

ESCOLA POLITÉCNICA DA UNIVERSIDADE DE SÃO PAULO  
Departamento de Engenharia Metalúrgica e de Materiais



Fundamentos de Ciência e Engenharia de Materiais

Prof. Dr. André Paulo Tschiptschin

CRISTALOGRAFIA E DIFRAÇÃO DE  
RAIOS-X

# RETICULADO CRISTALINO

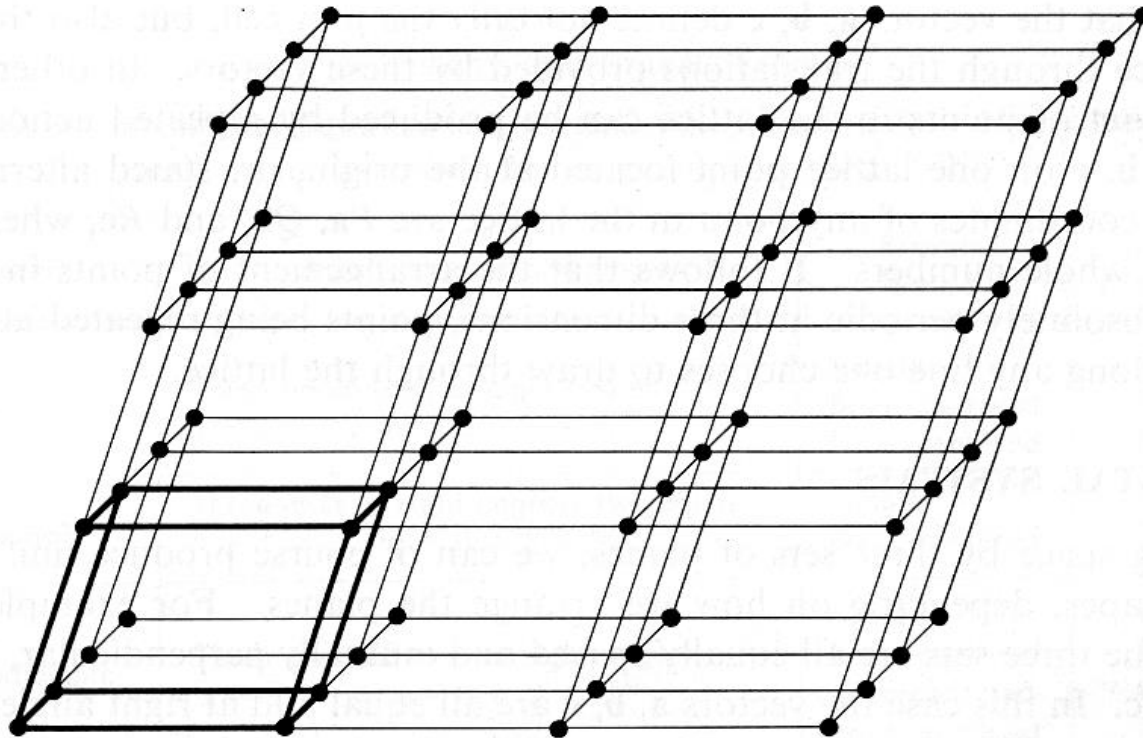
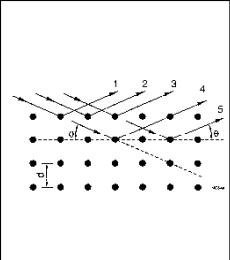
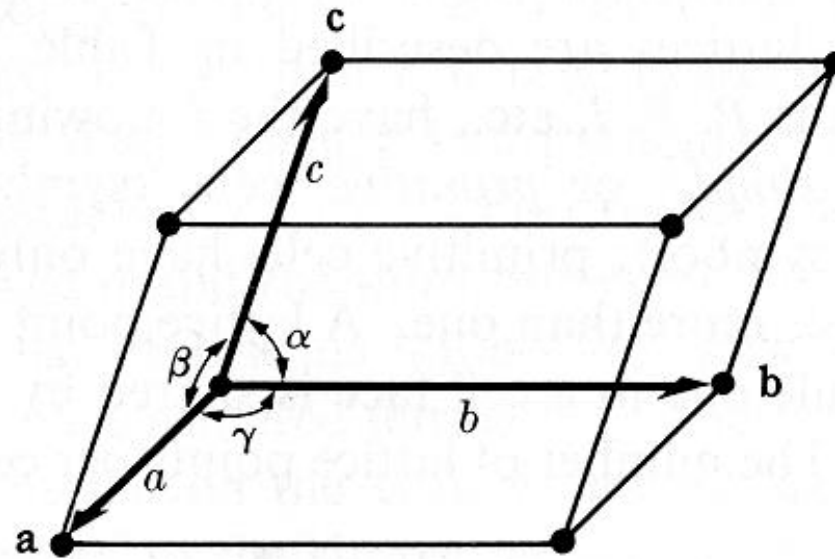
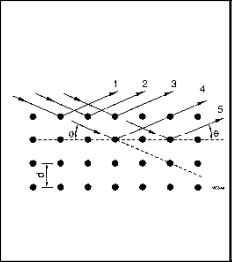


Fig. 2-1 A point lattice.

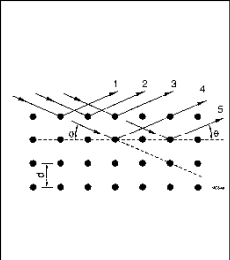
# CÉLULA UNITÁRIA



**Fig. 2-2** A unit cell.

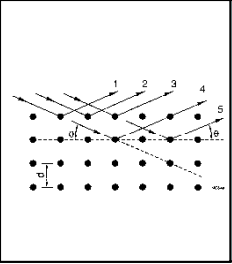
## CRYSTAL SYSTEMS AND BRAVAIS LATTICES

(The symbol  $\neq$  implies nonequality by reason of symmetry. Accidental equality may occur, as shown by an example in Sec. 2-4.)



System	Axials lengths and angles	Bravais lattice	Lattice symbol
Cubic	Three equal axes at right angles $a = b = c, \alpha = \beta = \gamma = 90^\circ$	Simple Body-centered Face-centered	P I F
Tetragonal	Three axes at right angles, two equal $a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	Simple Body-centered	P I
Orthorhombic	Three unequal axes at right angles $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	Simple Body-centered Base-centered Face-centered	P I C F
Rhombohedral*	Three equal axes, equally inclined $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	Simple	P
Hexagonal	Two equal coplanar axes at $120^\circ$ , third axis at right angles $a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	Simple	P
Monoclinic	Three unequal axes, one pair not at right angles $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$	Simple Base-centered	P C
Triclinic	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	Simple	P

\* Also called trigonal.



# CÉLULA UNITÁRIA

Qualquer reticulado cristalino pode ser descrito por um dos 14 reticulados de Bravais.

P = Primitivo (Simples)

F = Face centrada

I = Corpo centrado (Interior)

A, B, C = Base centrada

R = Romboédrico

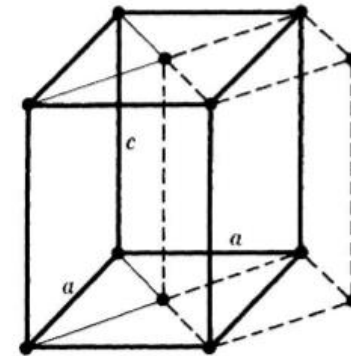


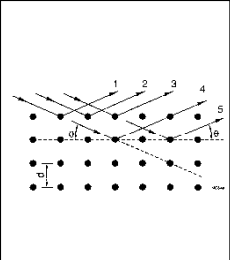
FIG. 2-4. Relation of tetragonal *C* lattice (full lines) to tetragonal *P* lattice (dashed lines).

O número de pontos I contribui com 1 átomo por célula

O número de pontos F contribui com  $\frac{1}{2}$  átomo por célula

O número de pontos P contribui com  $\frac{1}{8}$  átomo por célula

$$N = N_I + \frac{N_F}{2} + \frac{N_P}{8}$$



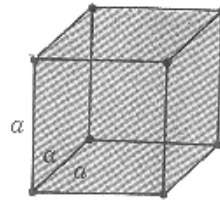
# Sistemas cristalinos

Existem somente sete diferentes combinações dos parâmetros de rede. Cada uma dessas combinações constitui um sistema cristalino.

Cubic

$$a = b = c$$

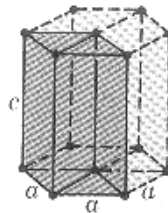
$$\alpha = \beta = \gamma = 90^\circ$$



Hexagonal

$$a = b \neq c$$

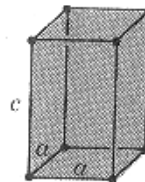
$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$



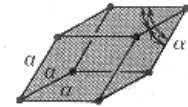
Tetragonal

$$a = b \neq c$$

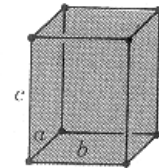
$$\alpha = \beta = \gamma = 90^\circ$$



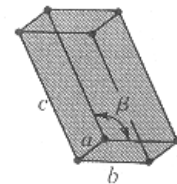
Rhombohedral  $a = b = c$   
 $\alpha = \beta = \gamma \neq 90^\circ$



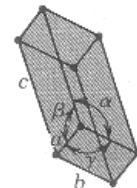
Orthorhombic  $a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$

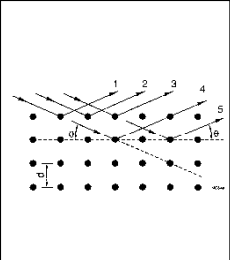


Monoclinic  $a \neq b \neq c$   
 $\alpha = \gamma = 90^\circ \neq \beta$



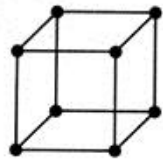
Triclinic  $a \neq b \neq c$   
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$



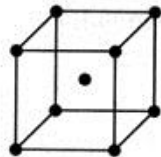


# Reticulados de Bravais

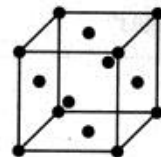
Bravais demonstrou em 1848 que qualquer reticulado cristalino pode ser descrito por um dos 14 reticulados de pontos.



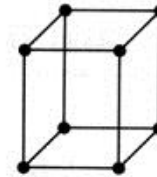
Simple cubic



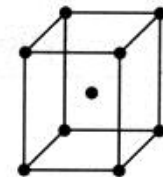
Body-centered cubic (bcc)



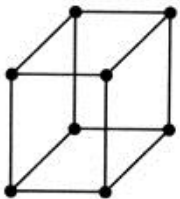
Face-centered cubic (fcc)



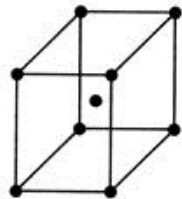
Simple tetragonal



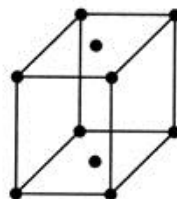
Body-centered tetragonal



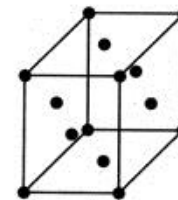
Simple orthorhombic



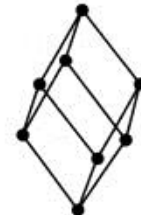
Body-centered orthorhombic



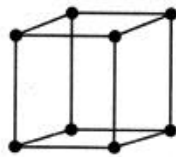
Base-centered orthorhombic



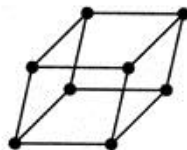
Face-centered orthorhombic



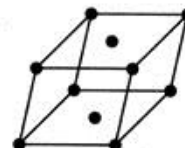
Rhombohedral



Hexagonal



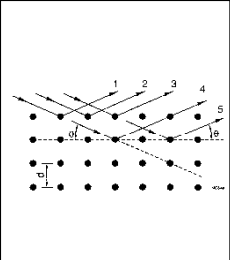
Simple monoclinic



Base-centered monoclinic



Triclinic



# Equivalência de reticulados

Qualquer ponto do reticulado não primitivo pode ser transladado para um equivalente pelos vetores  $a$ ,  $b$ ,  $c$  da mesma maneira que os pontos primitivos do reticulado.

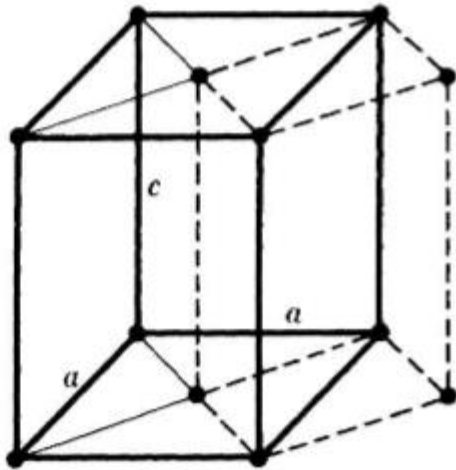


FIG. 2-4. Relation of tetragonal  $C$  lattice (full lines) to tetragonal  $P$  lattice (dashed lines).

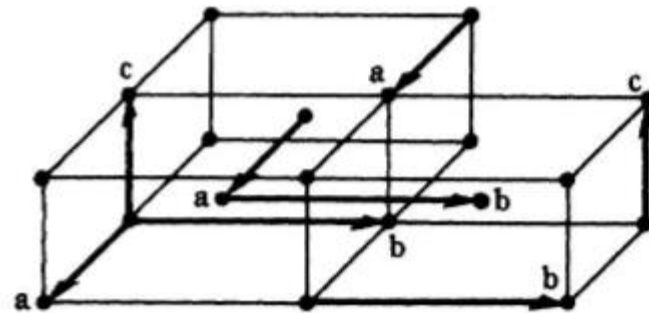


FIG. 2-5. Extension of lattice points through space by the unit cell vectors  $a$ ,  $b$ ,  $c$ .



# SIMETRIA

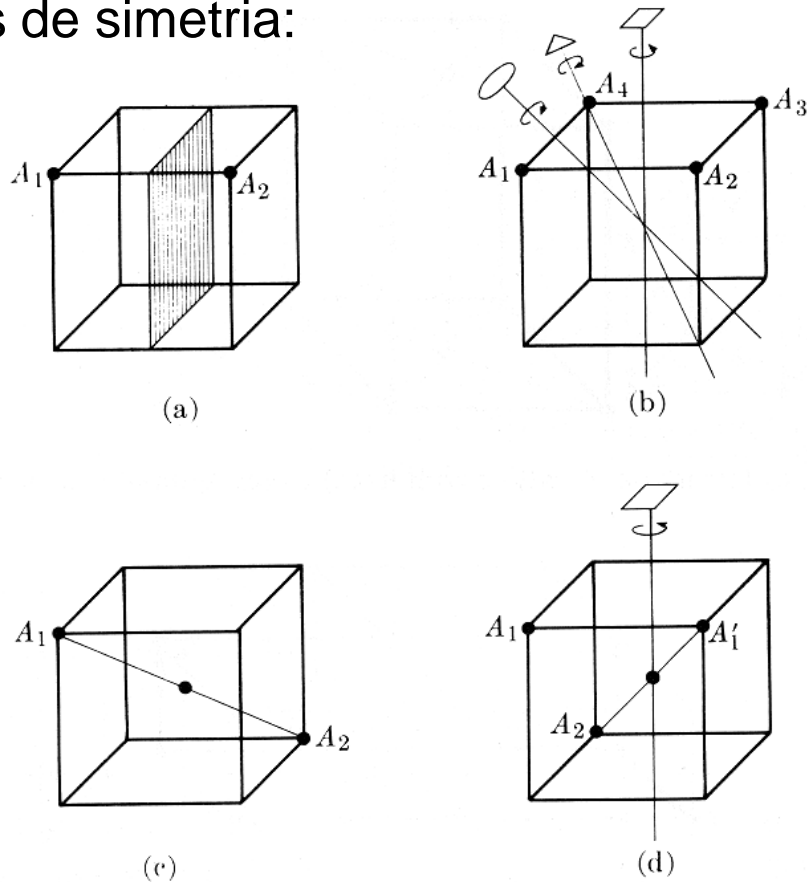
Possibilidade de 4 operações de simetria:

Reflexão;

Rotação;

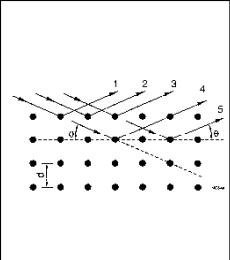
Inversão;

Rotação inversão.



**Fig. 2-6** Some symmetry elements of a cube. (a) Reflection plane.  $A_1$  becomes  $A_2$ . (b) Rotation axes. 4-fold axis:  $A_1$  becomes  $A_2$ ; 3-fold axis:  $A_1$  becomes  $A_3$ ; 2-fold axis:  $A_1$  becomes  $A_4$ . (c) Inversion center.  $A_1$  becomes  $A_2$ . (d) Rotation-inversion axis. 4-fold axis:  $A_1$  becomes  $A_1'$ ; inversion center:  $A_1'$  becomes  $A_2$ .

# SIMETRIA



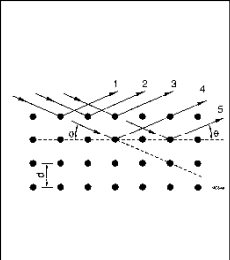
## SYMMETRY ELEMENTS

System	Minimum symmetry elements
Cubic	Four 3 - fold rotation axes
Tetragonal	One 4 - fold rotation (or rotation - inversion) axis
Orthorhombic	Three perpendicular 2 - fold rotation (or rotation - inversion) axes
Rhombohedral	One 3 - fold rotation (or rotation - inversion) axis
Hexagonal	One 6 - fold rotation (or rotation - inversion) axis
Monoclinic	One 2 - fold rotation (or rotation - inversion) axis
Triclinic	None

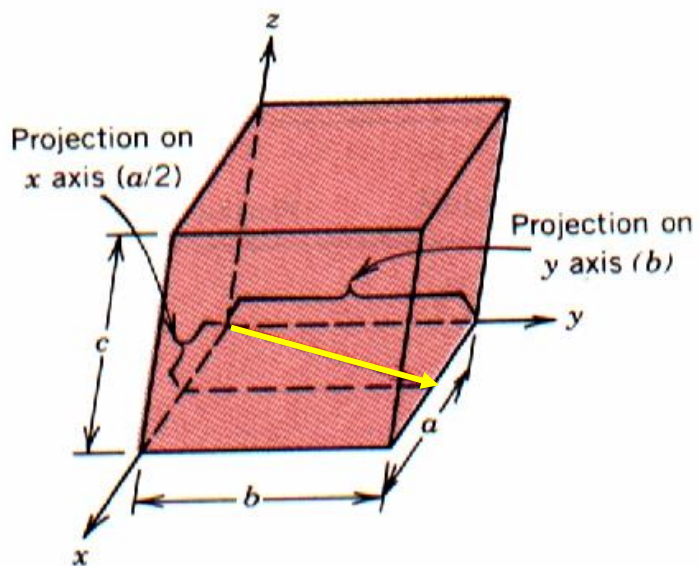


# Índices de Miller: direções cristalográficas

- **Direção cristalográfica:** vetor que une dois pontos da rede cristalina.
- Procedimento para determinação dos índices de Miller de uma direção cristalográfica:
  - transladar o “vetor direção” de maneira que ele passe pela origem do sistema de coordenadas.
  - determinar a projeção do vetor em cada um dos três eixos de coordenadas. Essas projeções devem ser medidas em termos dos parâmetros de rede (a,b,c)
  - multiplicar ou dividir esses três números por um fator comum, tal que os três números resultantes sejam os menores inteiros possíveis.
  - representar a direção escrevendo os três números entre colchetes: [u v w].



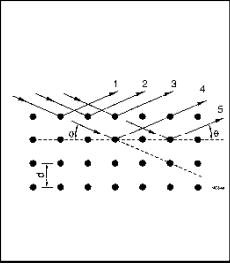
# Direções cristalográficas : exemplo



	x	y	z
projeções	$\frac{1}{2} \times a$	$1 \times b$	$0 \times c$
projeções em termos de a,b e c	$\frac{1}{2}$	1	0
redução a mínimos inteiros	1	2	0
notação	[120]		

Nota: uma **família de direções**, por exemplo [100],  $[\bar{1}00]$ , [010],  $[0\bar{1}0]$ , [001] e  $[00\bar{1}]$  é representada por **<100>**



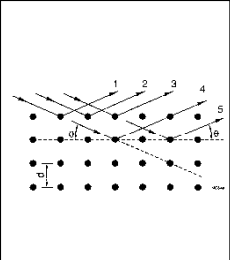


# Índices de Miller: Planos Cristalográficos

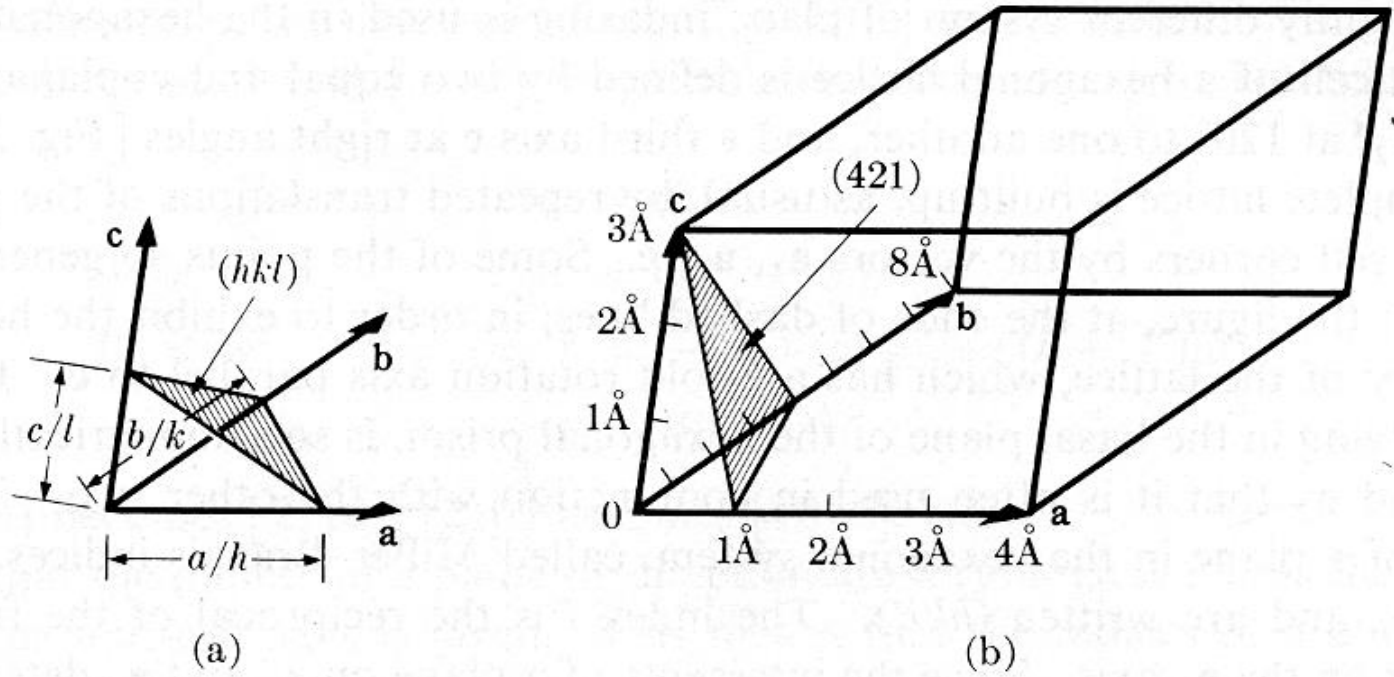
Determinação dos índices de Miller de um plano cristalográfico:

- determinar os interceptos do plano com os eixos do sistema de coordenadas em termos dos parâmetros de rede  $a$ ,  $b$  e  $c$ . Se o plano passar pela origem, transladar o plano para uma nova posição no sistema de coordenadas.
- obter os recíprocos desses três interceptos. Se o plano for paralelo a um dos eixos, considera-se o intercepto infinito e o seu recíproco zero.
- representar na forma  $( h k l )$

**Nota** : às vezes é necessário multiplicar os três números resultantes por um fator comum para assim obter três índices inteiros.

