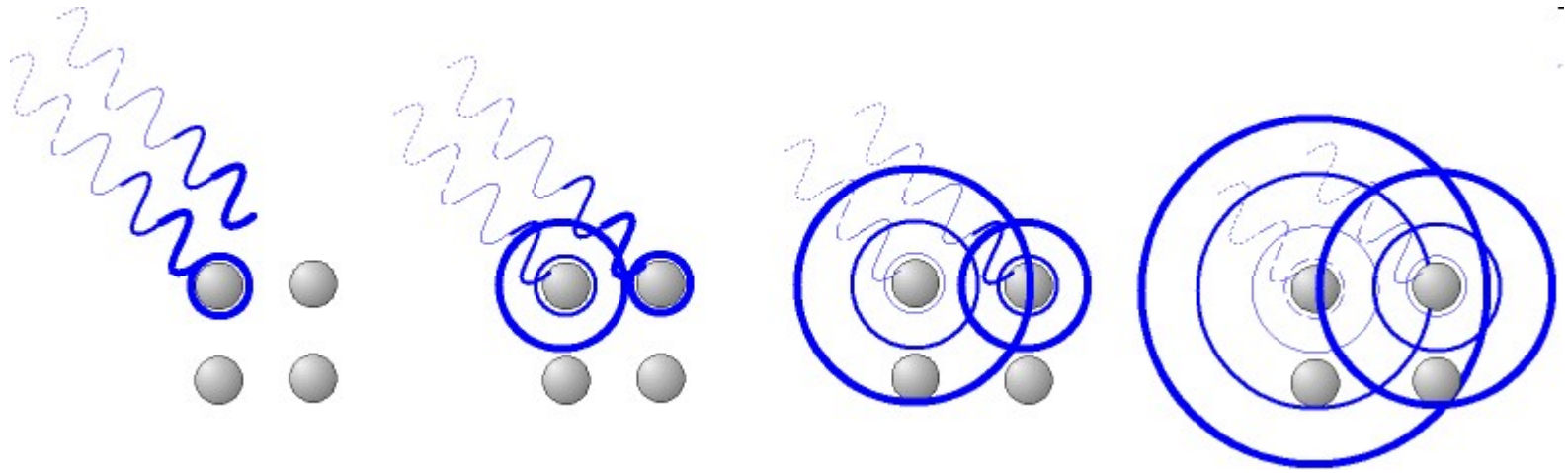




Interstícios

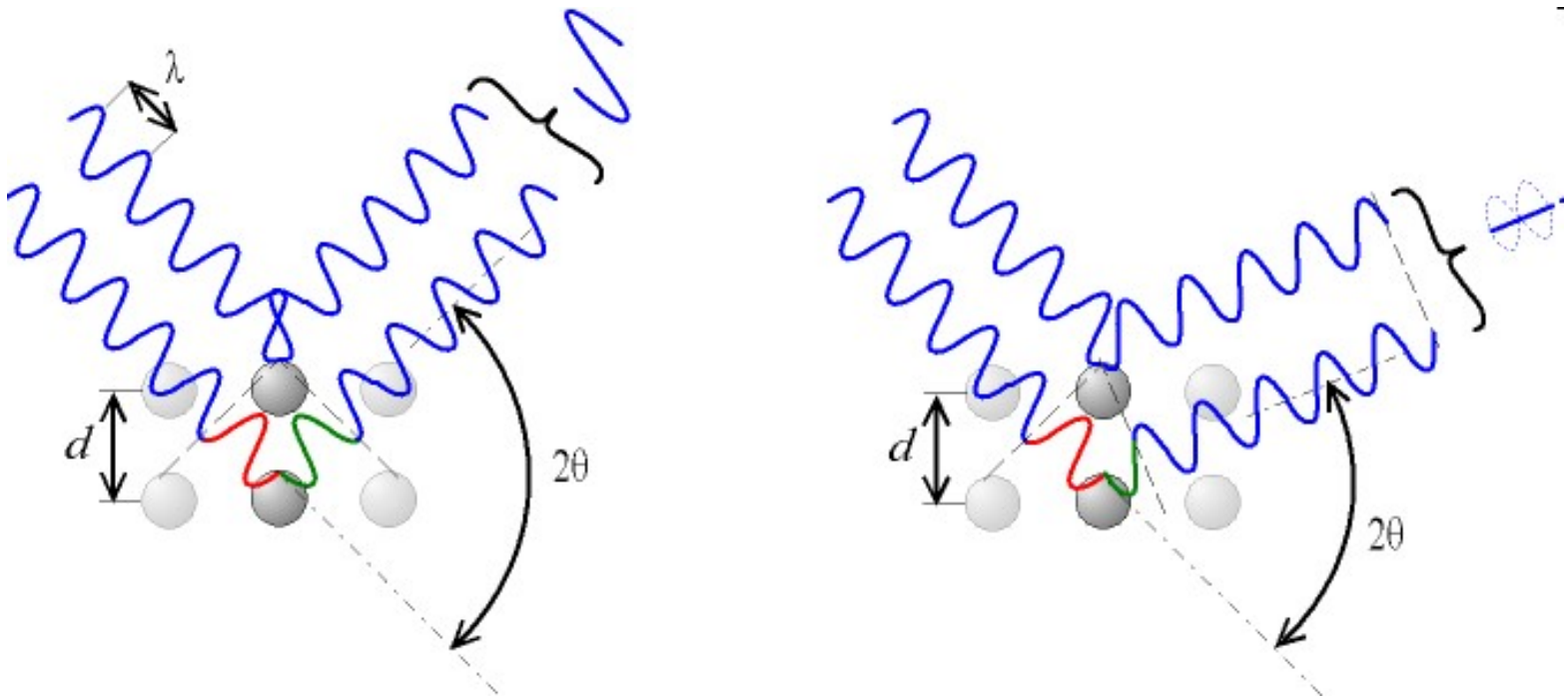


Espalhamento de raios-X pelos átomos



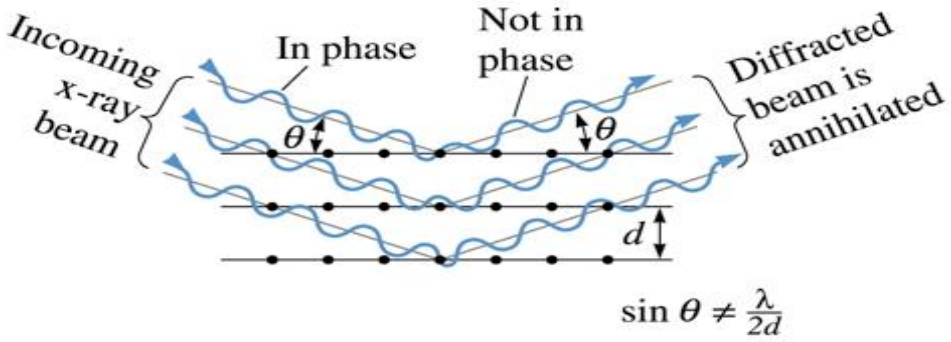
Cada átomo é um centro de espalhamento do raio-X incidente para todas as direções

O fenômeno da Difração

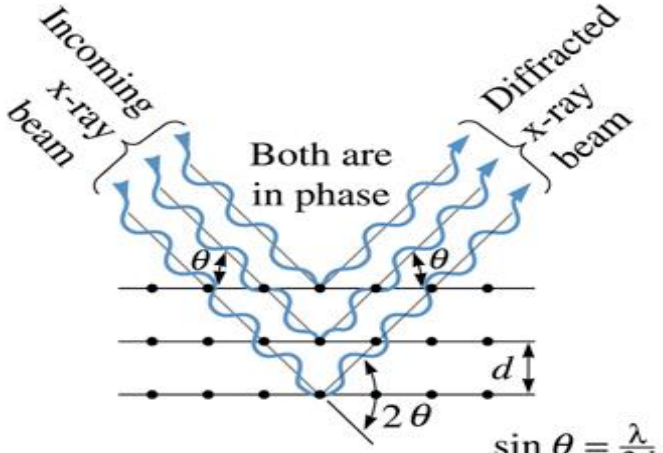


Somente direções específicas produzem interferência construtiva

A Lei de Bragg



(a)



(b)

Lei de Bragg

É necessária mas não suficiente para a difração.

Fator estrutural para a difração

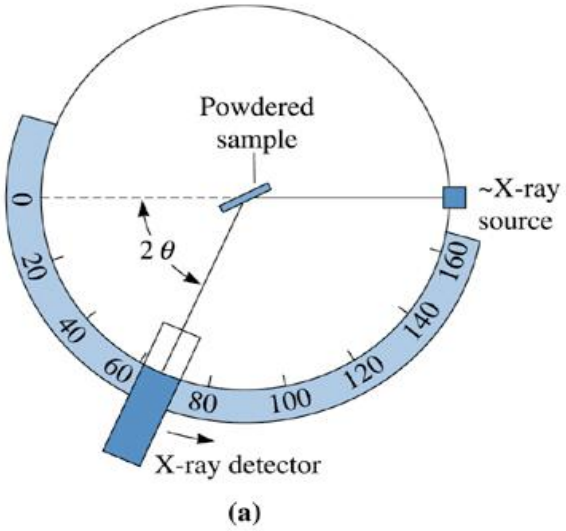