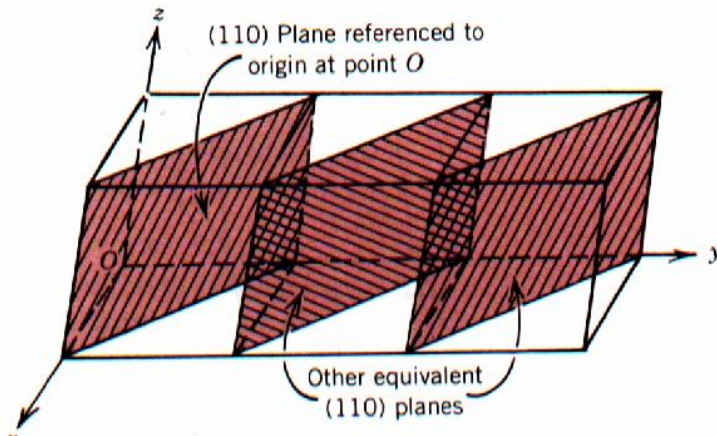
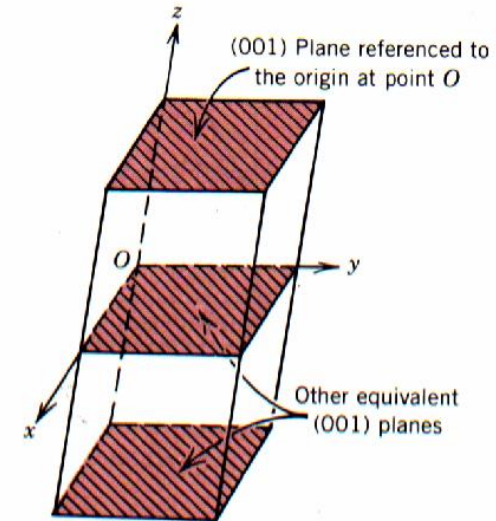
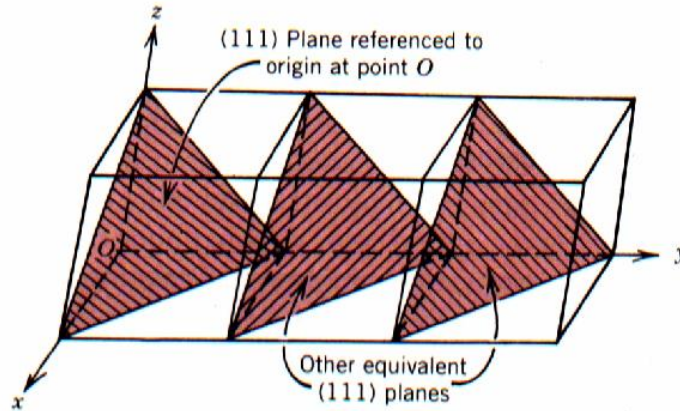
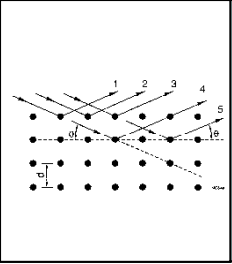


# ÍNDICES DE MILLER (Planos)



**Fig. 2-9** Plane designation by Miller indices.

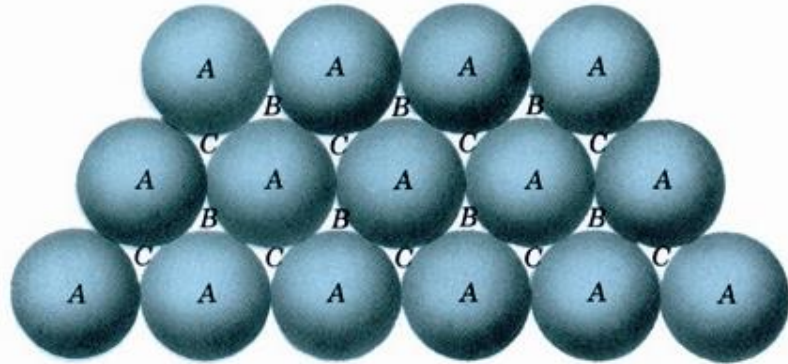
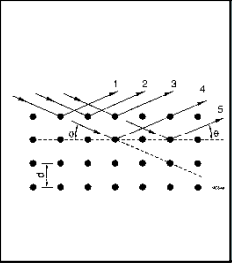
# Planos cristalográficos



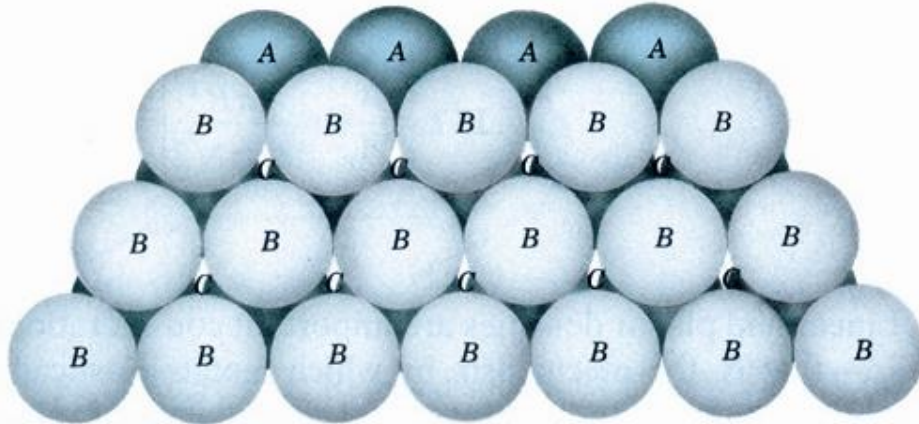
Nota: uma **família de planos**, como por exemplo  $\bar{1}11$ ,  $1\bar{1}1$ ,  $11\bar{1}$ ,  $\bar{1}\bar{1}1$ ,  $1\bar{1}\bar{1}$ ,  $\bar{1}1\bar{1}$  e  $111$  é representada por **{111}**



# Estruturas compactas – HC



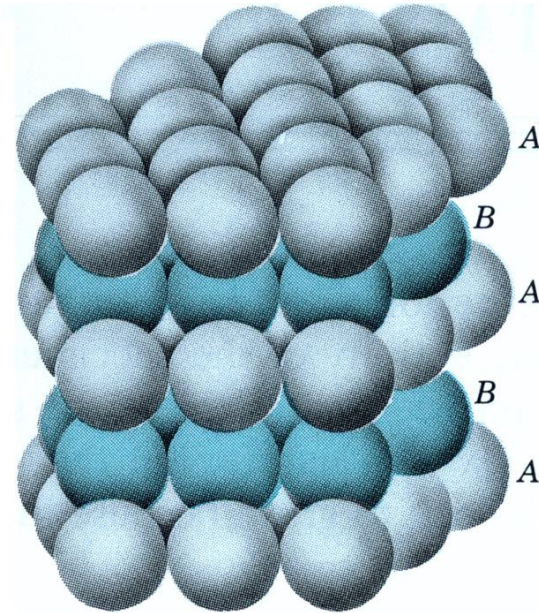
(a)



(b)

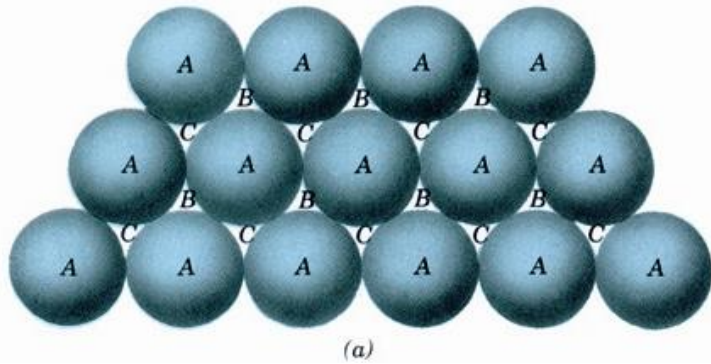
*Empilhamento de dois planos compactos.*

*Plano compacto formado por esferas rígidas (A). Observam-se dois tipos de interstícios, que são assinalados como B e C.*

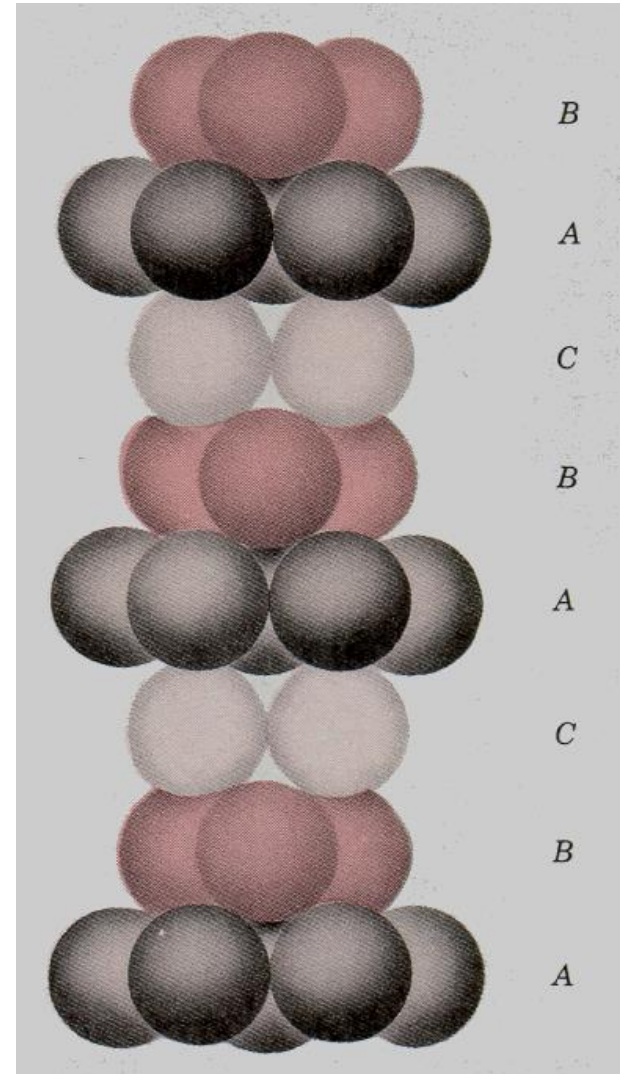
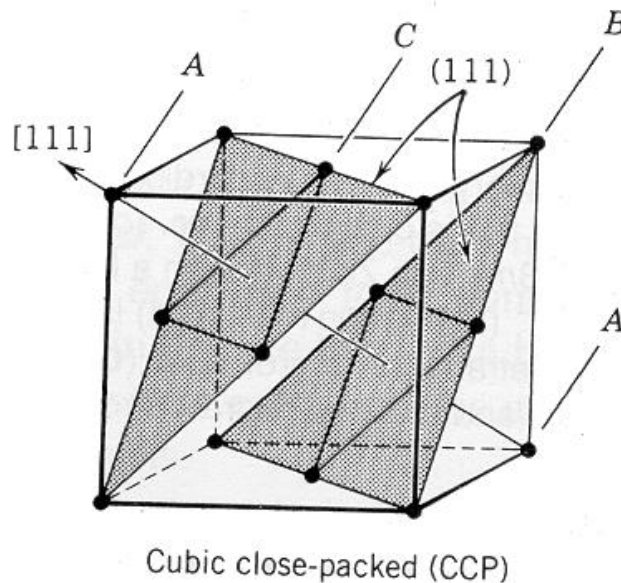


*Empilhamento de planos compactos formando uma estrutura HC.*

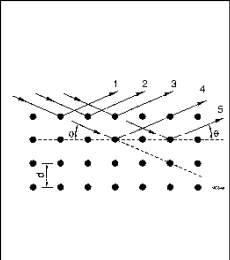
# Estruturas compactas - CFC



*Plano compacto formado por esferas rígidas (A). Observam-se dois tipos de interstícios, que são assinalados como B e C.*



*Empilhamento de planos compactos formando uma estrutura CFC.*



# Fator de empacotamento atômico (FEA)

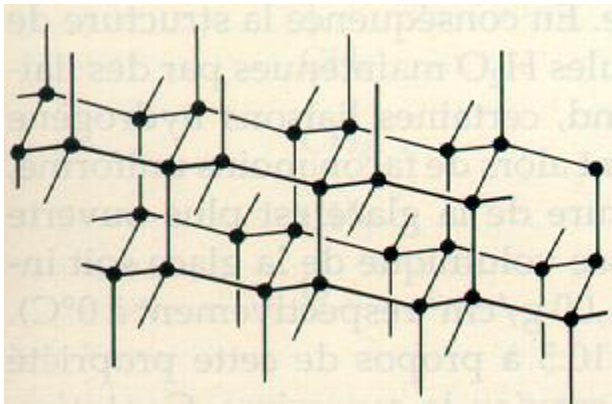
$$FEA = \frac{V_{\text{átomos}}}{V_{\text{célula}}}$$

$$FEA_{CFC} = \frac{4 \left( \frac{4\pi R^3}{3} \right)}{a^3} = \frac{4 \left( \frac{4\pi R^3}{3} \right)}{(2R\sqrt{2})^3} = 0,74$$

# Alotropia e polimorfismo

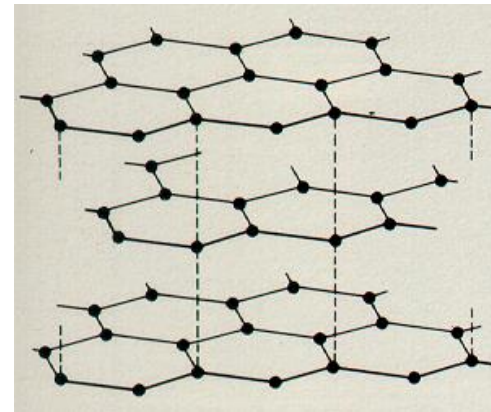
- **Polimorfismo:** fenômeno no qual um sólido (metálico ou não metálico) pode apresentar mais de uma estrutura cristalina, dependendo da temperatura e da pressão (por exemplo, a sílica,  $\text{SiO}_2$  como quartzo, cristobalita e tridimita).
- **Alotropia:** polimorfismo em elementos puros.

Exemplo: o diamante e o grafite são constituídos por átomos de carbono arranjados em diferentes estruturas cristalinas.



Diamante

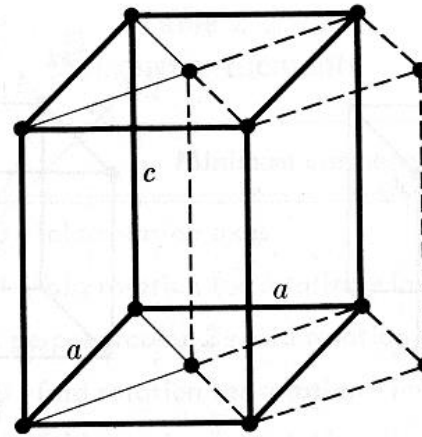
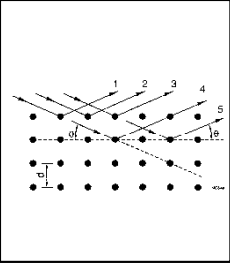
Hibridização  $sp^3$



Grafite

Hibridização  $sp^2$

# RELAÇÃO ENTRE RETICULADOS



**Fig. 2-4** Relation of tetragonal *C* lattice (full lines) to tetragonal *P* lattice (dashed lines).

# ÍNDICES DE MILLER E DISTÂNCIAS INTERPLANARES

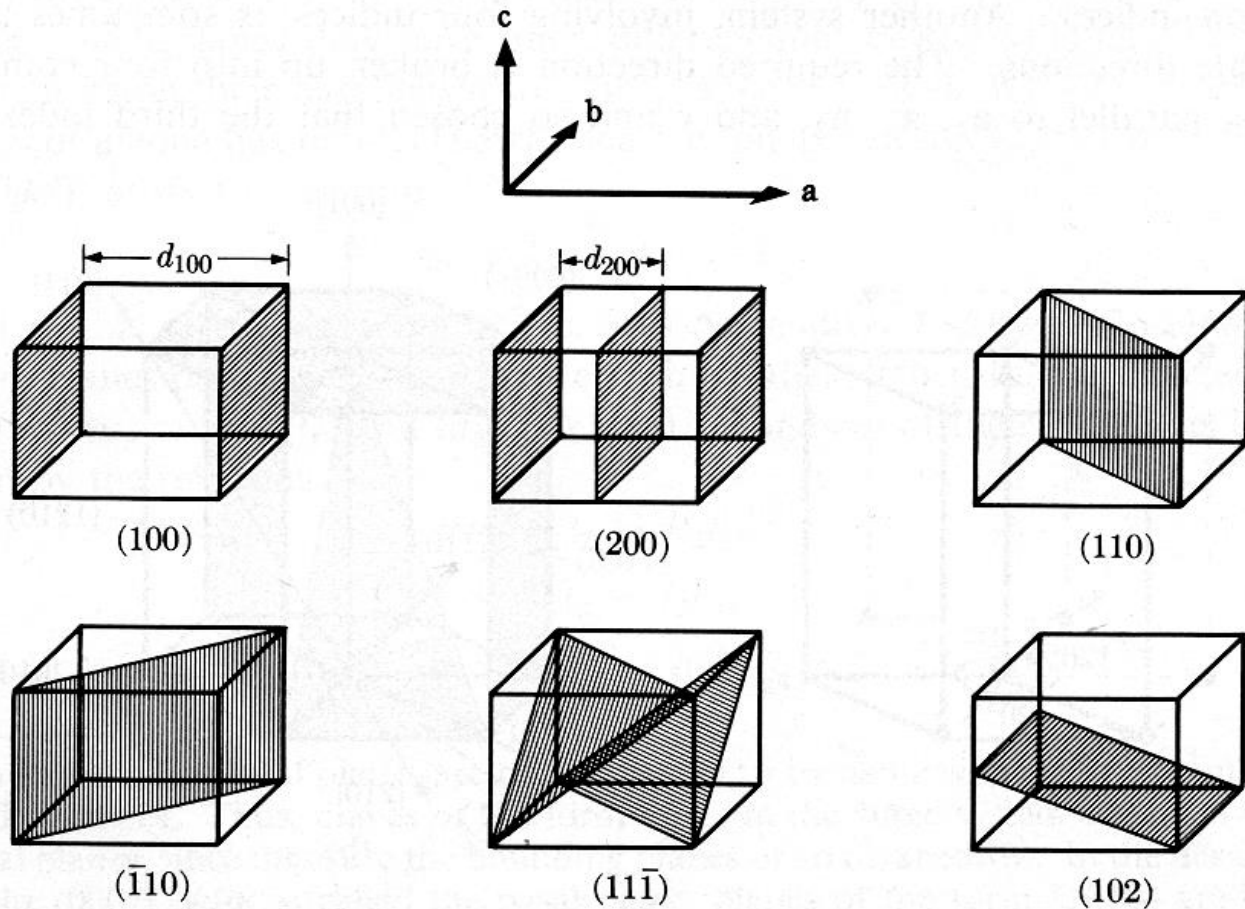
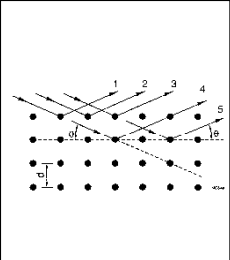
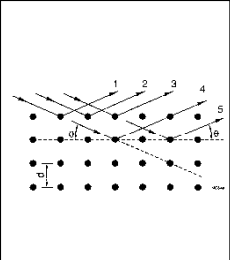
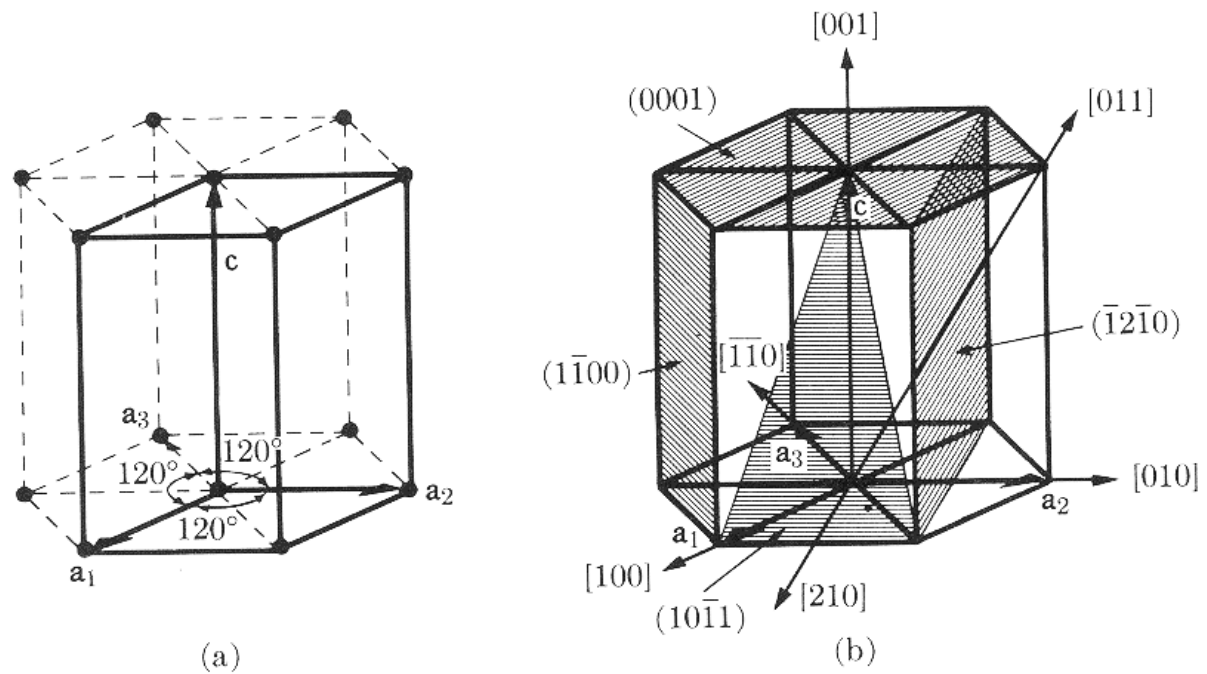


Fig. 2-10 Miller indices of lattice planes. The distance  $d$  is the plane spacing.



# ÍNDICES DE MILLER-BRAVAIS



**Fig. 2-11** (a) The hexagonal unit cell (heavy lines) and (b) indices of planes and directions.

# ÍNDICES DE MILLER E DISTÂNCIAS INTERPLANARES

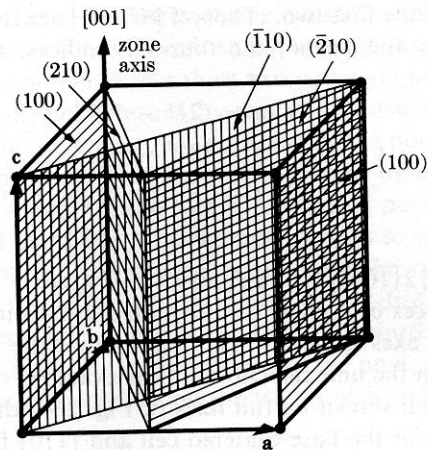
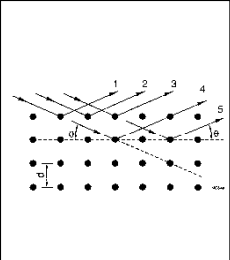


Fig. 2-12 All shaded planes in the cubic lattice shown are planes of the zone [001].

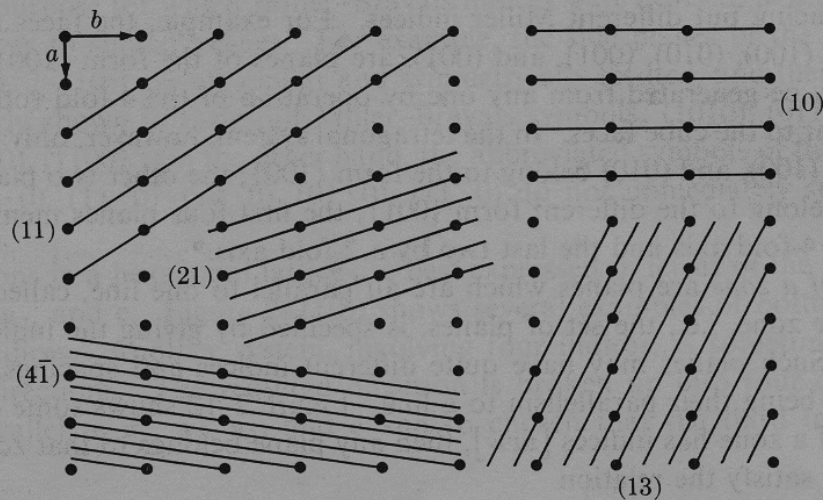
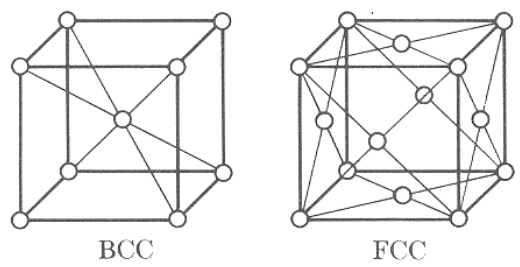
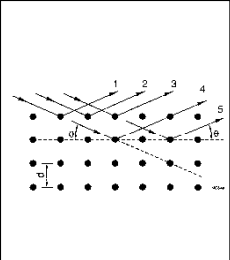


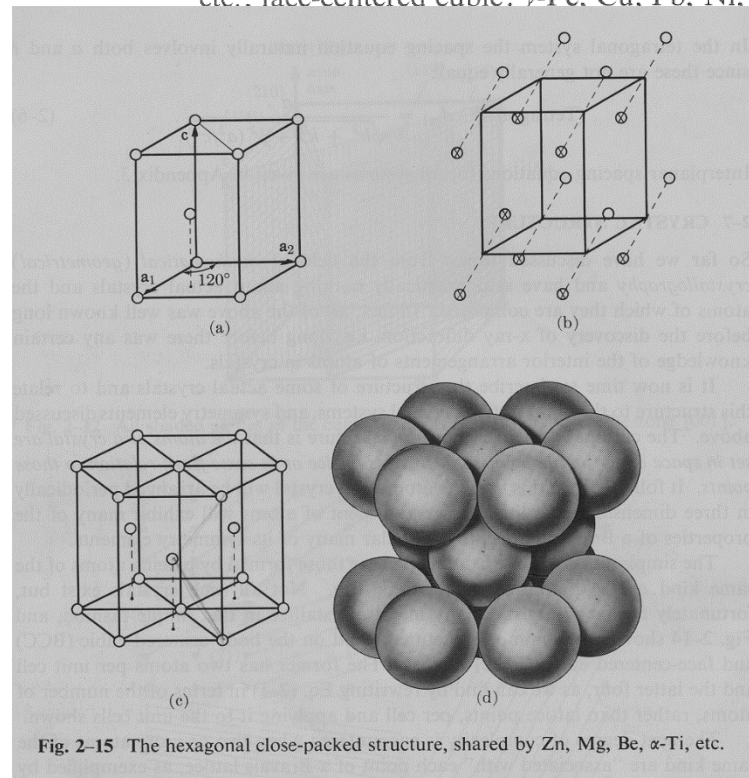
Fig. 2-13 Two-dimensional lattice, showing that lines of lowest indices have the greatest spacing and the greatest density of lattice points.