p/ CCC

$$F_{hkl} = \begin{cases} 2f, & h+k+l = par \\ 0, & h+k+l = \acute{i}mpar \end{cases}$$

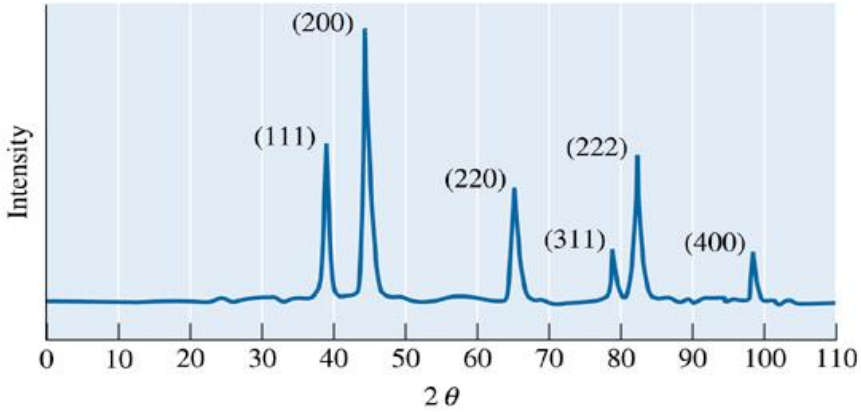
p/ CFC

$$F_{hkl} = \begin{cases} 4f, & h,k,l \rightarrow \acute{i}mpares \\ 4f, & h,k,l \rightarrow pares \\ 0, & h,k,l \rightarrow mistos \end{cases}$$

Difratograma



(a)



(b)

Metais Amorfos

- Exibem somente ordem de curto alcance
- Cristalizam no aquecimento
- Podem apresentar transição vítrea
- Propriedades diferentes com relação aos equivalentes cristalinos, maior RM, menor E, maior dureza, maior resist. à corrosão, etc.