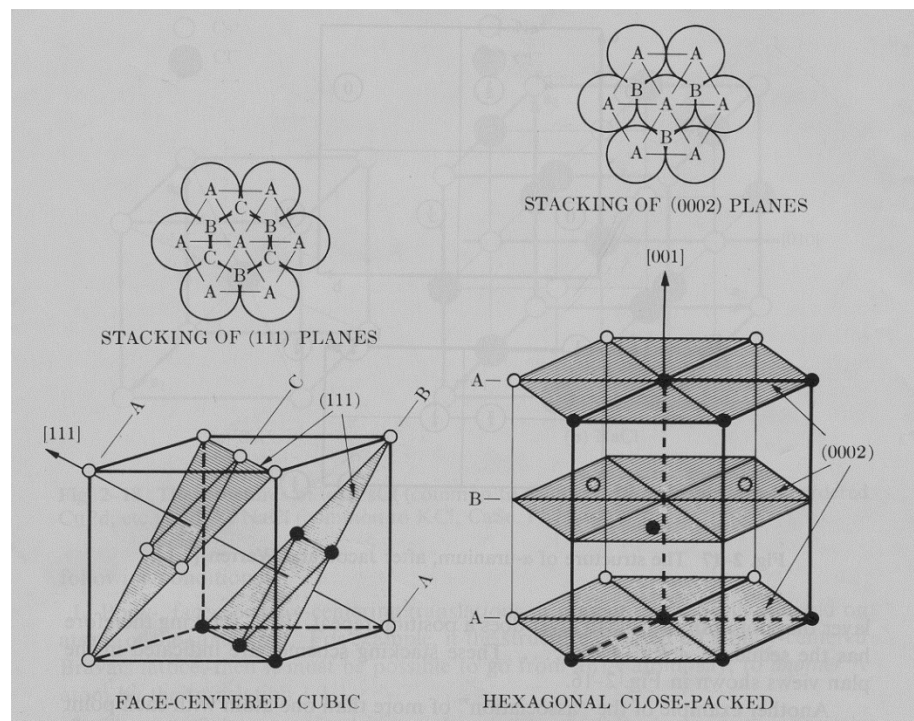
# CRISTAIS METÁLICOS



**Fig. 2-14** Structures of some common metals. Body-centered cubic:  $\alpha$ -Fe, Cr, Mo, V, etc.; face-centered cubic:  $\gamma$ -Fe, Cu, Pb, Ni, etc.

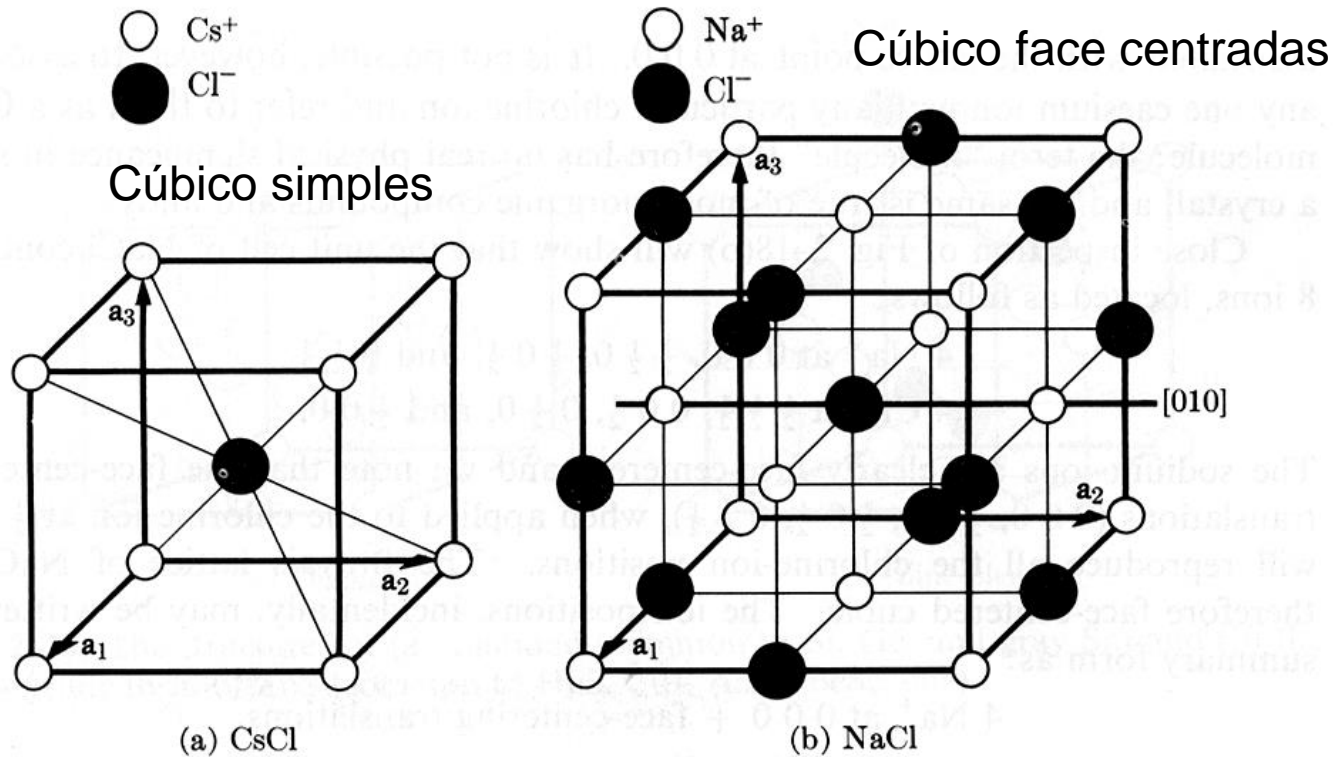


**Fig. 2-15** The hexagonal close-packed structure, shared by Zn, Mg, Be,  $\alpha$ -Ti, etc.



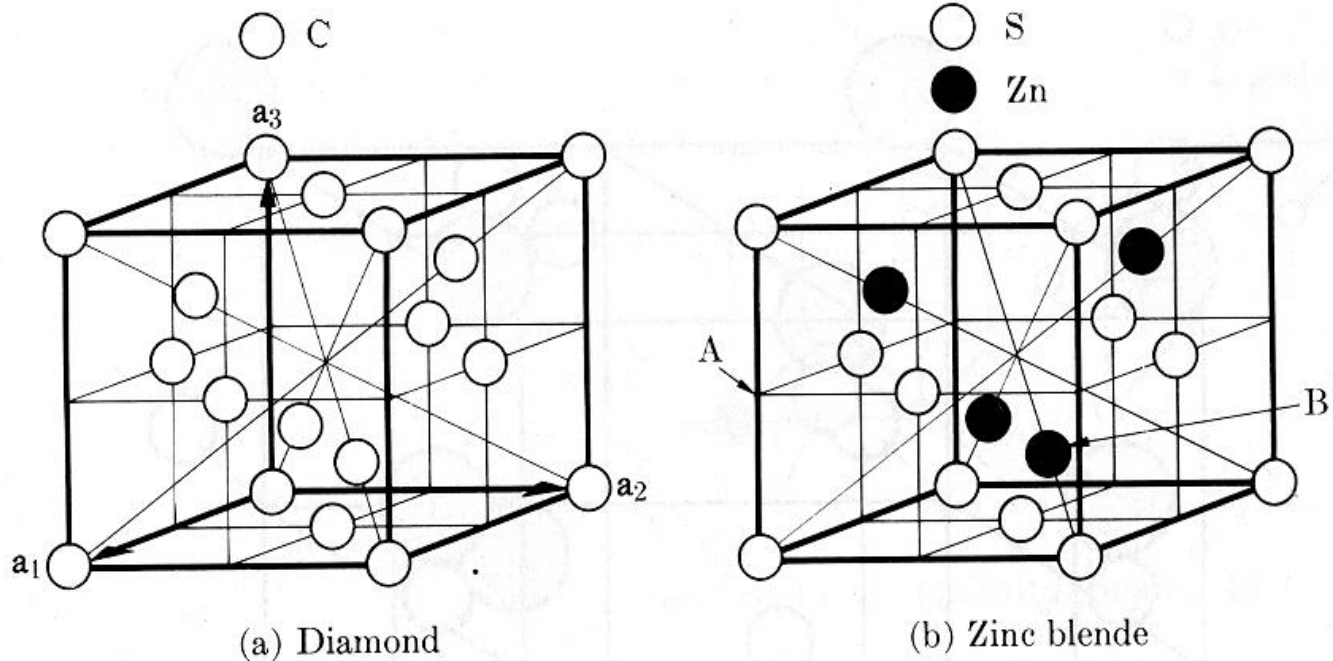
**Fig. 2-16** Comparison of FCC and HCP structures. The black atoms in the FCC drawing delineate half a hexagon, which is completed on the same plane extended into the next unit cell below (not shown).

# CRISTAIS IÔNICOS



**Fig. 2-18** The structures of (a) CsCl (common to CsBr, NiAl, ordered  $\beta$ -brass, ordered CuPd, etc.) and (b) NaCl (common to KCl, CaSe, PbTe, etc.).

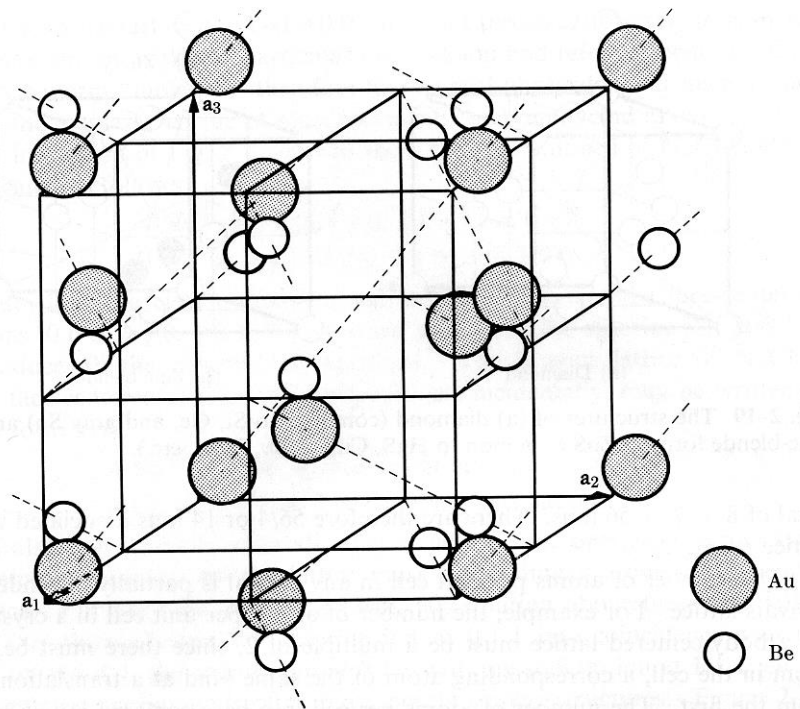
# CRISTAIS COVALENTES



**Fig. 2-19** The structures of (a) diamond (common to Si, Ge, and gray Sn) and (b) the zinc-blende form of ZnS (common to HgS, CuI, AlSb, BeSe, etc.).

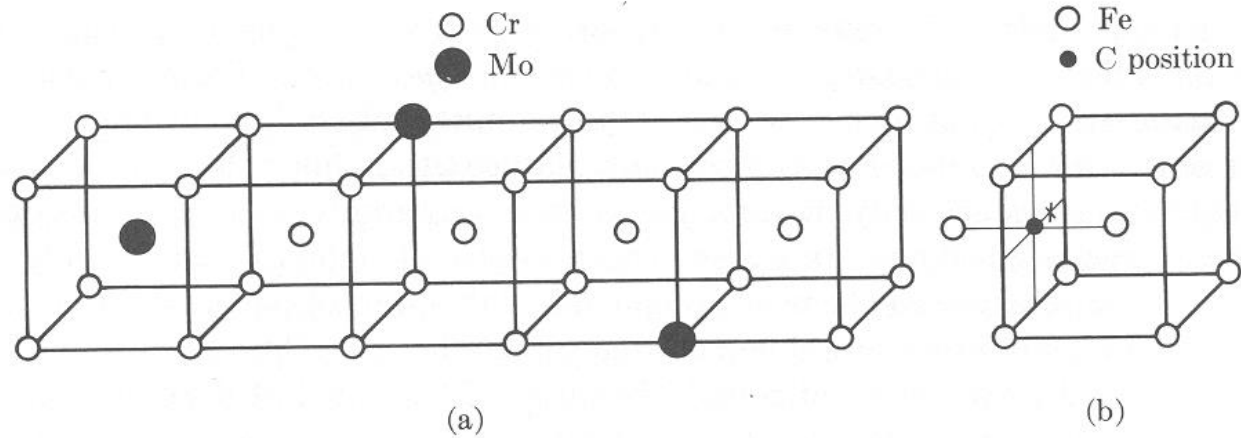
Cúbico faces centradas

# CRISTAIS ORDENADOS



**Fig. 2-20** The structure of AuBe, shared by FeSi, NiSi, CoSi, MnSi, etc. It is known as the FeSi structure [2.2].

# SOLUÇÕES SÓLIDAS



**Fig. 2-21** Structure of solid solutions: (a) Mo in Cr (substitutional); (b) C in  $\alpha$ -Fe (interstitial).

# CRISTAIS MACLADOS

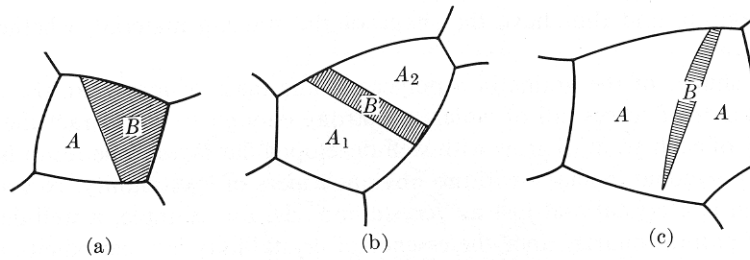


Fig. 2-23 Twinned grains: (a) and (b) FCC annealing twins; (c) HCP deforma

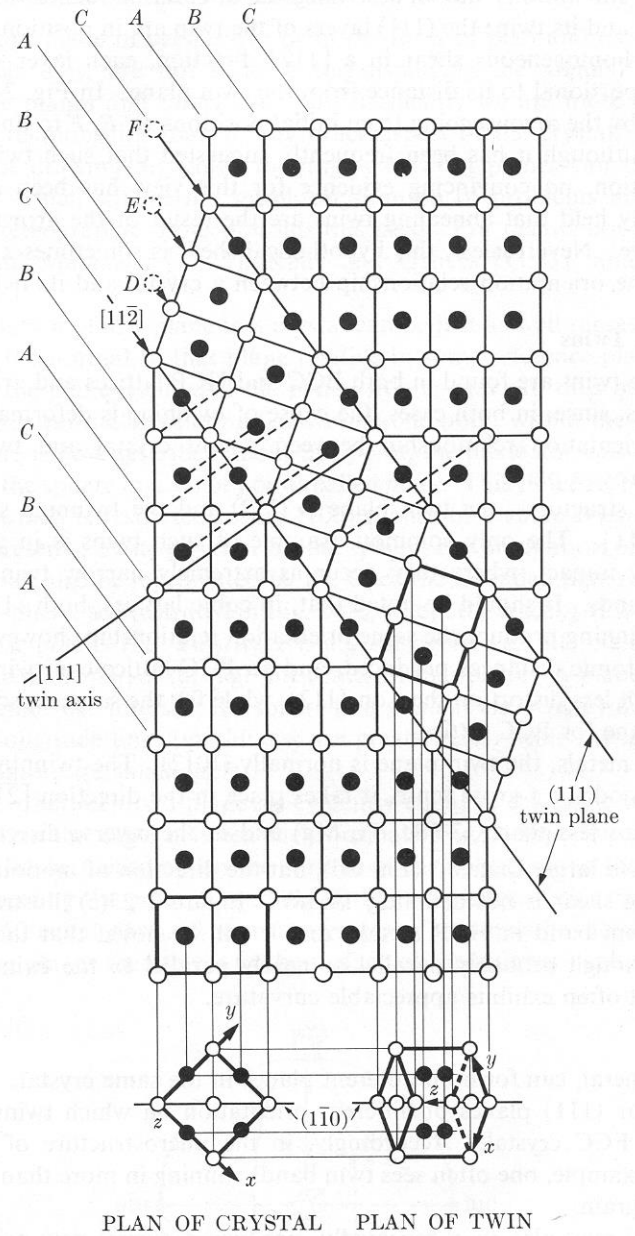


Fig. 2-24 Twin band in FCC lattice. Plane of main drawing is  $(1\bar{1}0)$ .

# PROJEÇÃO ESTEREOGRÁFICA

1 crystal

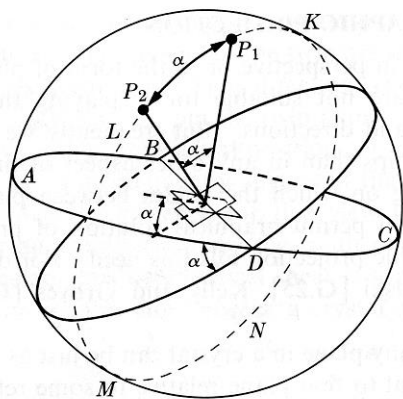


Fig. 2-26 Angle between two planes.

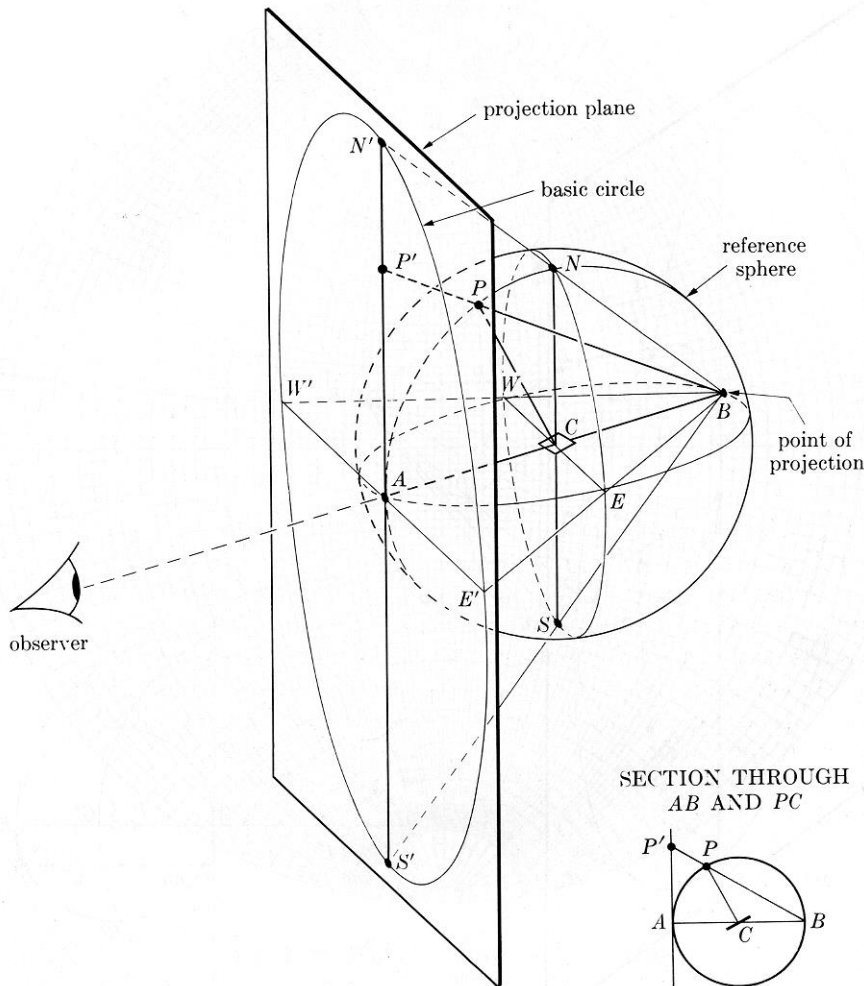


Fig. 2-27 The stereographic projection.

# PROJEÇÃO ESTEREOGRÁFICA

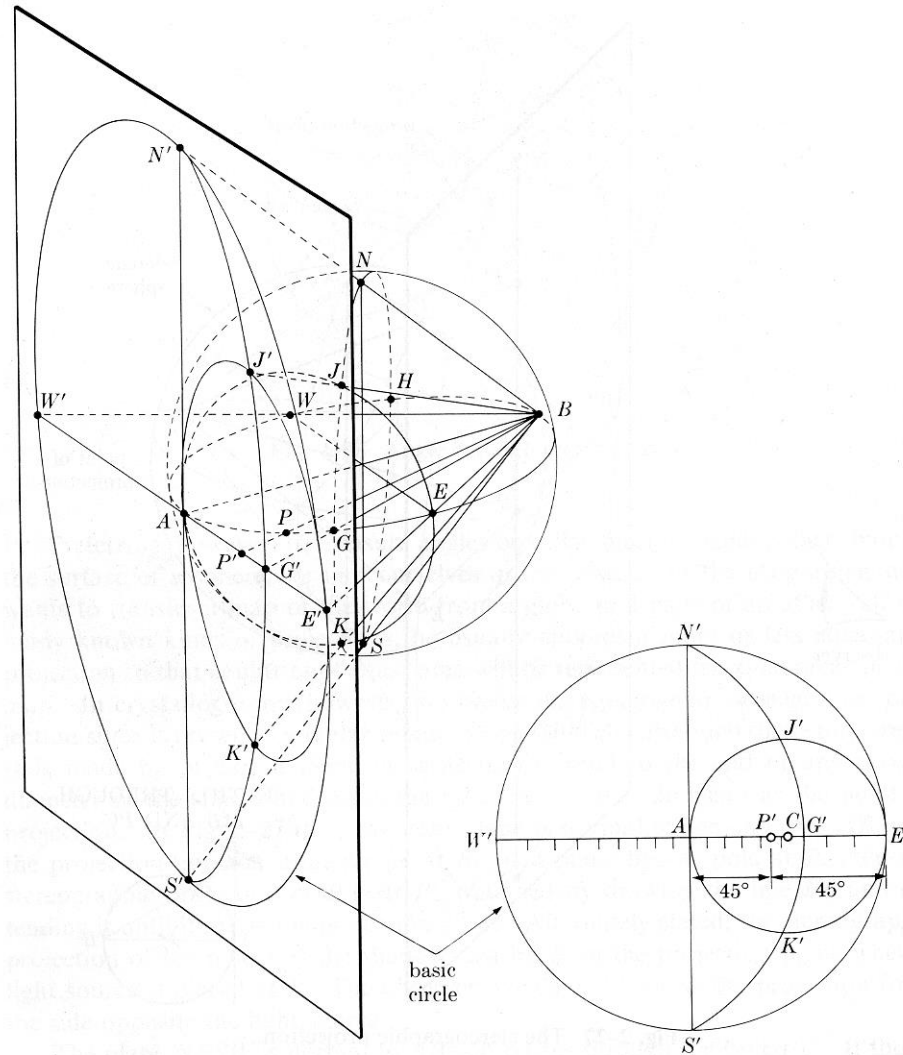
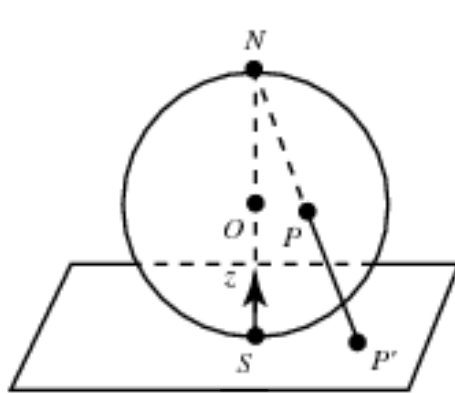


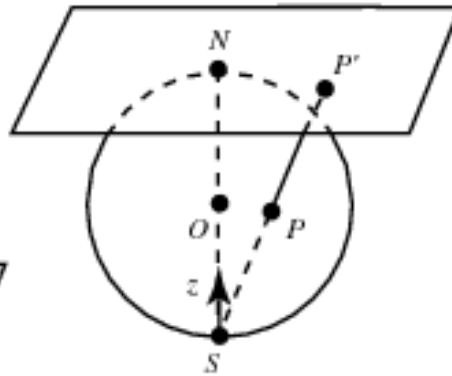
Fig. 2-28 Stereographic projection of great and small circles.



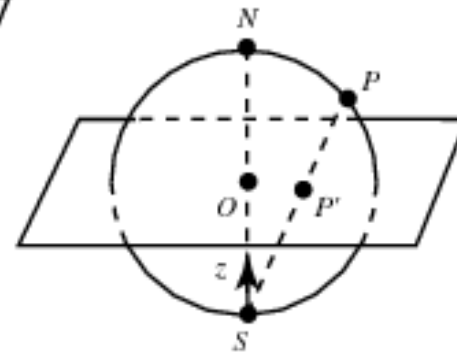
# PROJEÇÃO ESTEREOGRÁFICA



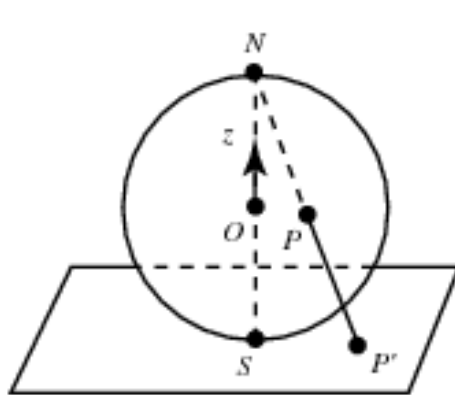
$$P' = \frac{2r}{2r-z} P$$



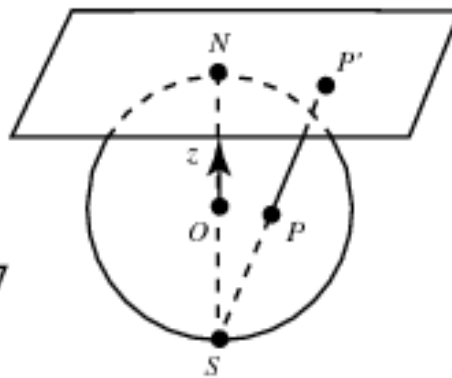
$$P' = \frac{2r}{z} P$$



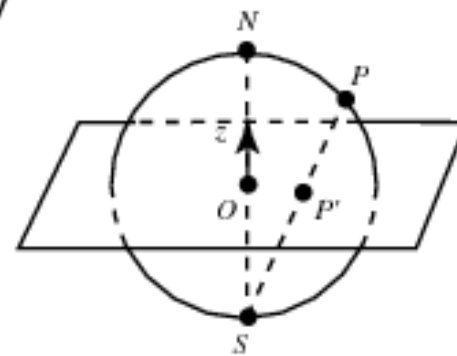
$$P' = \frac{r}{z} P$$



$$P' = \frac{2r}{r-z} P$$

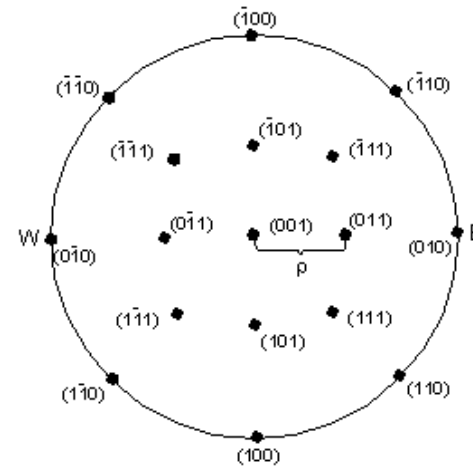
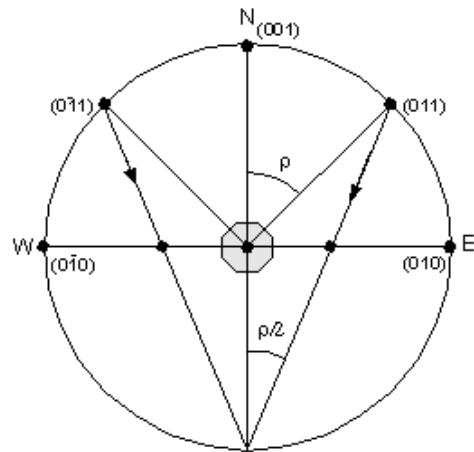
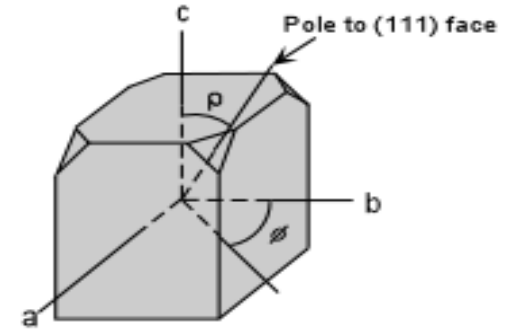
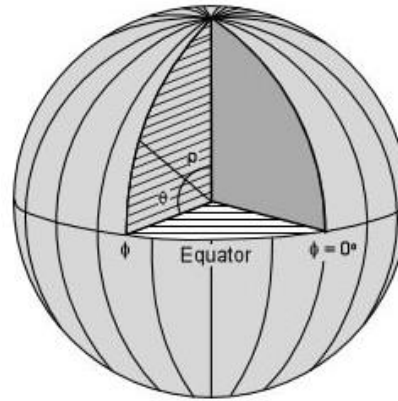
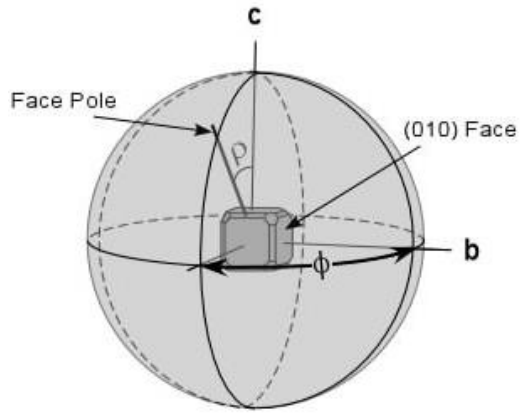
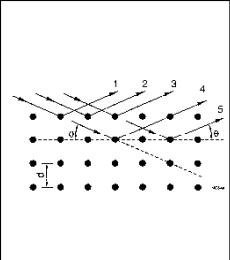


$$P' = \frac{2r}{r+z} P$$

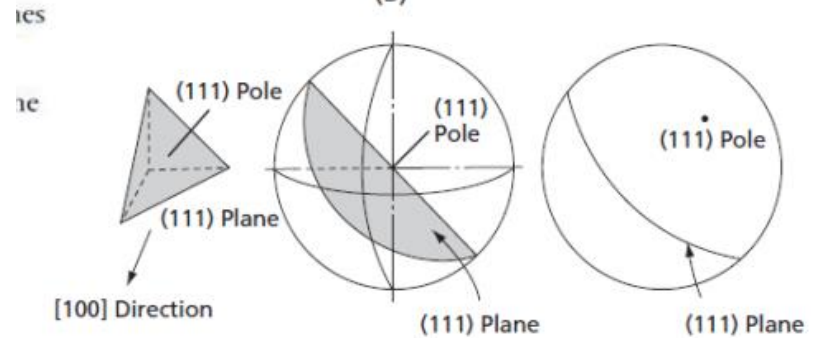
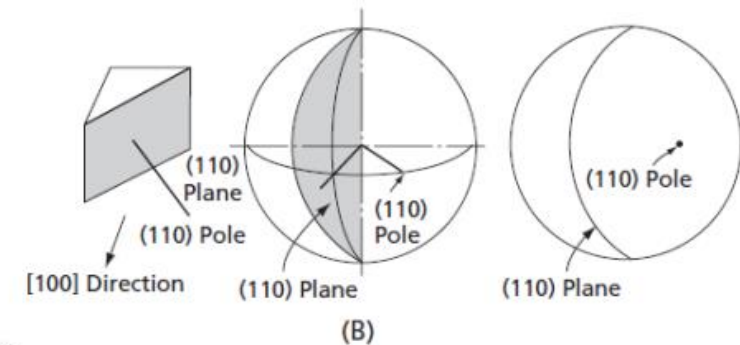
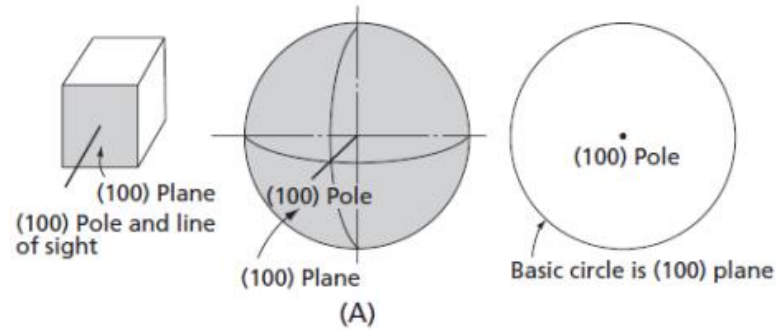
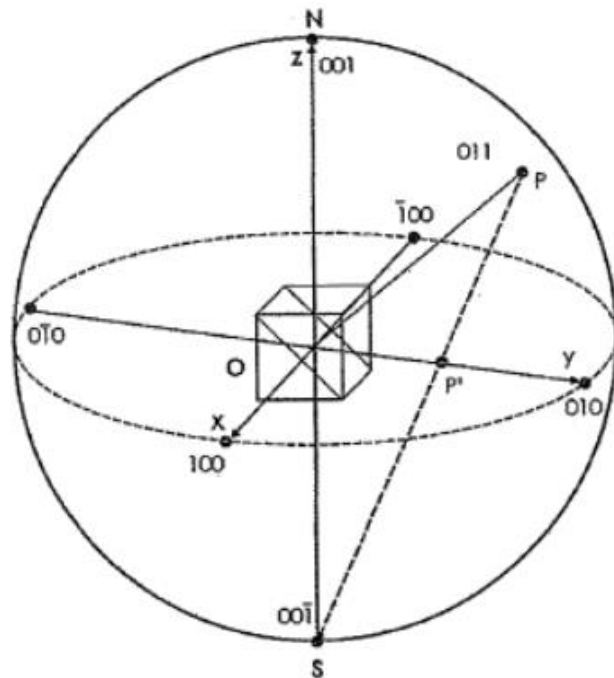
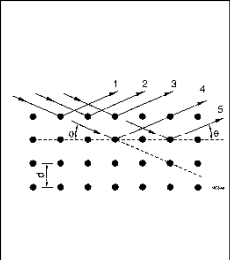


$$P' = \frac{r}{r+z} P$$

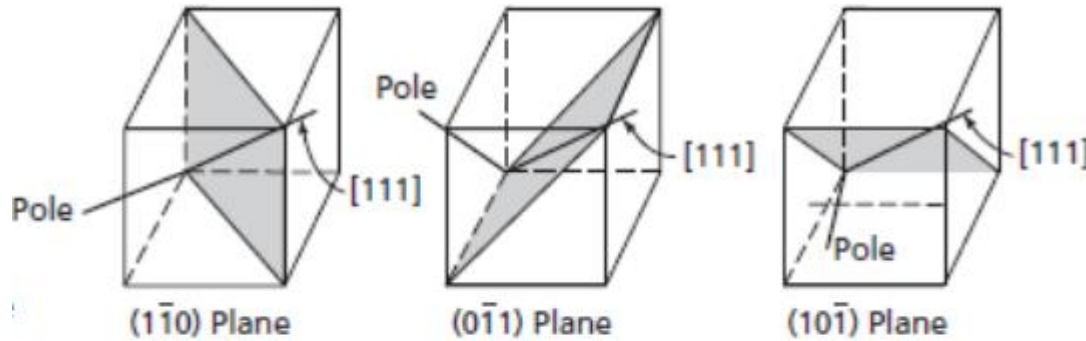
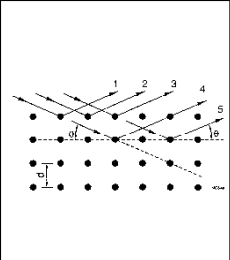
# PROJEÇÃO ESTEREOGRÁFICA



# PROJEÇÃO ESTEREOGRÁFICA NO SISTEMA CÚBICO

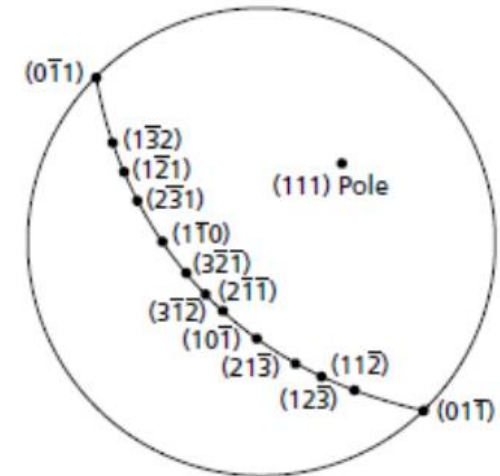
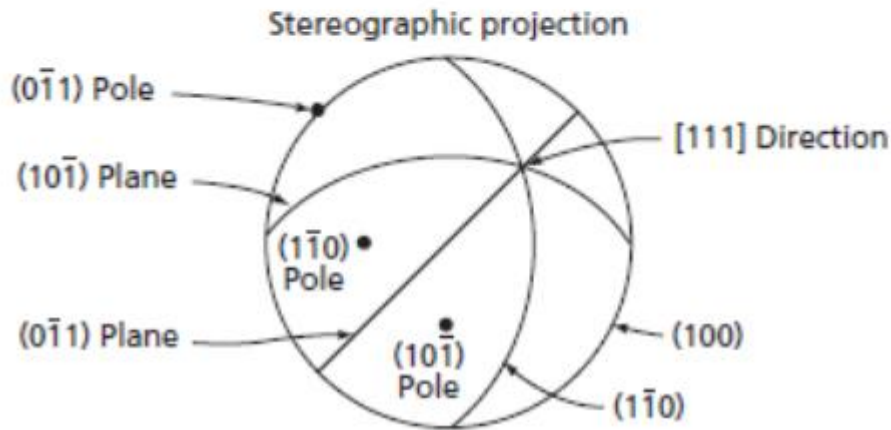


# EIXOS DE ZONA [111]

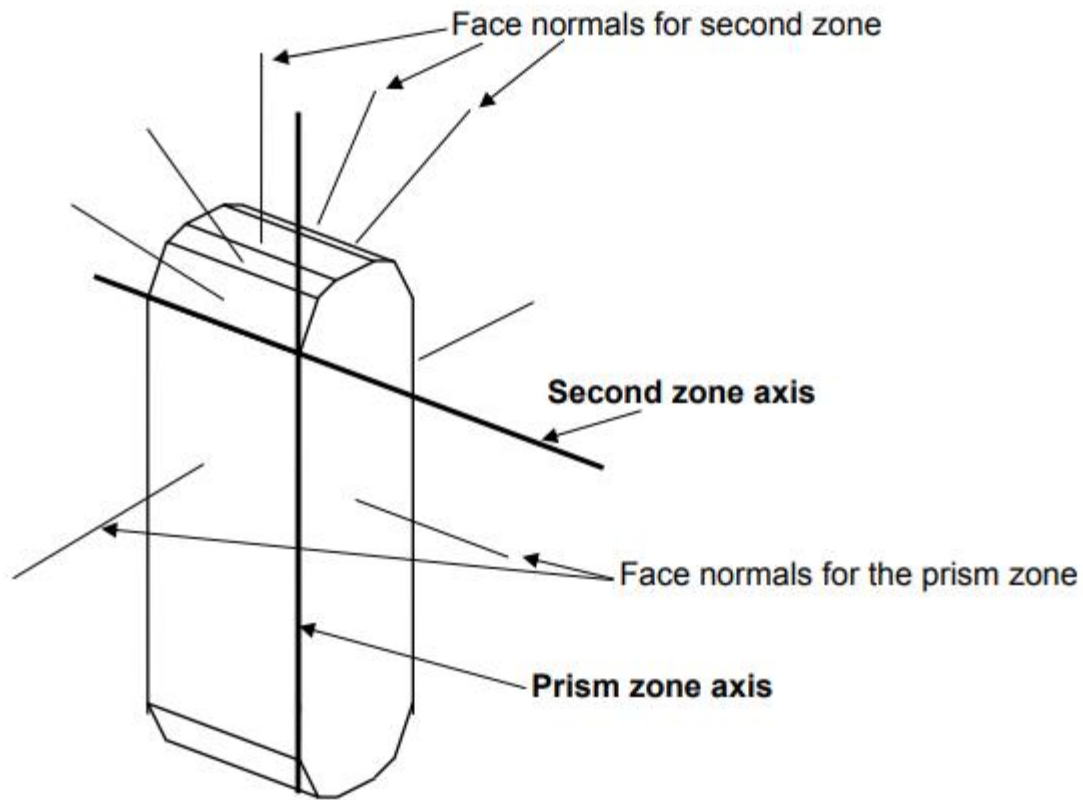


Existem 3 planos  $\{110\}$  que passam pela direção  $[111]$   
 Existem, também, 3 planos  $\{112\}$  e seis planos  $\{123\}$ , bem como um número maior de planos de mais alto índice que possuem o mesmo eixo de zona.

## [111] zone axis

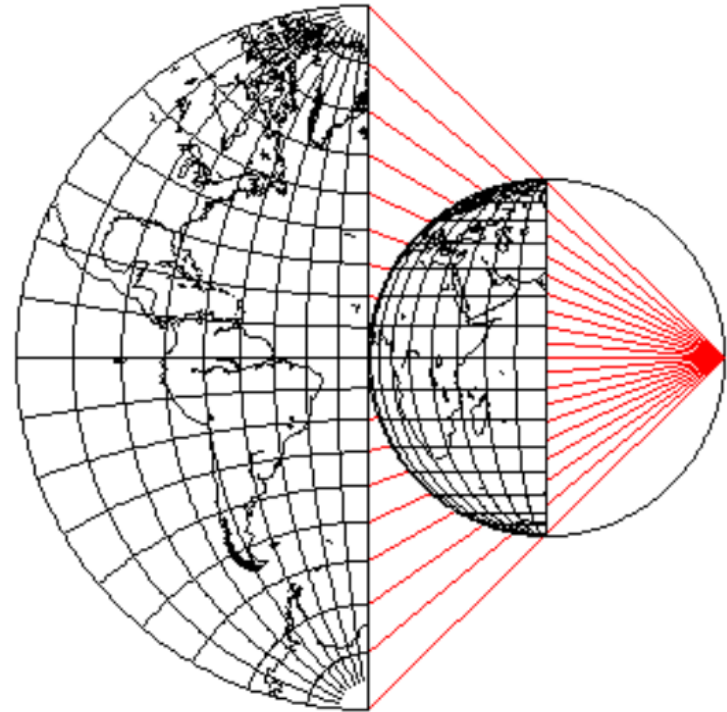
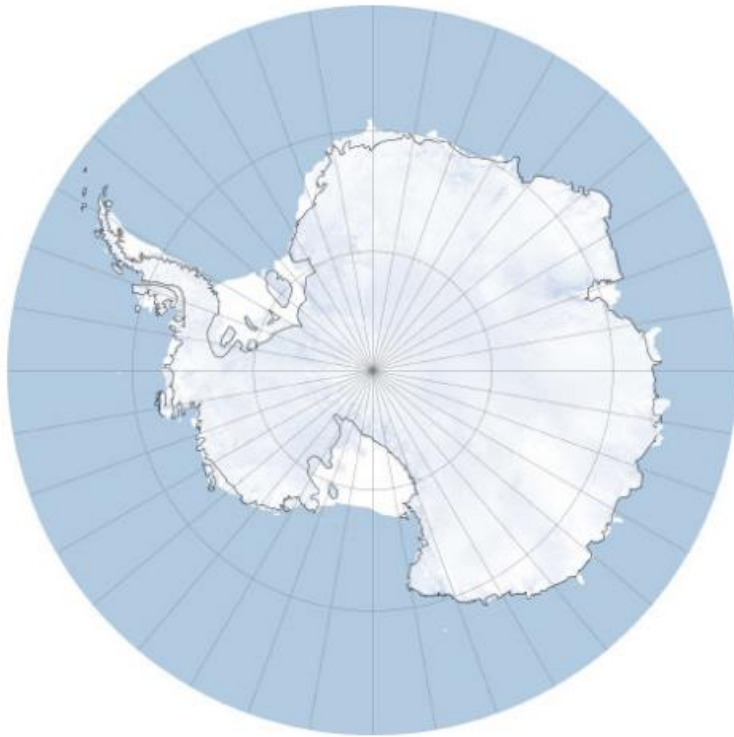
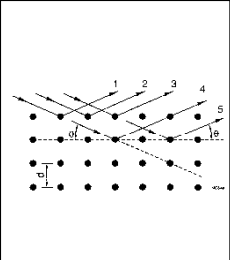


# PROJEÇÃO ESTEREOGRÁFICA NO SISTEMA CÚBICO

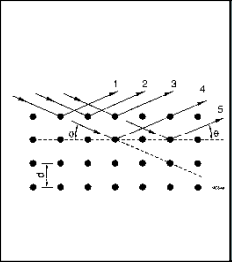


*Fig 9. Simple crystal showing two zones of faces, their zone axes, and their sets of face normals each lying in a single plane*

# PROJEÇÃO ESTEREOGRÁFICA



# PROJEÇÃO ESTEREOGRÁFICA



# PROJEÇÃO ESTEREOGRÁFICA

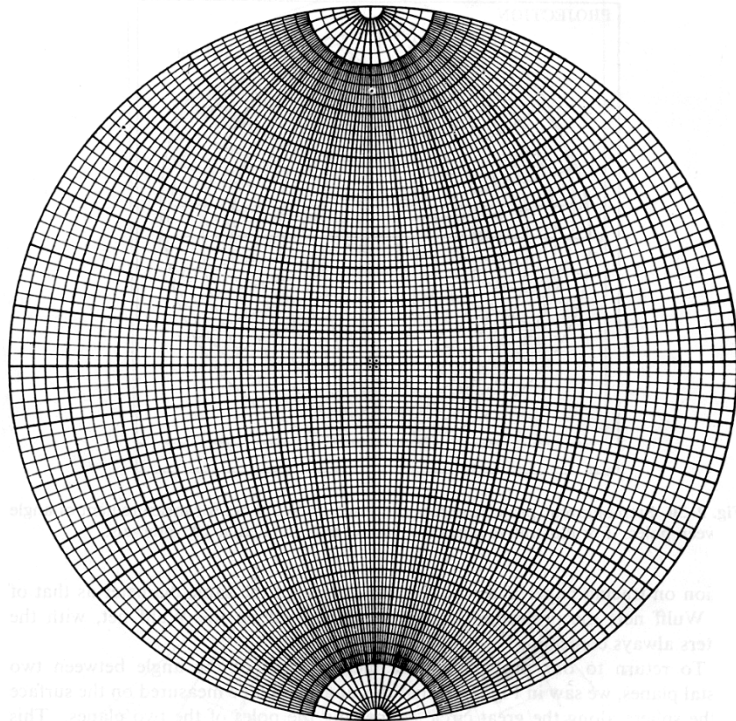
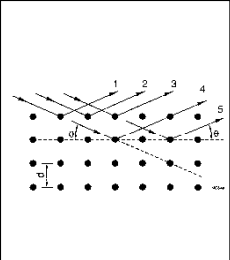


Fig. 2-29 Wulff net drawn to 2° intervals.

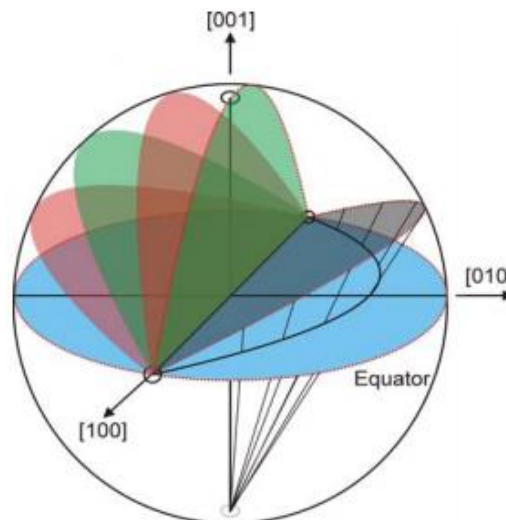


Fig. 8a

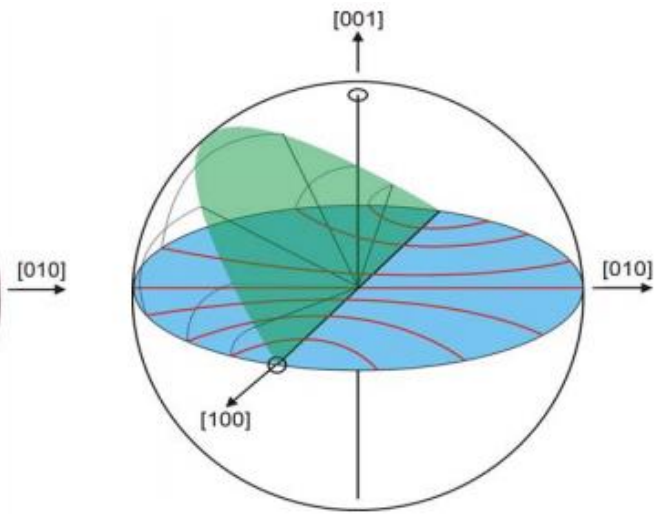


Fig. 8b



# PROJEÇÃO ESTEREOGRÁFICA

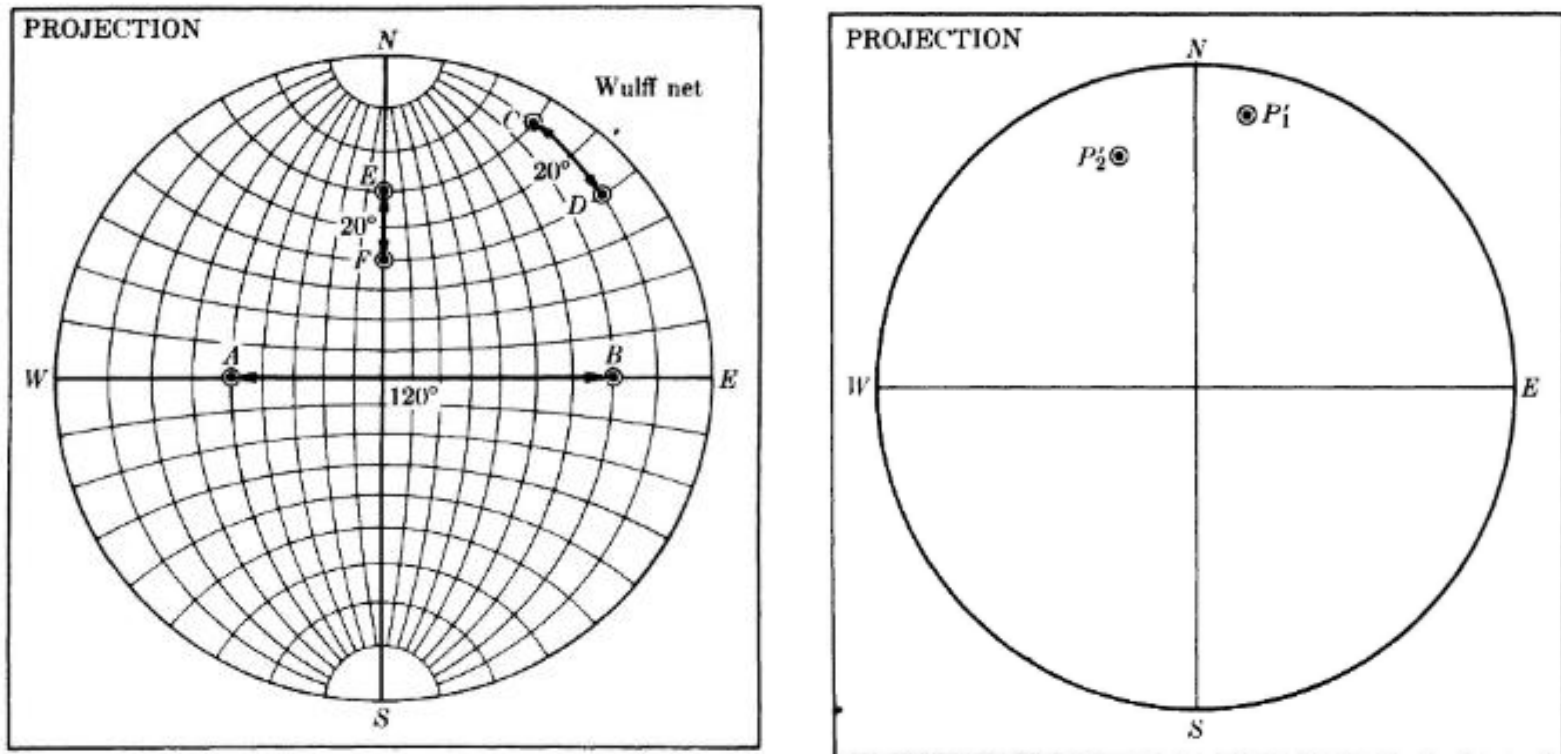


FIG. 2-30. Stereographic projection superimposed on Wulff net for measurement of angle between poles.

# PROJEÇÃO ESTEREOGRÁFICA

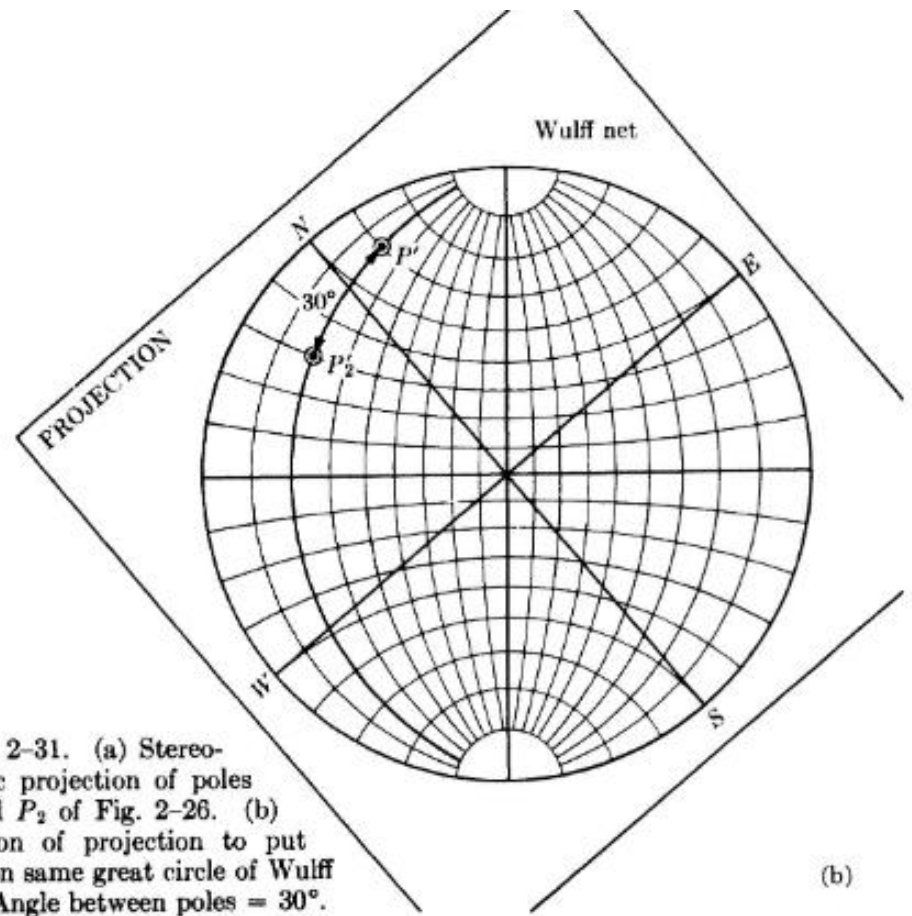
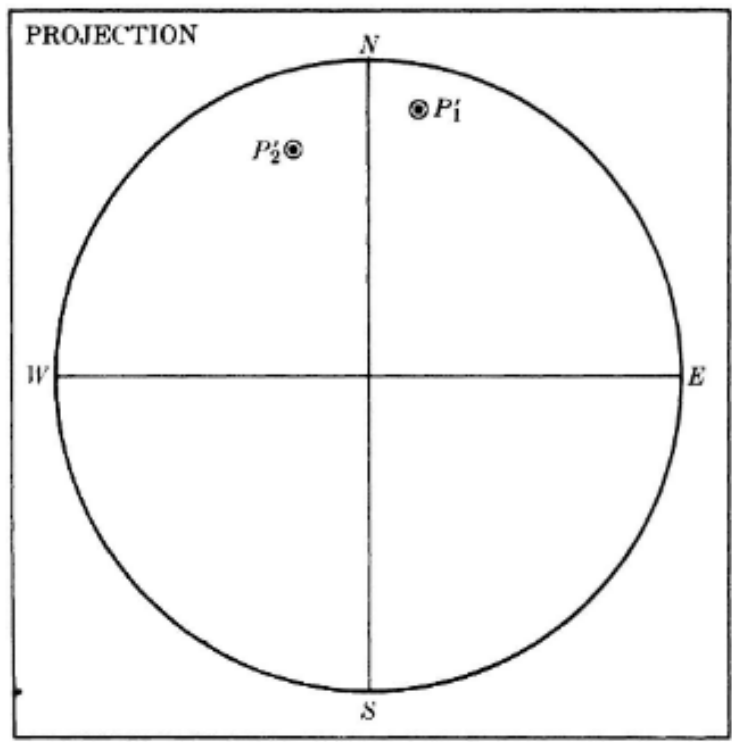
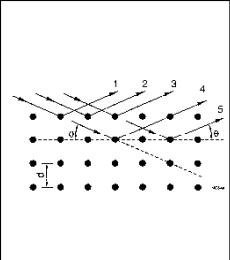


FIG. 2-31. (a) Stereographic projection of poles  $P_1$  and  $P_2$  of Fig. 2-26. (b) Rotation of projection to put poles on same great circle of Wulff net. Angle between poles =  $30^\circ$ .

(b)

# PROJEÇÃO ESTEREOGRÁFICA

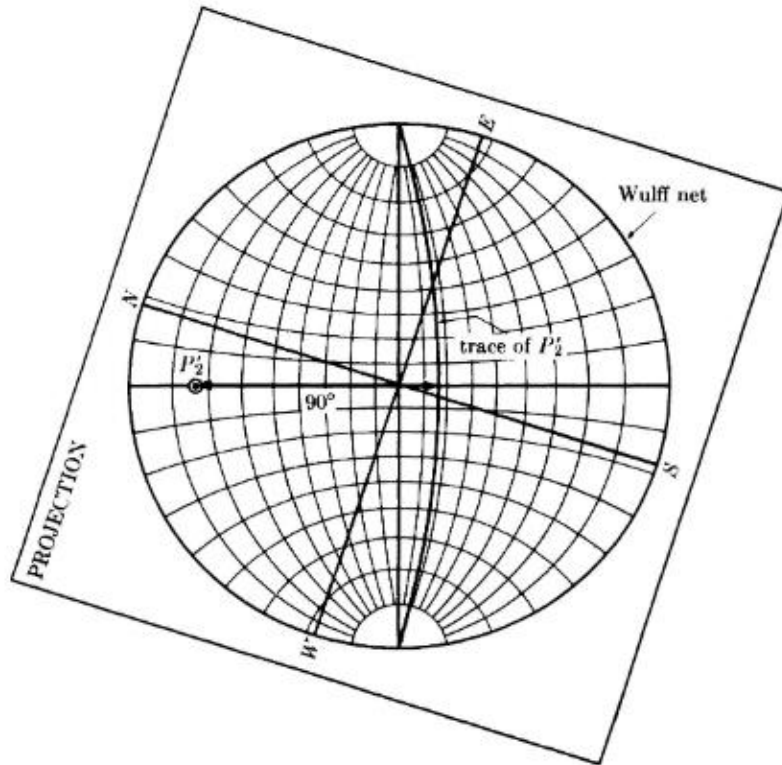
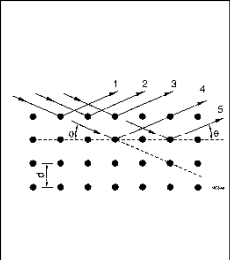


FIG. 2-32. Method of finding the trace of a pole (the pole  $P_2'$  in Fig. 2-31).

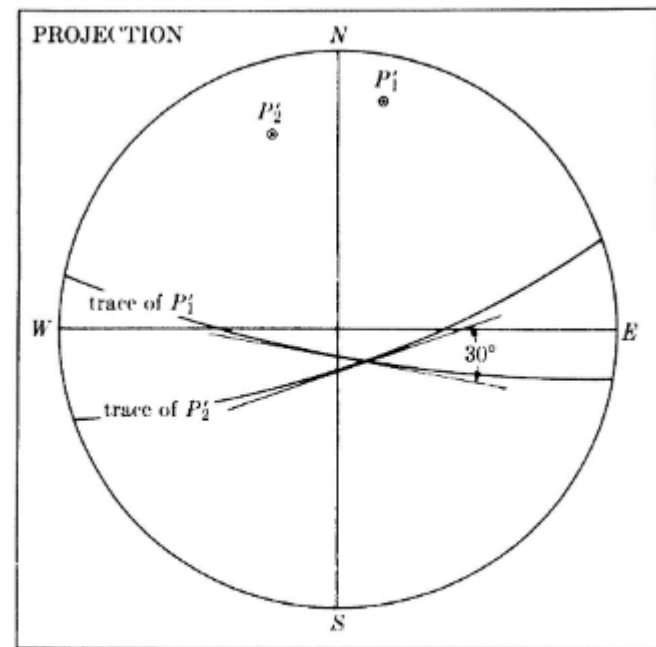


FIG. 2-33. Measurement of an angle between two poles ( $P_1$  and  $P_2$  of Fig. 2-26) by measurement of the angle of intersection of the corresponding traces.

# PROJEÇÃO ESTEREOGRÁFICA

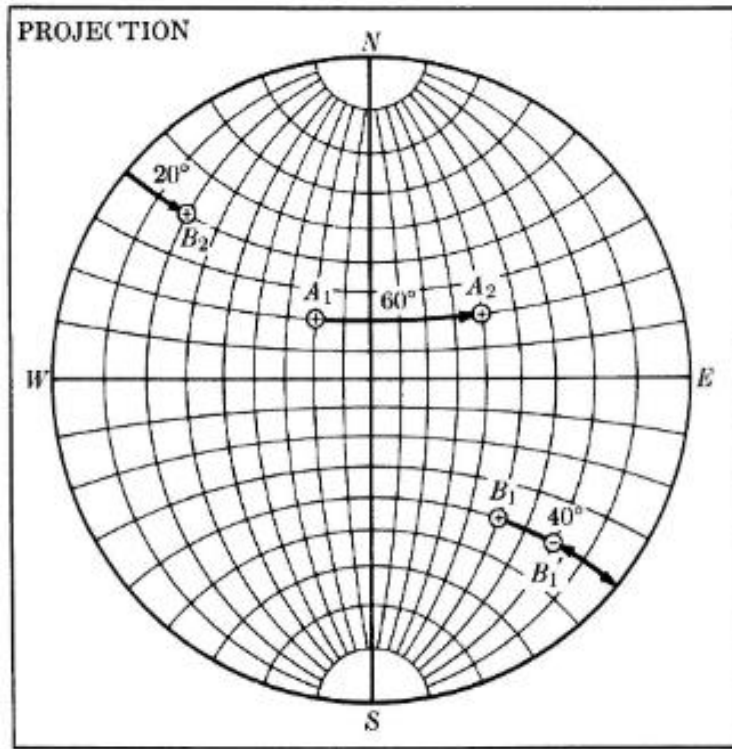


FIG. 2-34. Rotation of poles about *NS* axis of projection.

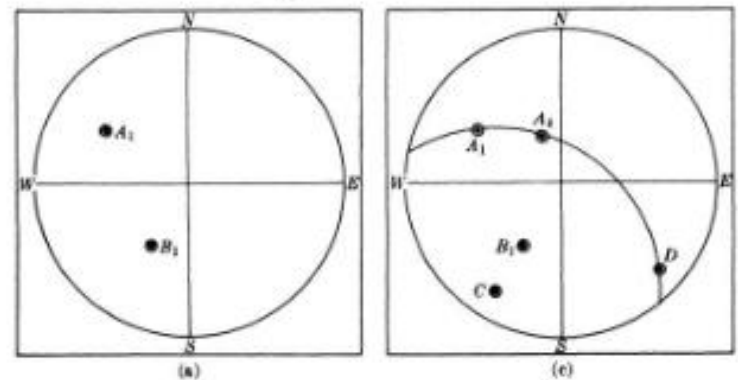
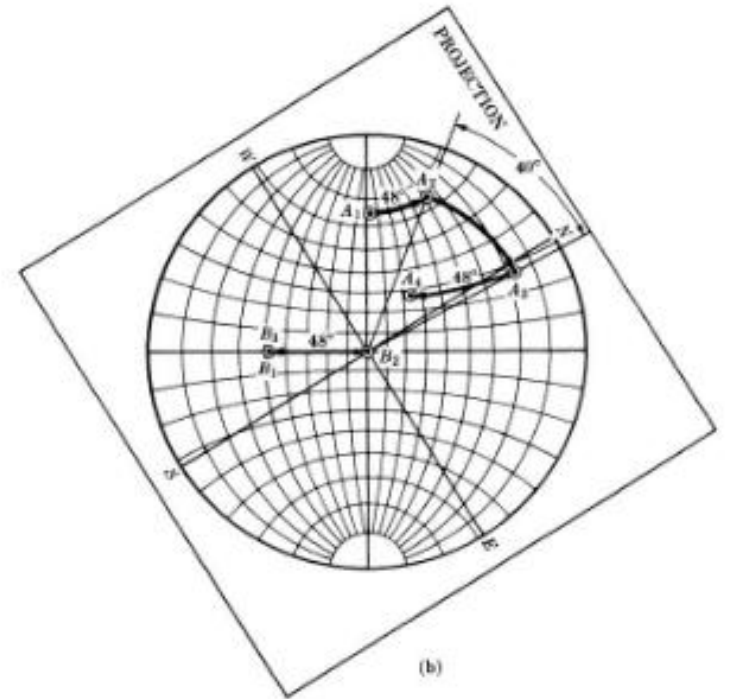
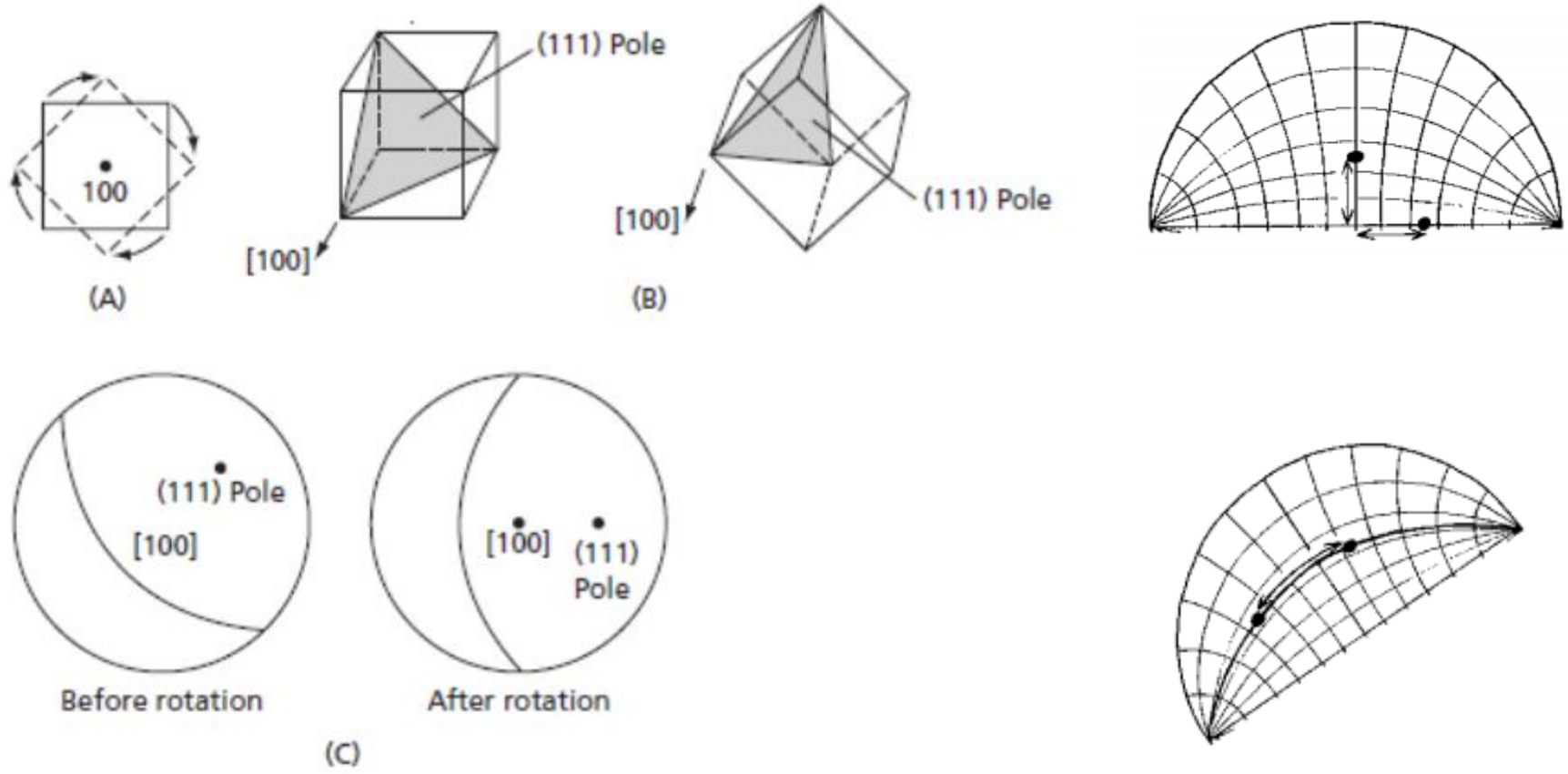
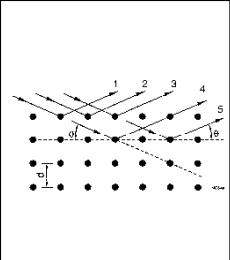
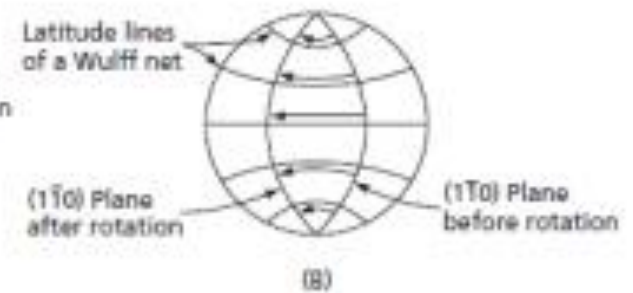
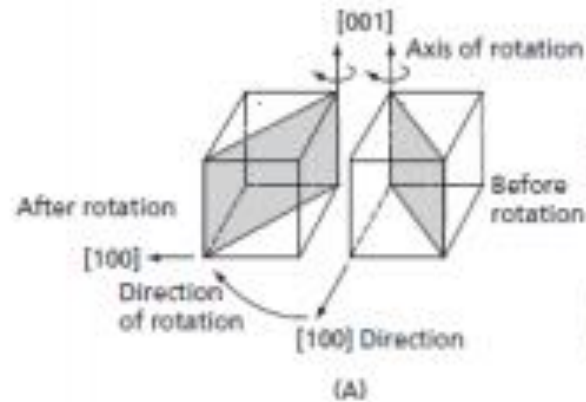
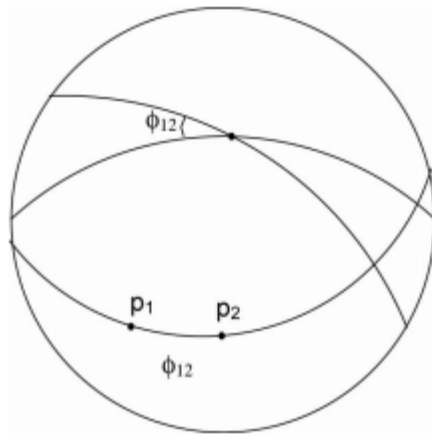
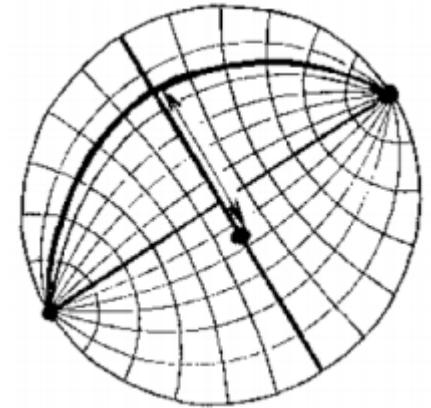
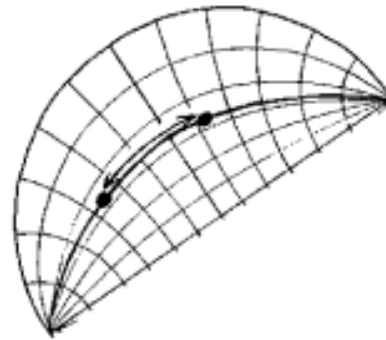
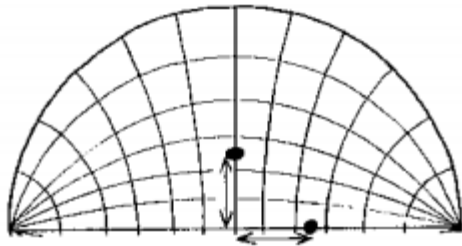
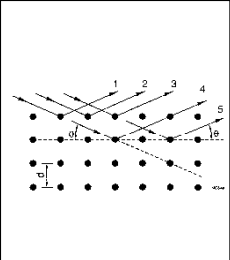


FIG. 2-35. Rotation of a pole about an inclined axis.

# PROJEÇÃO ESTEREOGRÁFICA



# PROJEÇÃO ESTEOROGRÁFICA



# PROJEÇÃO ESTEREOGRÁFICA

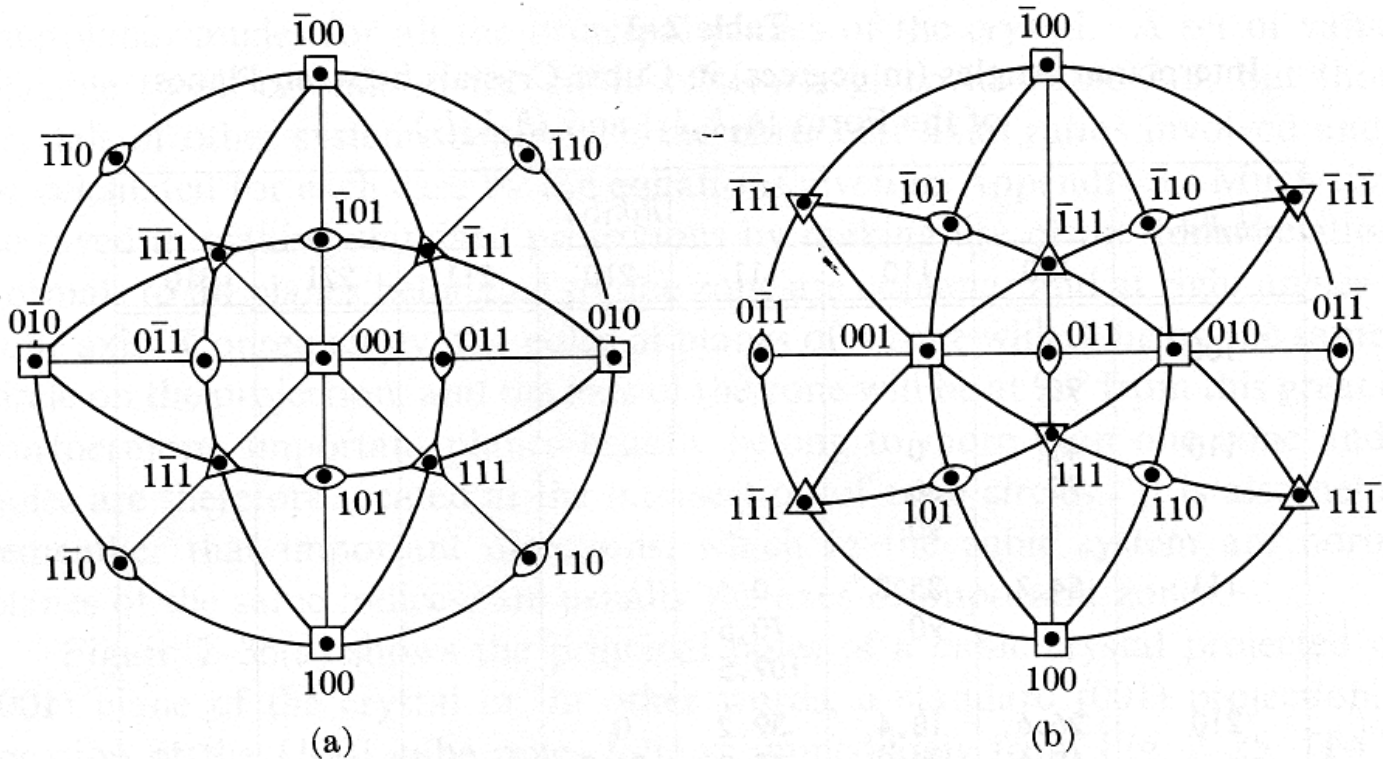
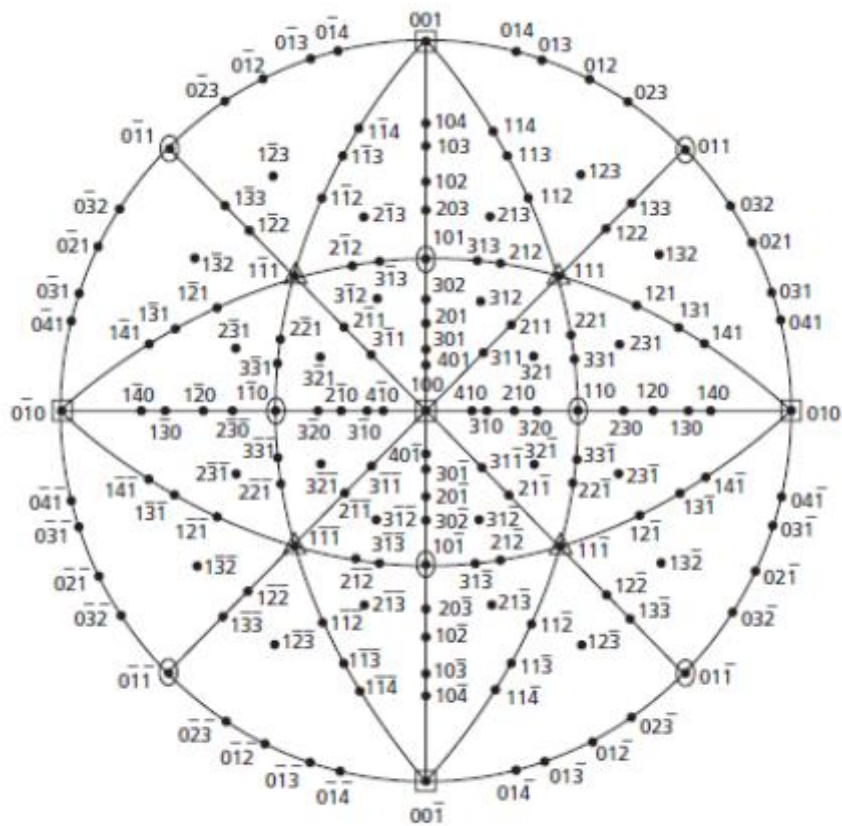
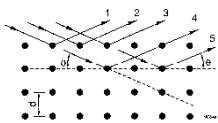
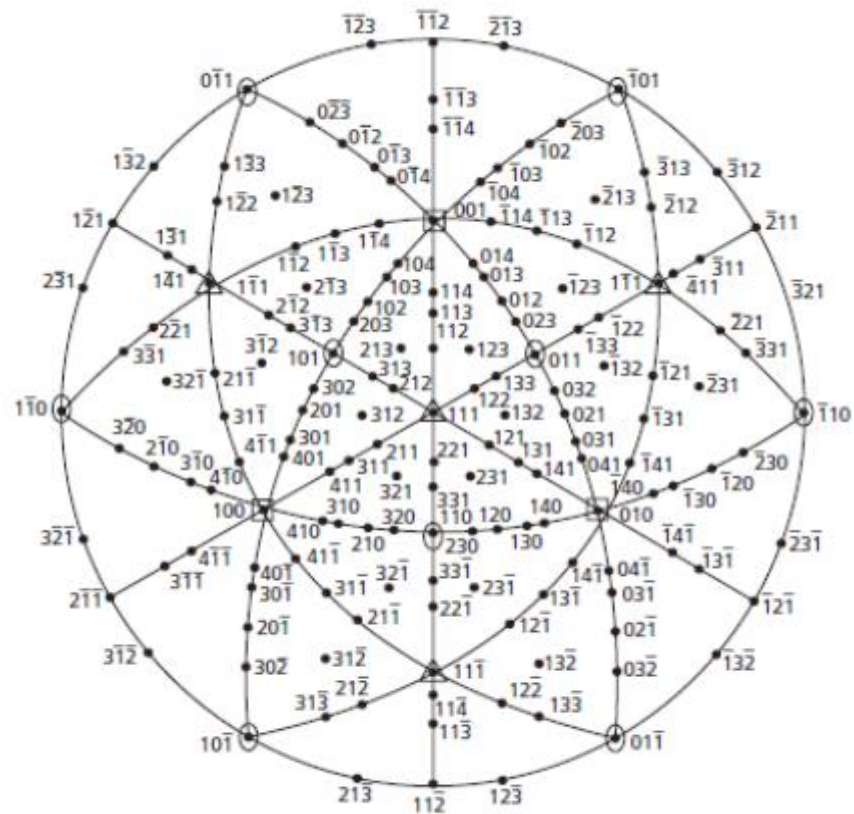


Fig. 2-36 Standard projections of cubic crystals, (a) on (001) and (b) on (011).

# PROJEÇÃO ESTEREOGRÁFICA



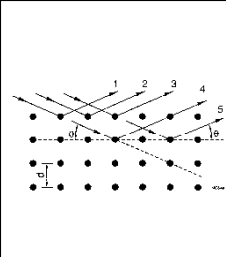
**FIG. 1.31** A 100 standard stereographic projection of a cubic crystal showing additional poles



**FIG. 1.32** A 111 standard projection of a cubic crystal



# ÂNGULOS ENTRE PLANOS CRISTALINOS EM CRISTAIS CÚBICOS



$ h_2k_2l_2 $	$ h_1k_1l_1 $						
	100	110	111	210	211	221	310
100	0						
90							
110	45	0					
90		60					
90							
111	54.7	35.3	0				
		90	70.5				
			109.5				
210	26.6	18.4	39.2	0			
63.4		50.8	75.0	36.9			
90		71.6		53.1			
211	35.3	30	19.5	24.1	0		
65.9		54.7	61.9	43.1	33.6		
		73.2	90	56.8	48.2		
		90					
221	48.2	19.5	15.8	26.6	17.7	0	
70.5		45	54.7	41.8	35.3	27.3	
		76.4	78.9	53.4	47.1	39.0	
		90					
310	18.4	26.6	43.1	8.1	25.4	32.5	0
71.6		47.9	68.6	58.1	49.8	42.5	25.9
90		63.4		45	58.9	58.2	36.9
		77.1					
311	25.2	31.5	29.5	19.3	10.0	25.2	17.6
72.5		64.8	58.5	47.6	42.4	45.3	40.3
		90	80.0	66.1	60.5	59.8	55.1
320	33.7	11.3	61.3	7.1	25.2	22.4	15.3
56.3		54.0	71.3	29.8	37.6	42.3	37.9
90		66.9		41.9	55.6	49.7	52.1
321	36.7	19.1	22.2	17.0	10.9	11.5	21.6
57.7		40.9	51.9	33.2	29.2	27.0	32.3
74.5		55.5	72.0	53.3	40.2	36.7	40.5
			90				
331	46.5	13.1	22.0				

# PROJEÇÃO ESTEREOGRÁFICA

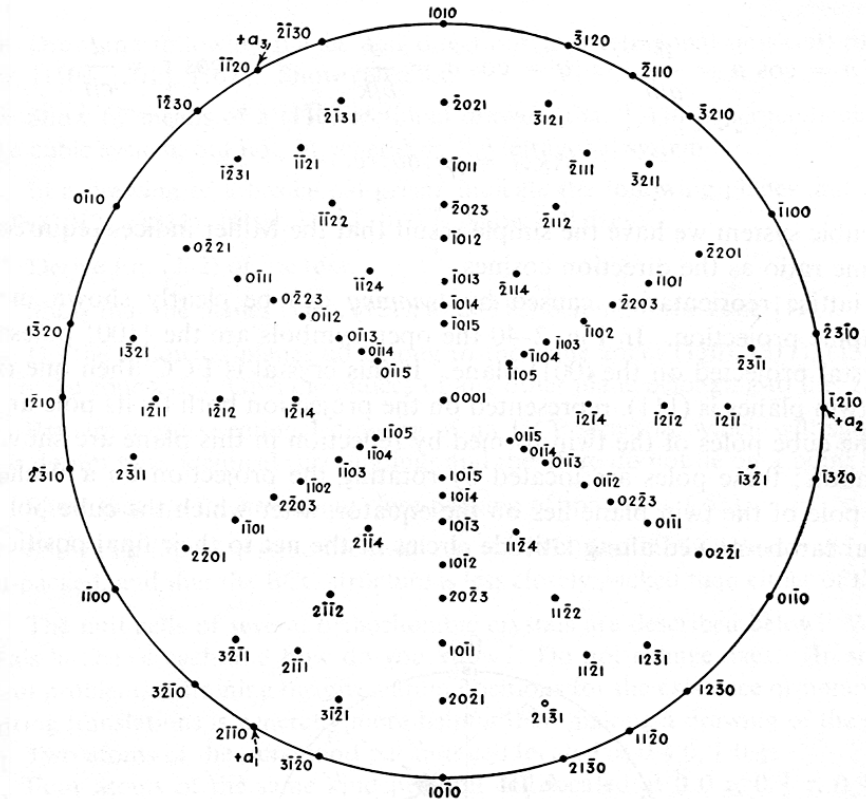
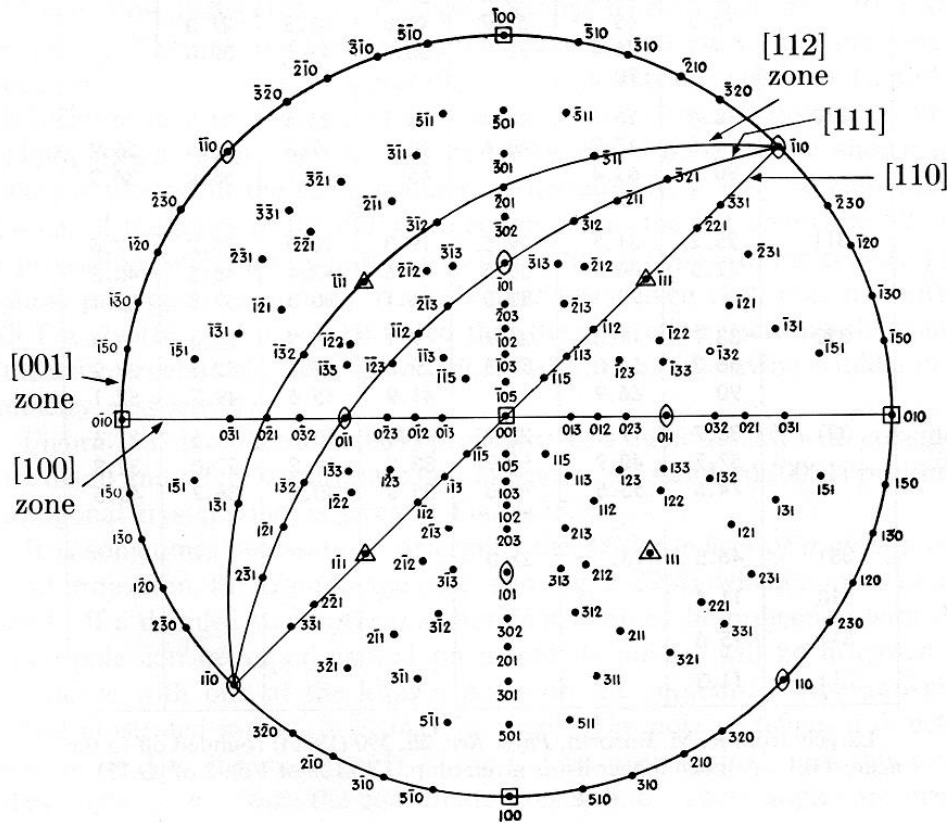
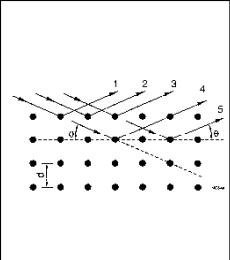


Fig. 2-37 Standard (001) projection of a cubic crystal, after Barrett [1.7].

2-38 Standard (001) projection for zinc (hexagonal,  $c/a = 1.86$ ) after Barr

# DETERMINAÇÃO DOS ÍNDICES DE MILLER DE UM POLO

$$p = \cos \rho = \frac{d}{a/h}, \quad q = \cos \sigma = \frac{d}{b/k}, \quad r = \cos \tau = \frac{d}{c/l}$$

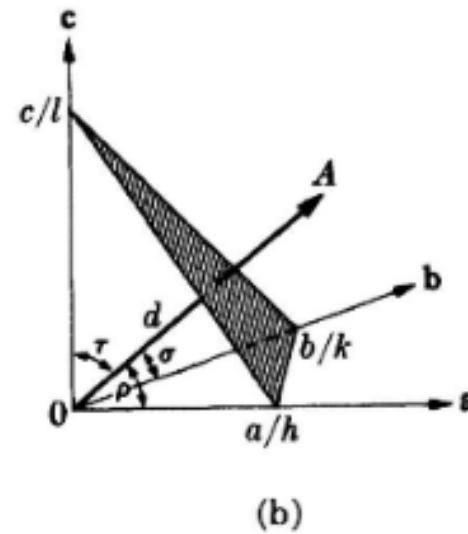
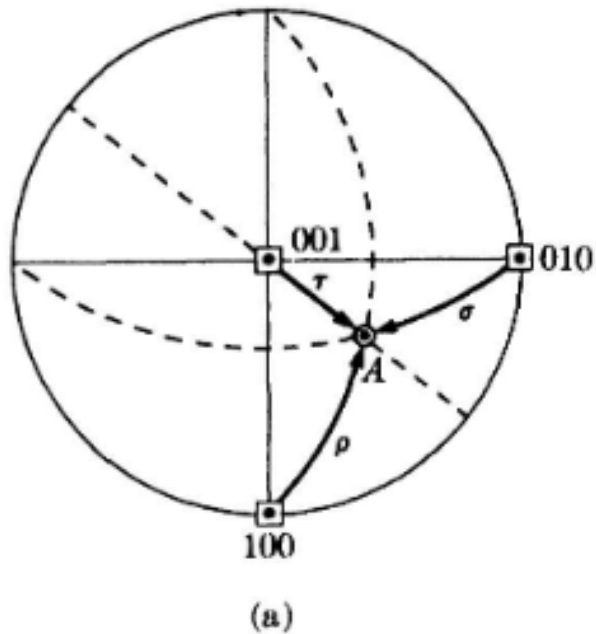
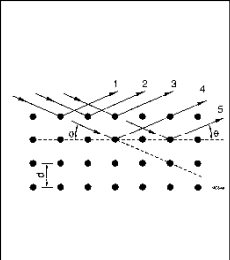
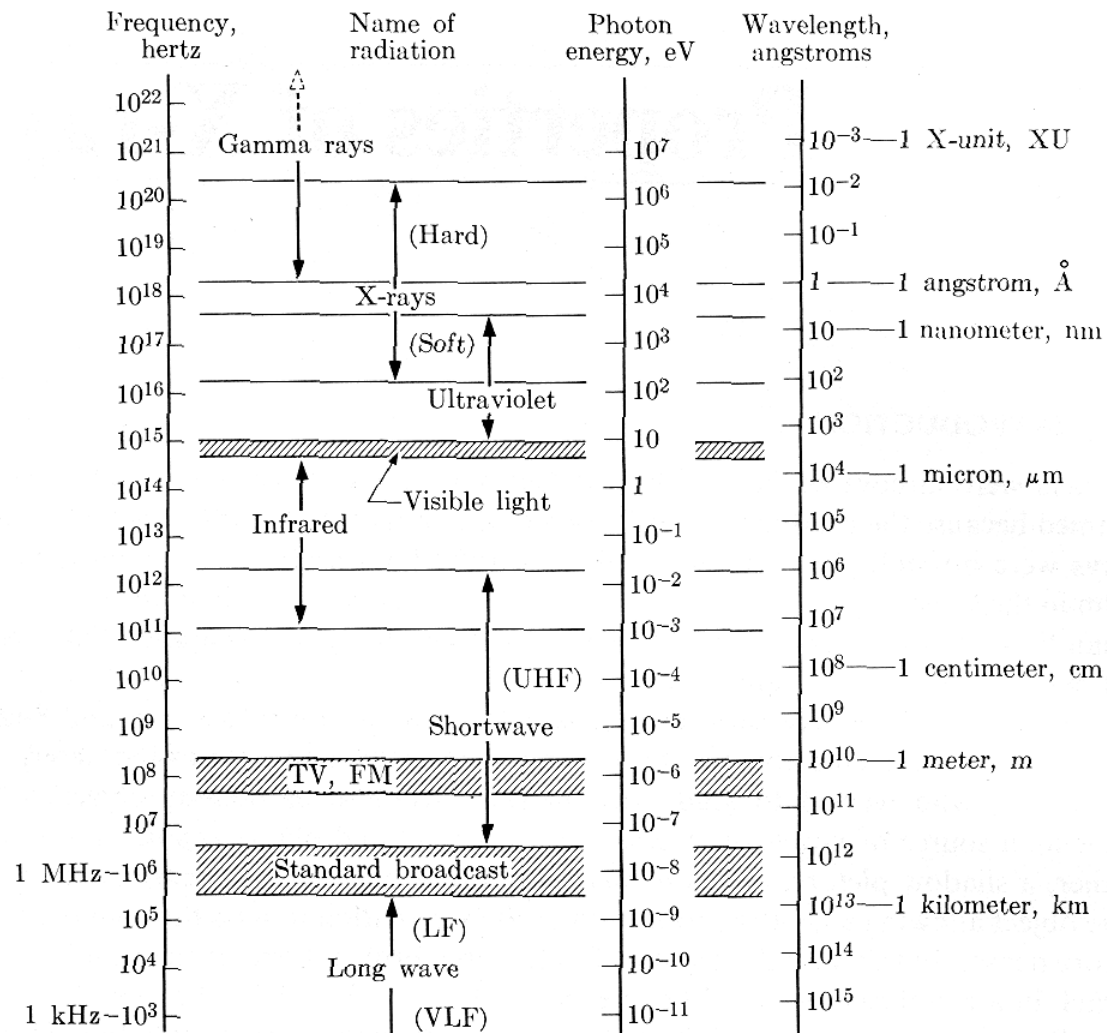


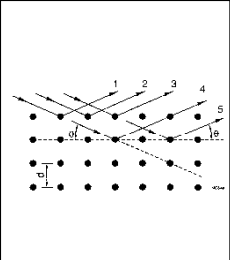
FIG. 2-39. Determination of the Miller indices of a pole.

$$h:k:l = pa:qb:rc.$$

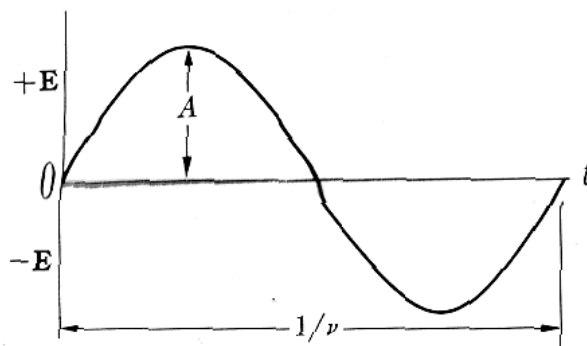
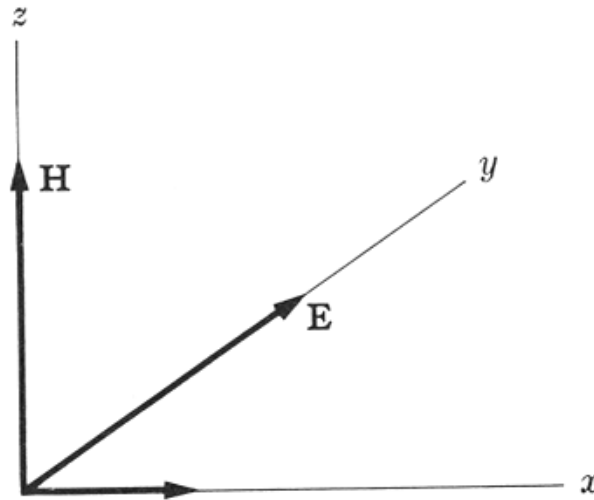


# DIFRAÇÃO DE RAIOS-X

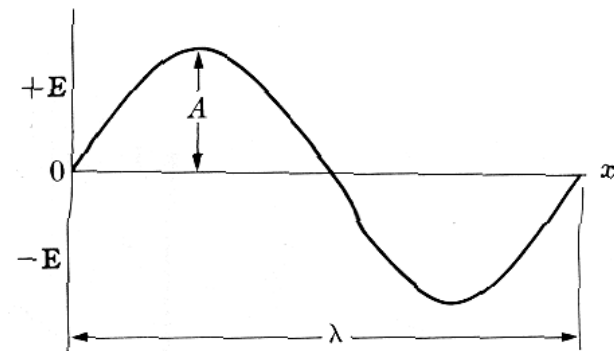




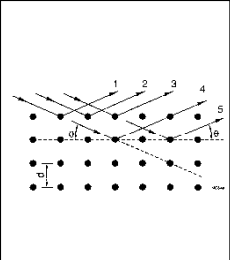
# ONDAS ELETROMAGNÉTICAS



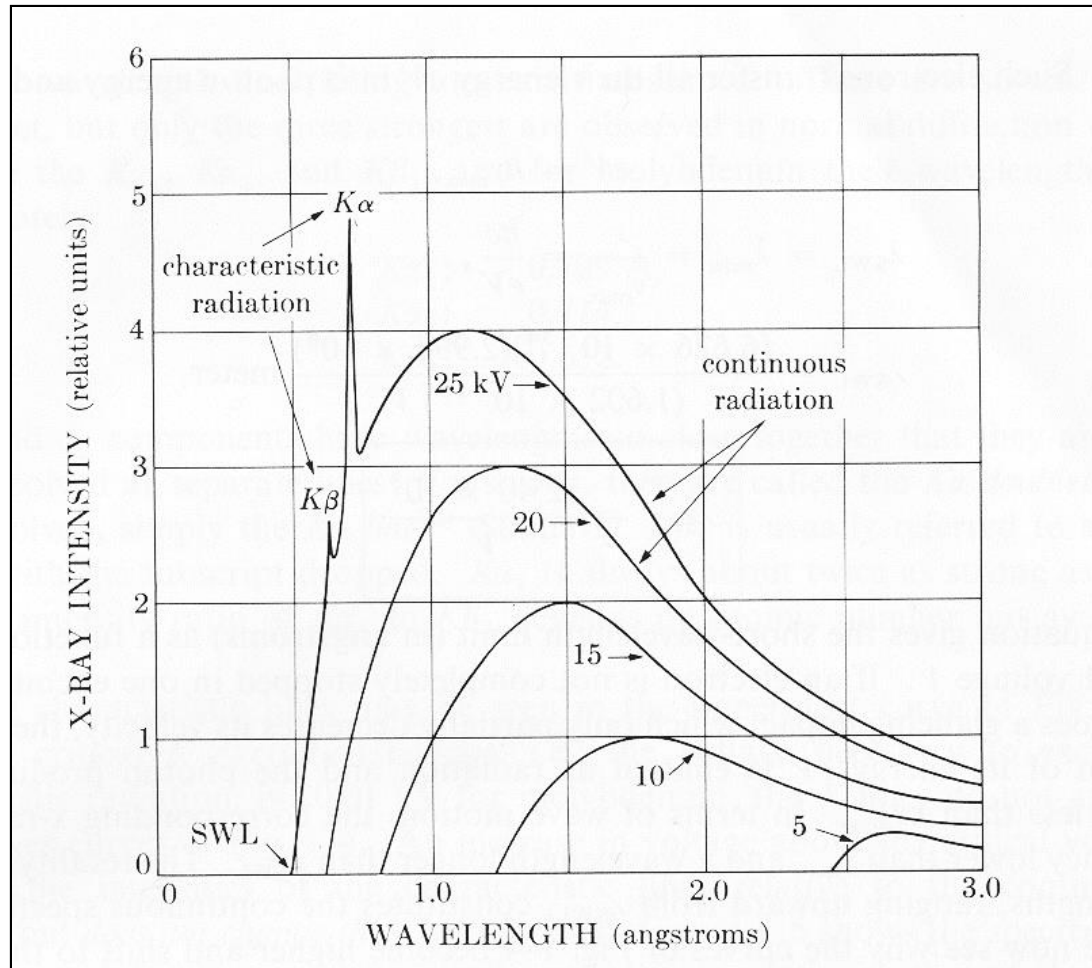
(a)

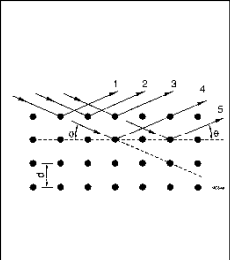


(b)

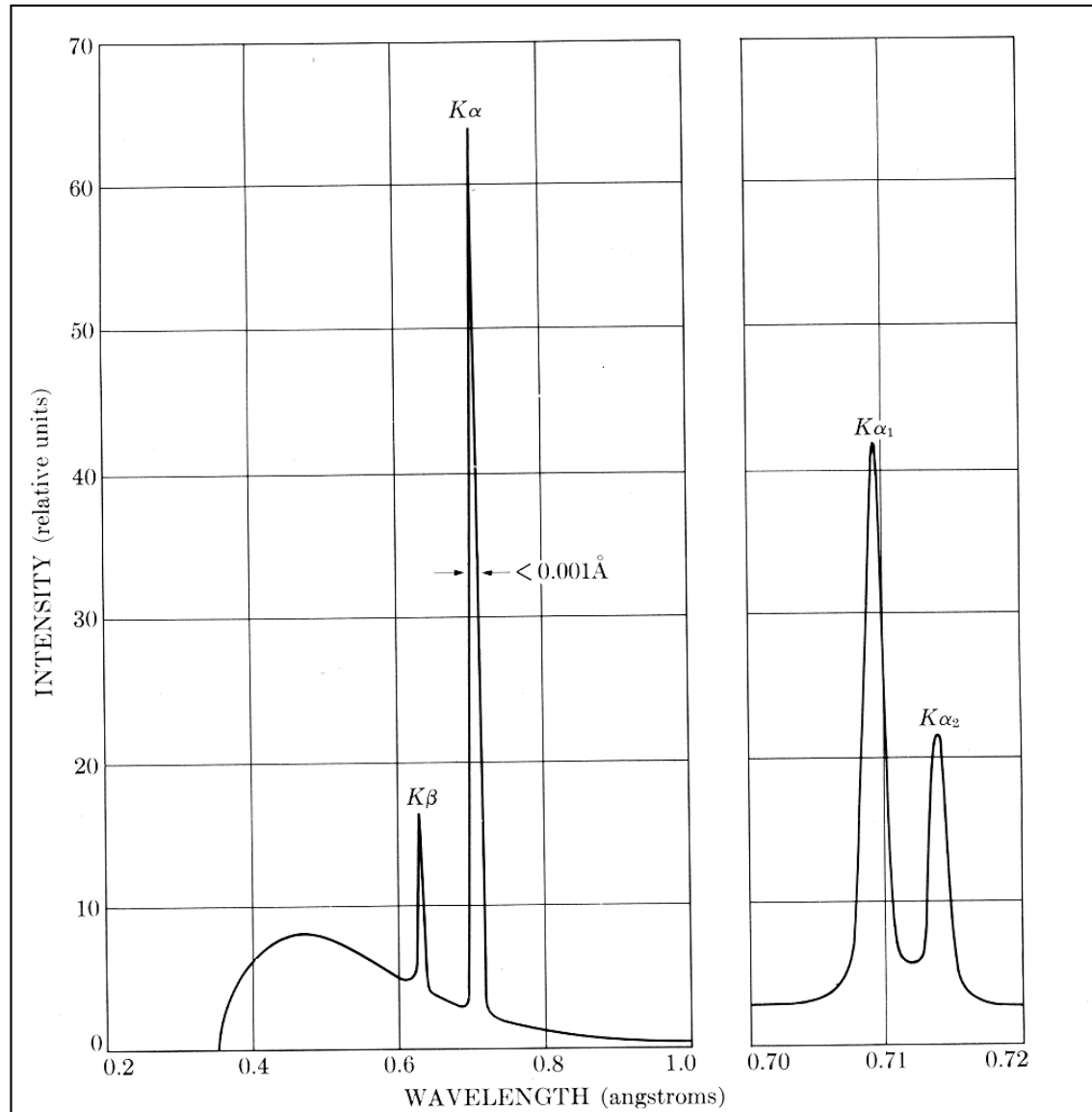


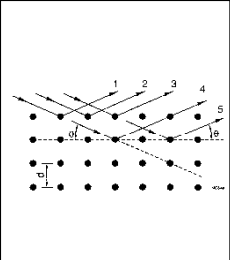
# INTENSIDADE DE RAIOS-X



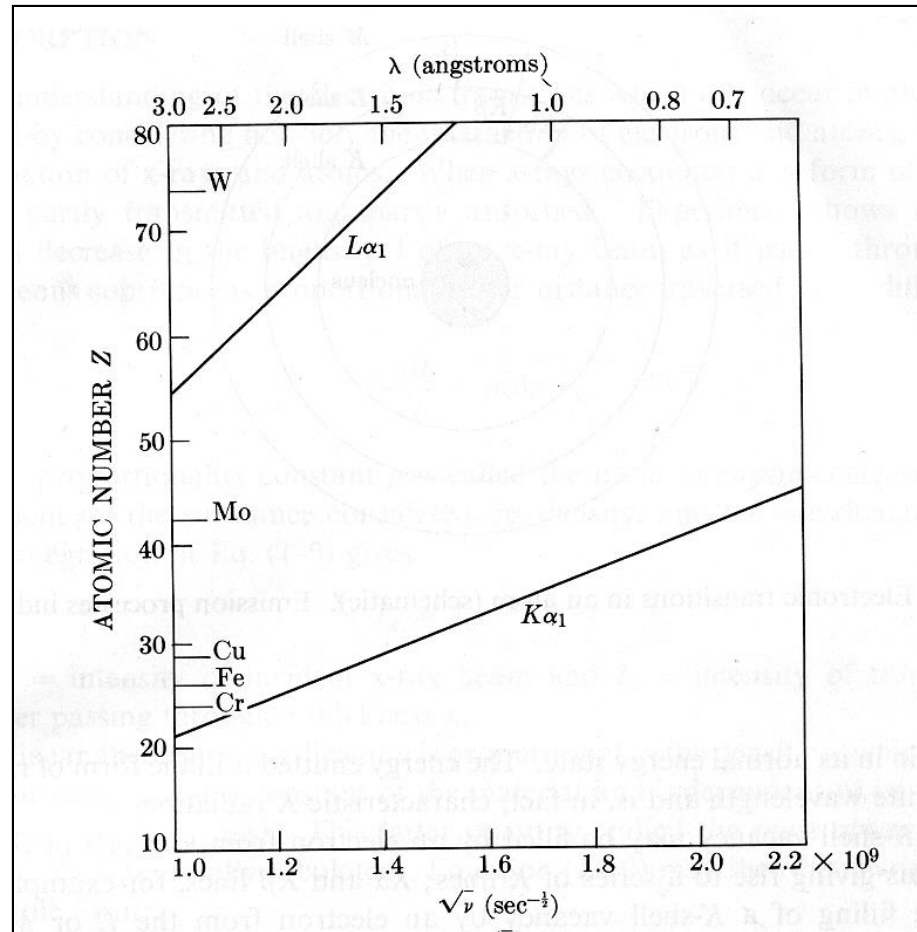


# INTENSIDADE DE RAIOS-X

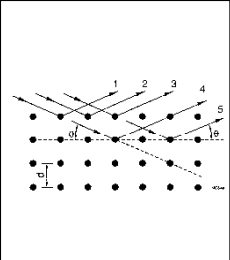




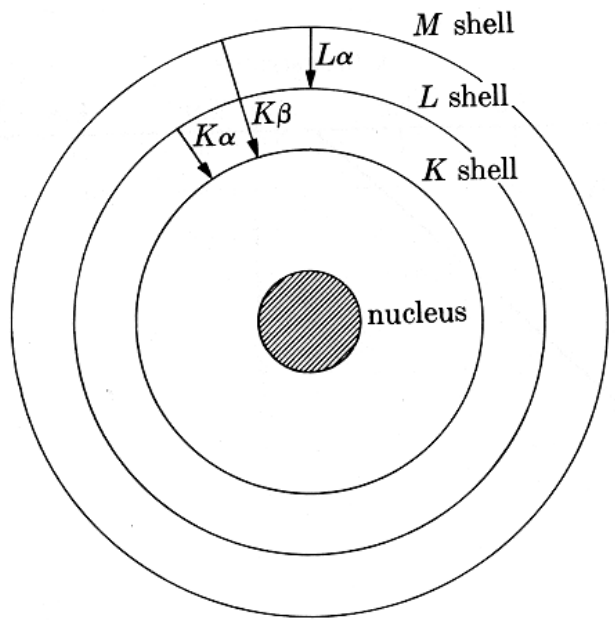
# INTENSIDADE DE RAIOS-X



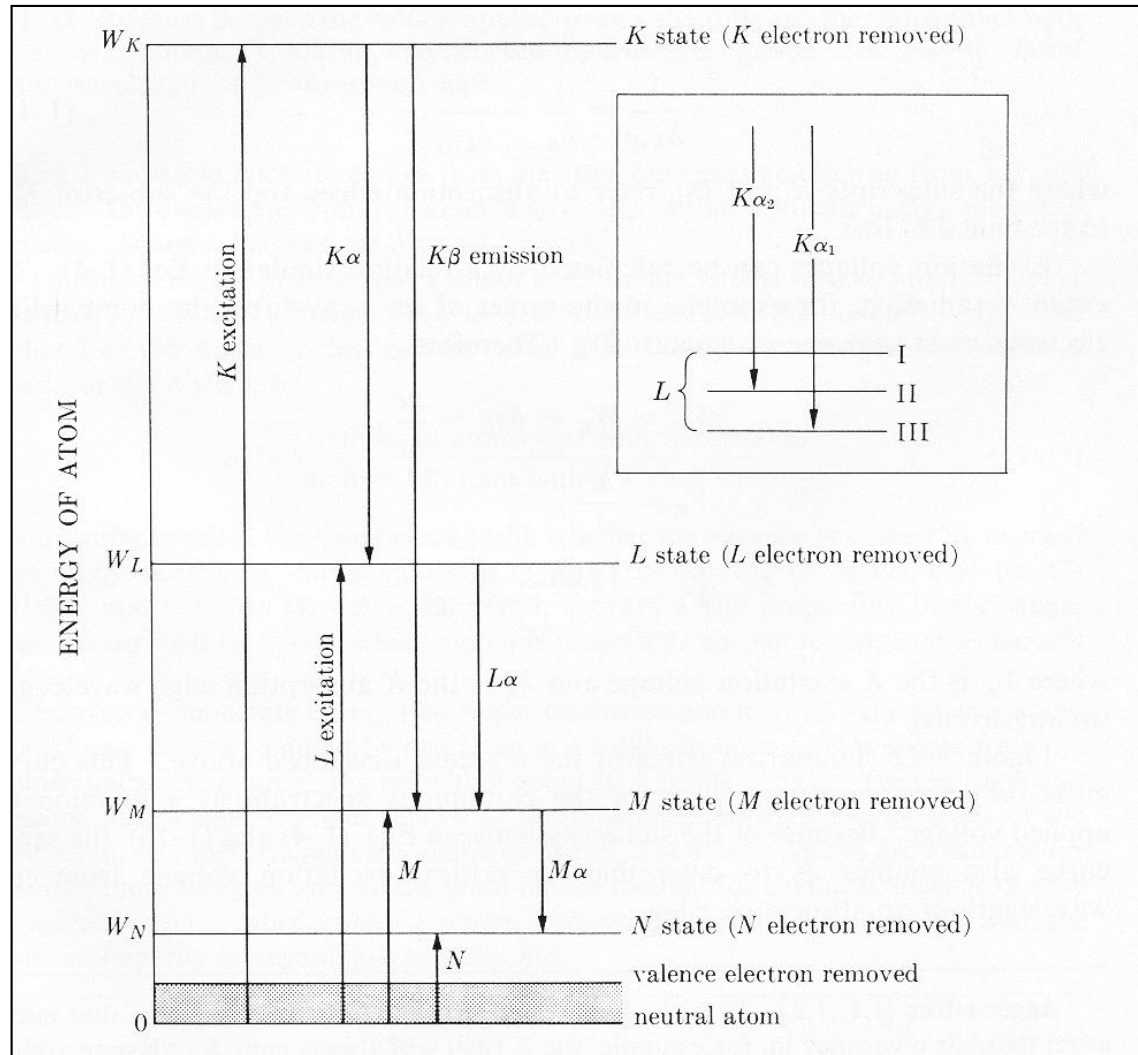




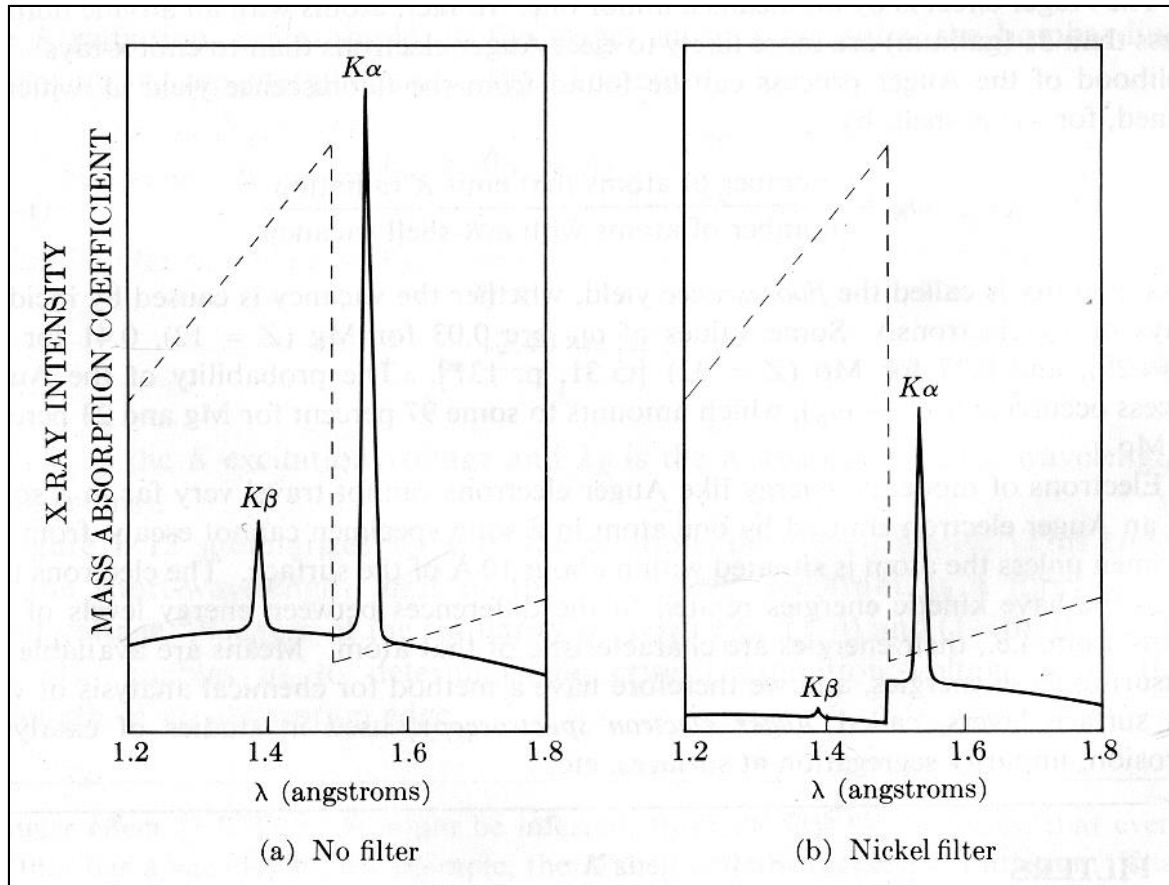
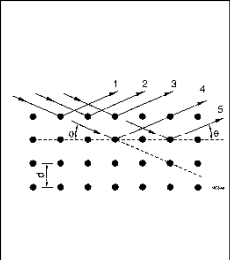
# DECAIMENTO DE ELÉTRONS



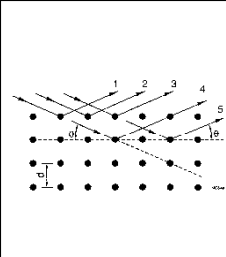
# DECAIMENTO DE ELÉTRONS



# APLICAÇÃO DE FILTROS



# APLICAÇÃO DE FILTROS



**Table 1-1**  
Filters for Suppression of  $K\beta$  Radiation

Target	Filter	Incident beam* $\frac{I(K\alpha)}{I(K\beta)}$	Filter thickness for $\frac{I(K\alpha)}{I(K\beta)} = \frac{500}{1}$ in trans. beam		$\frac{I(K\alpha) \text{ trans.}}{I(K\alpha) \text{ incident}}$
			mg/cm <sup>2</sup>	in.	
Mo	Zr	5.4	77	0.0046	0.29
Cu	Ni	7.5	18	0.0008	0.42
Co	Fe	9.4	14	0.0007	0.46
Fe	Mn	9.0	12	0.0007	0.48
Cr	V	8.5	10	0.0006	0.49

# TUBOS DE RAIOS-X

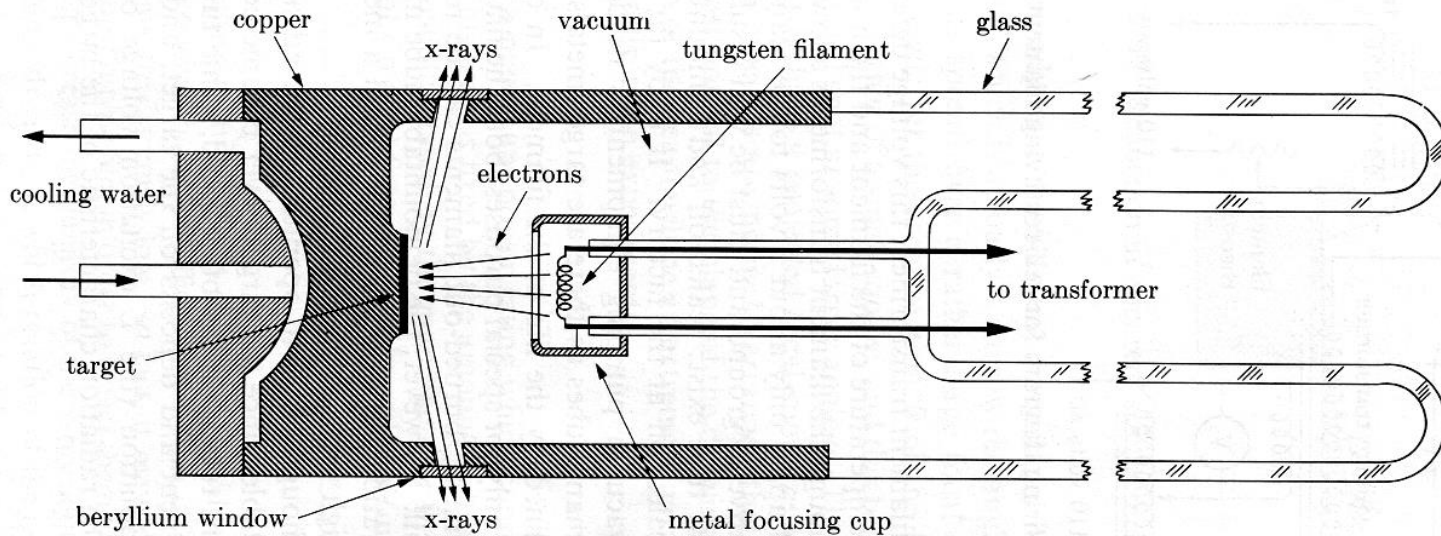
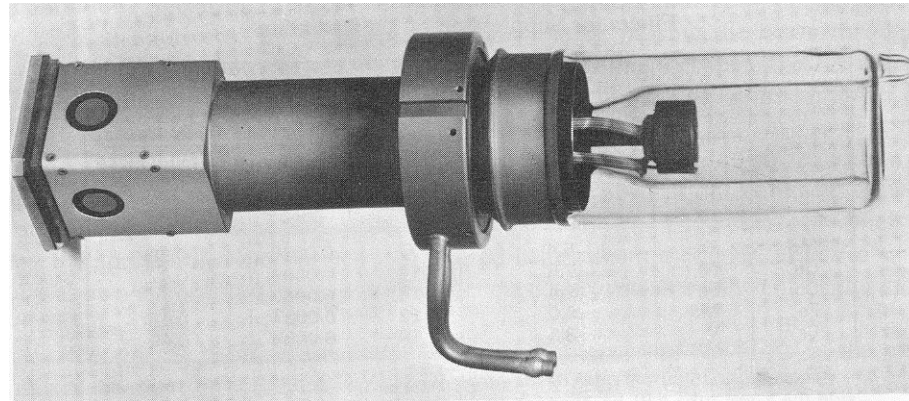
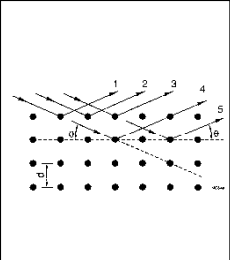
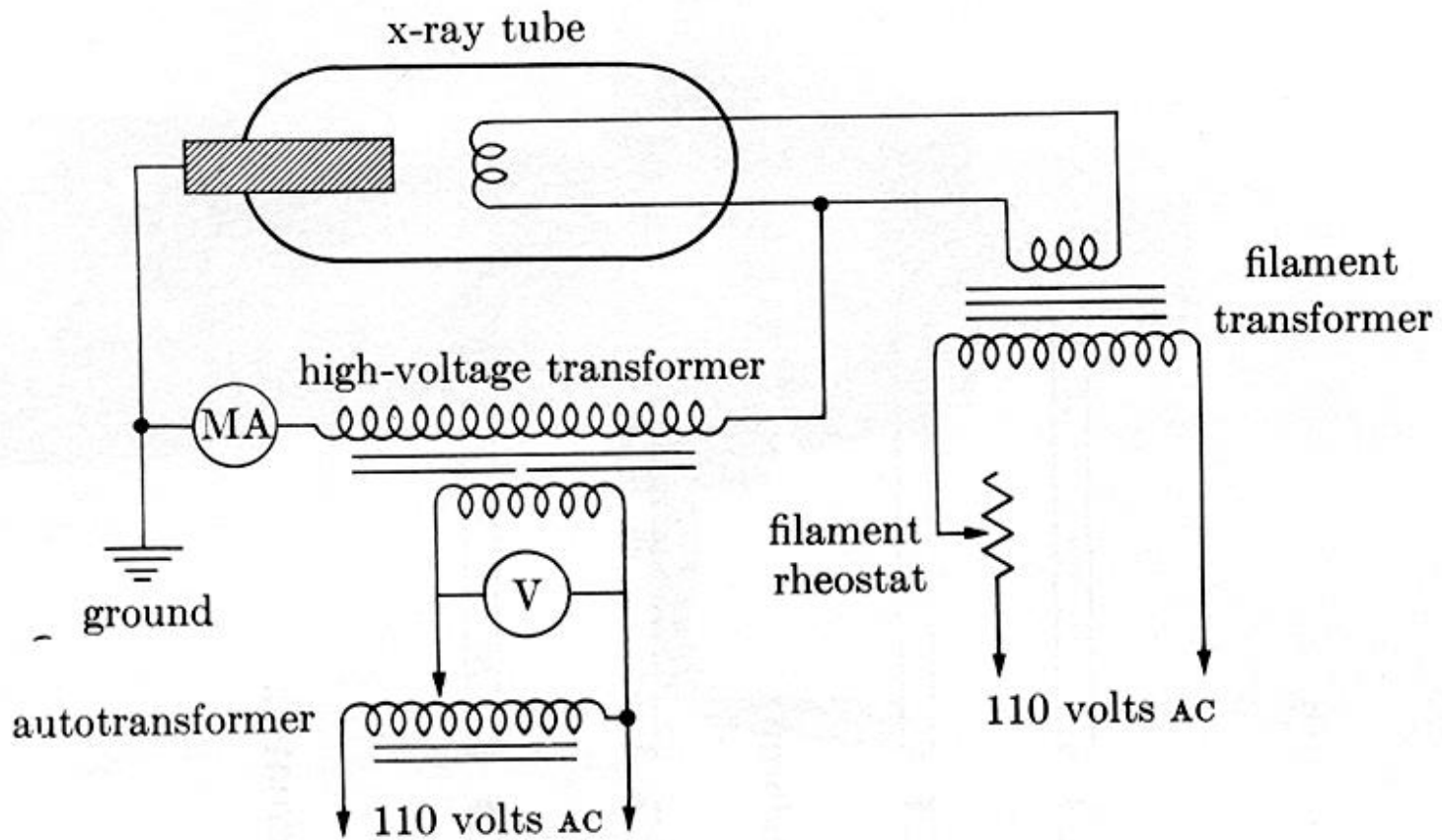


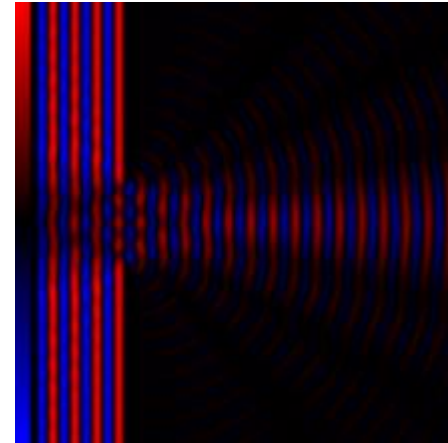
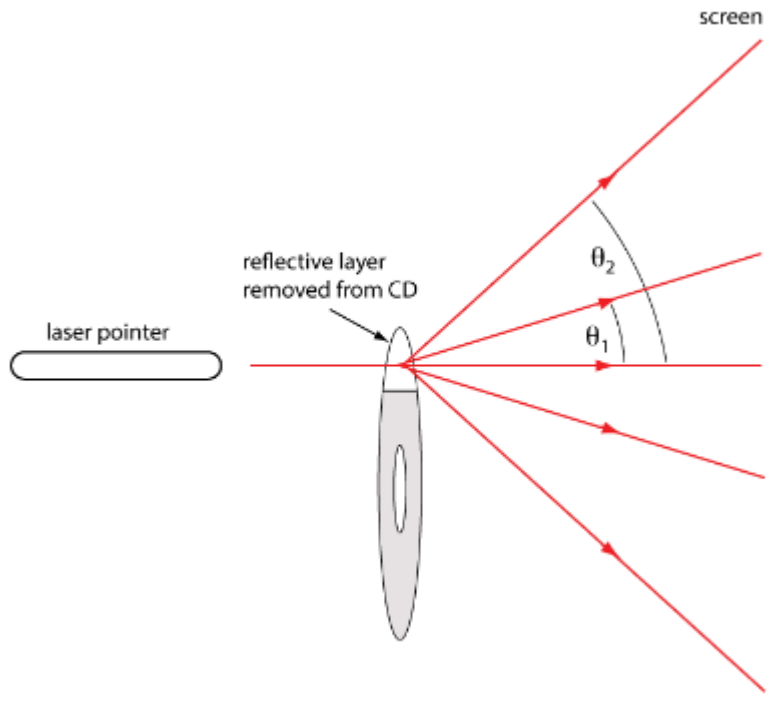
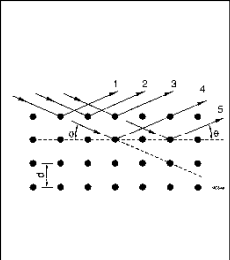
Fig. 1-15 Cross section of sealed-off filament x-ray tube (schematic).



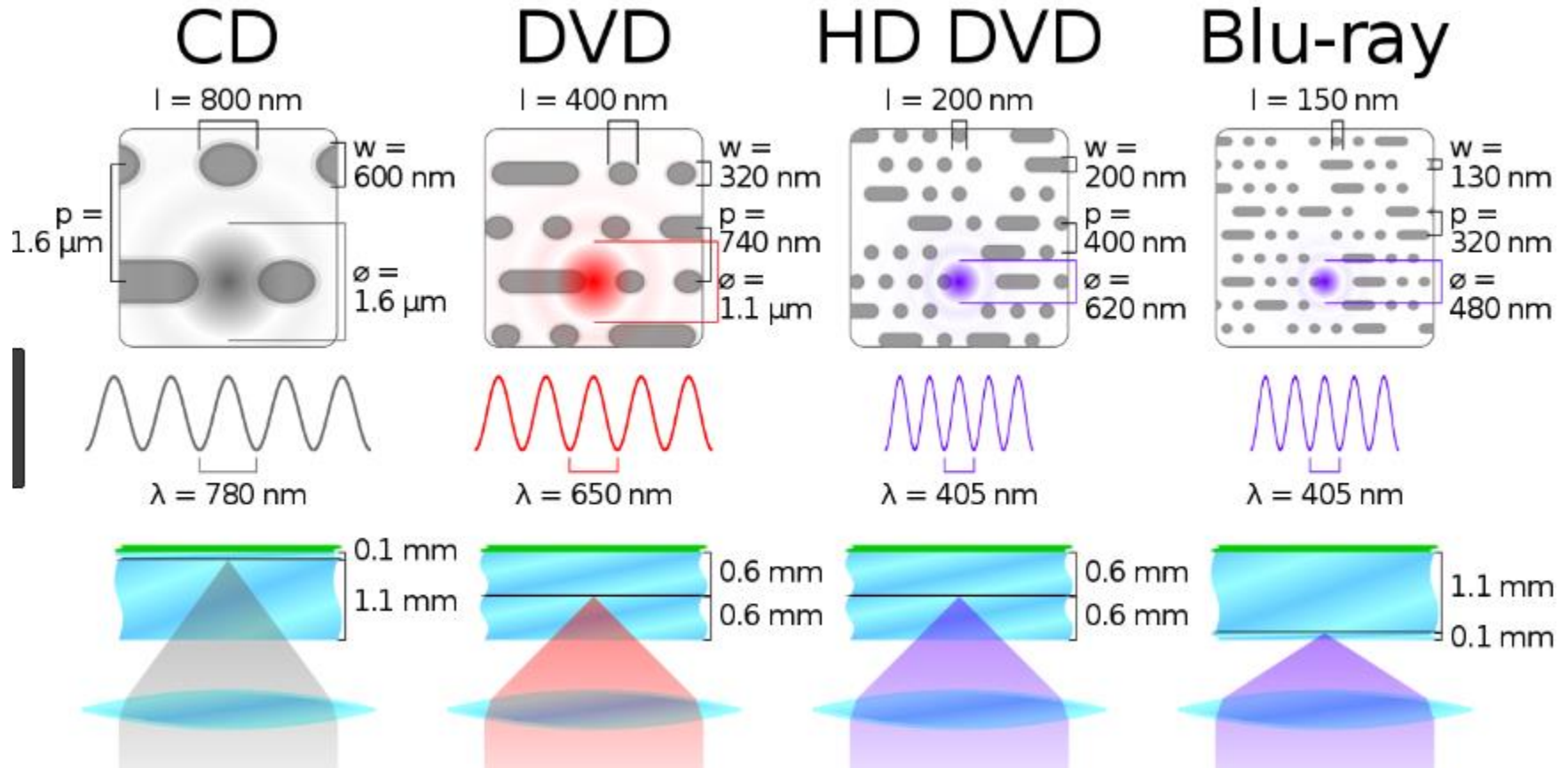
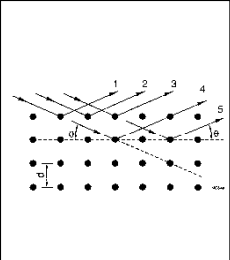
# TUBOS DE RAIOS-X



# DIFRAÇÃO DE ONDAS ELETROMAGNÉTICAS

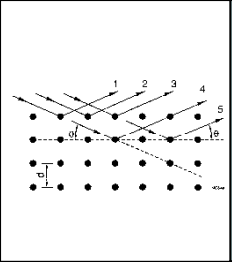


# DIFRAÇÃO DE ONDAS ELETROMAGNÉTICAS

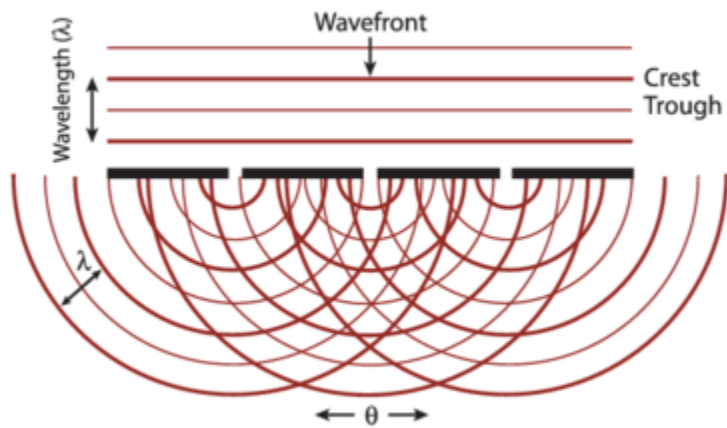




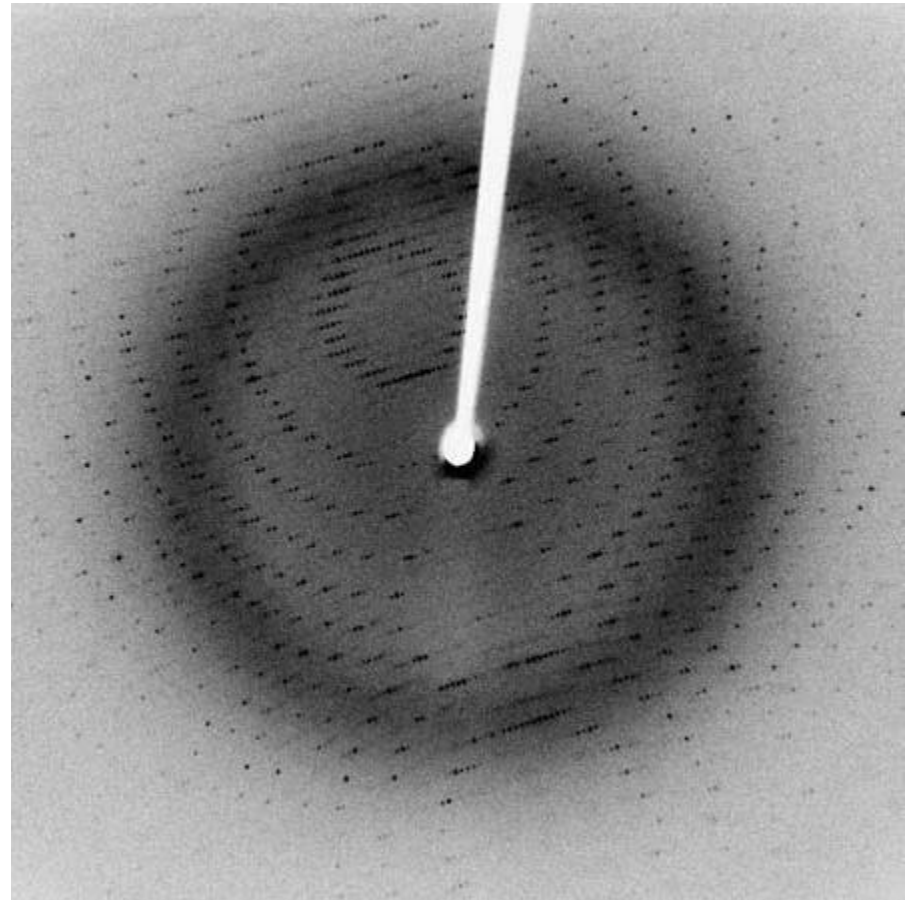
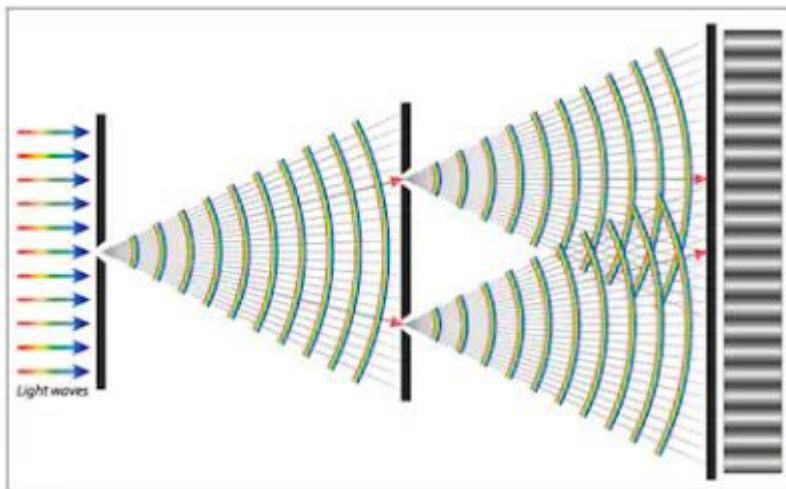
# DIFRAÇÃO DE ONDAS ELETROMAGNÉTICAS

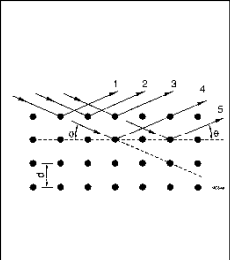


Diffraction Mechanism

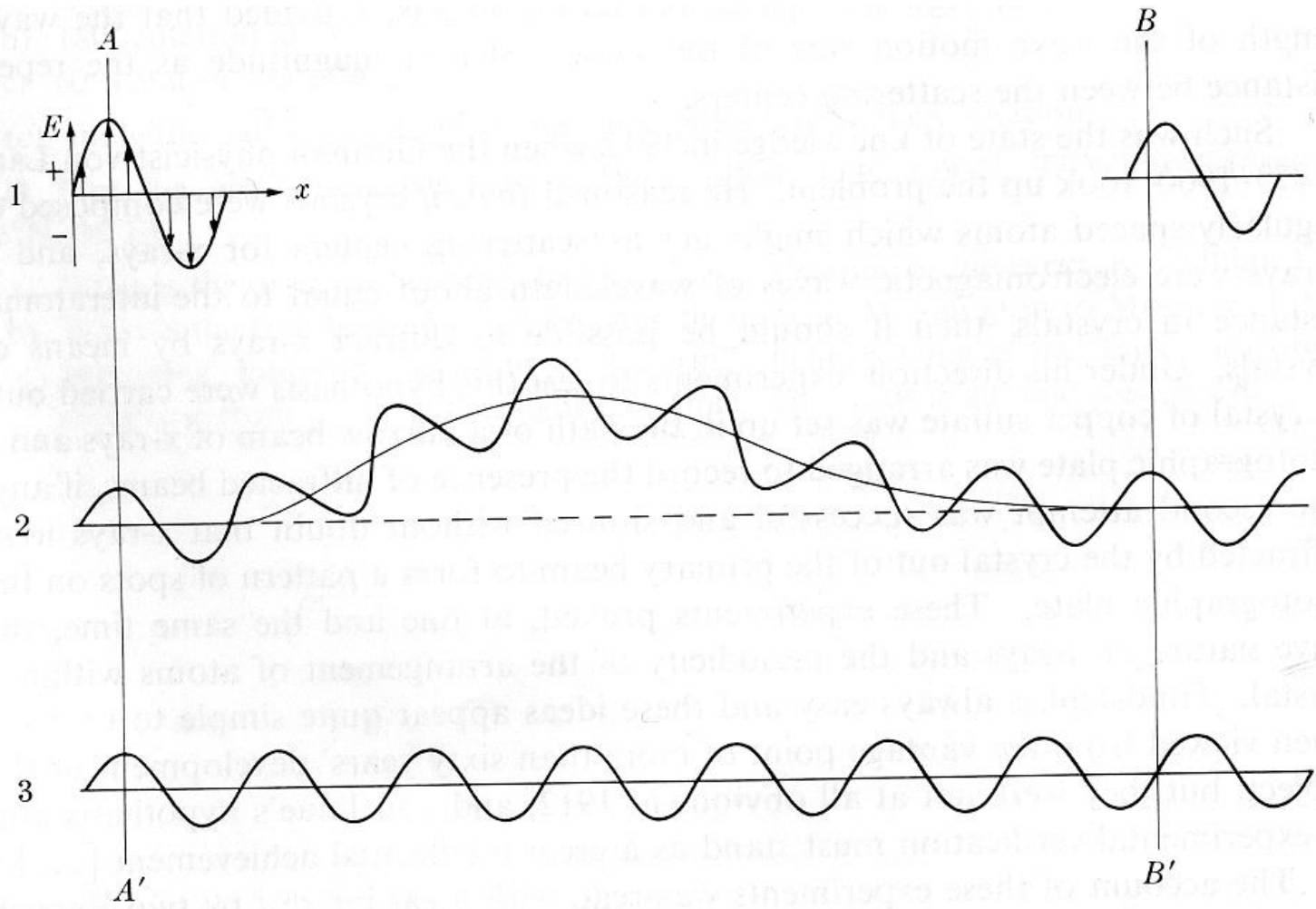


Diffraction Intensity

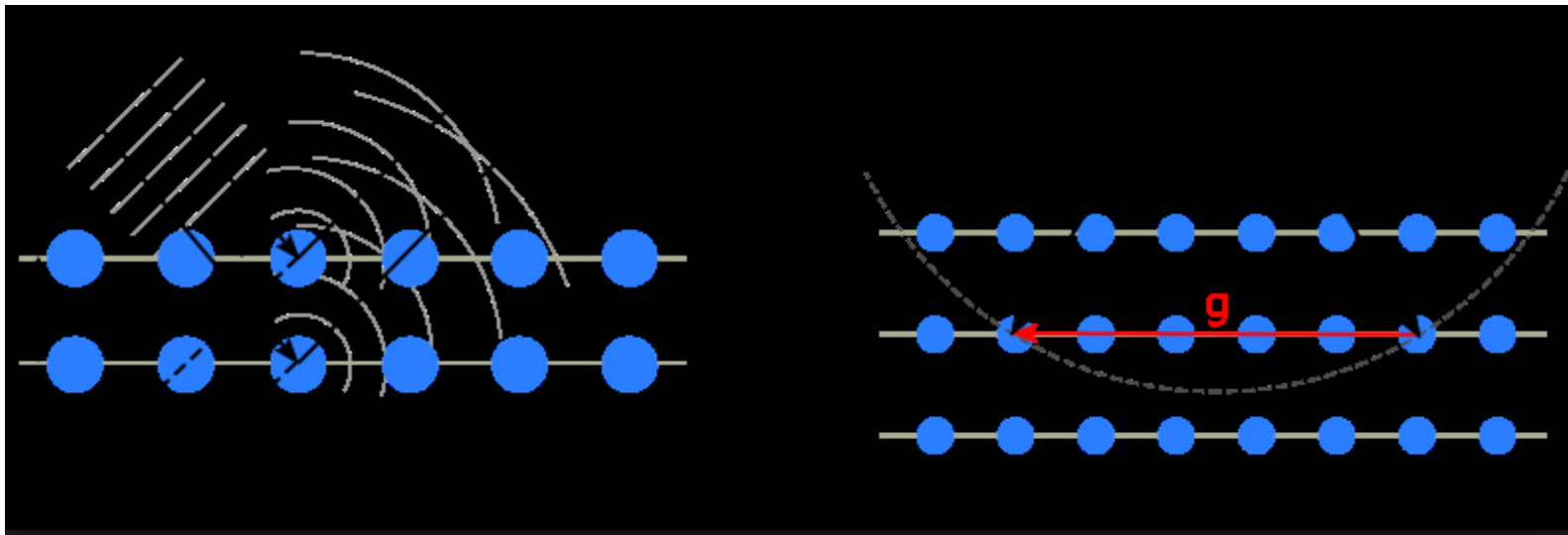
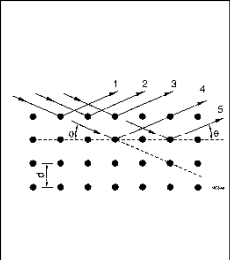




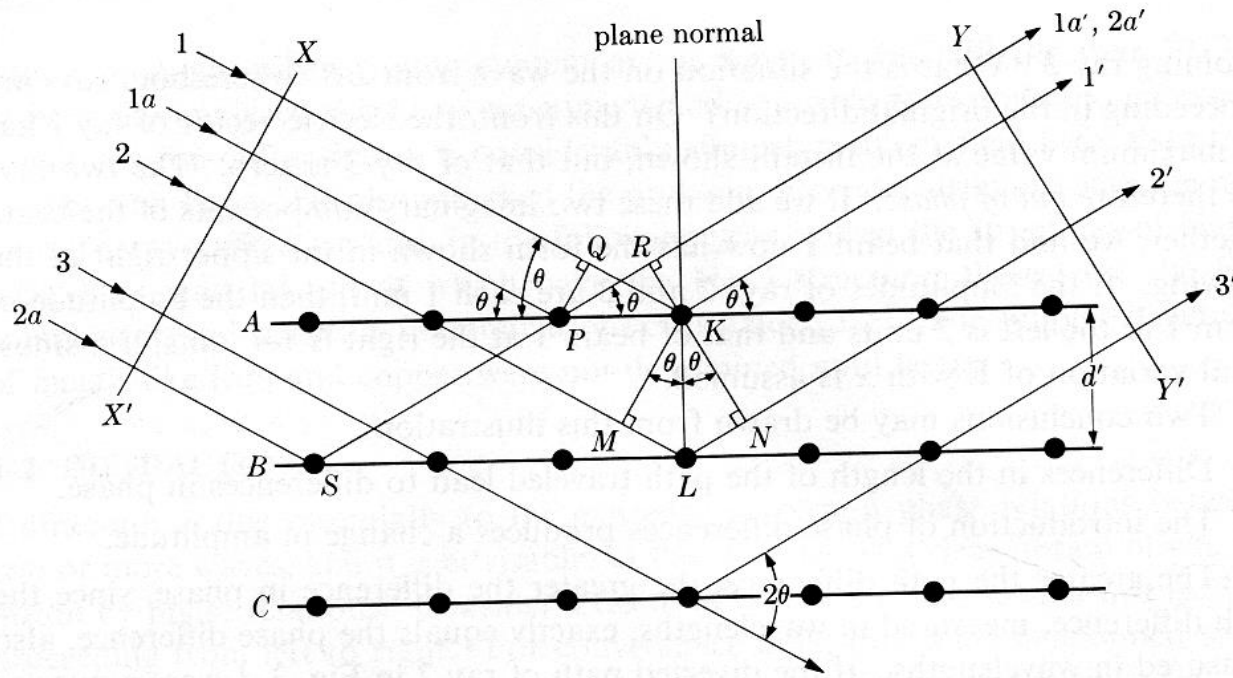
# DIFERENÇA DE TRAJETÓRIAS DE ONDAS ELETROMAGNÉTICAS



# DIFERENÇA DE TRAJETÓRIAS DE ONDAS ELETROMAGNÉTICAS



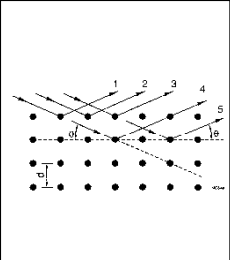
# LEI DE BRAGG



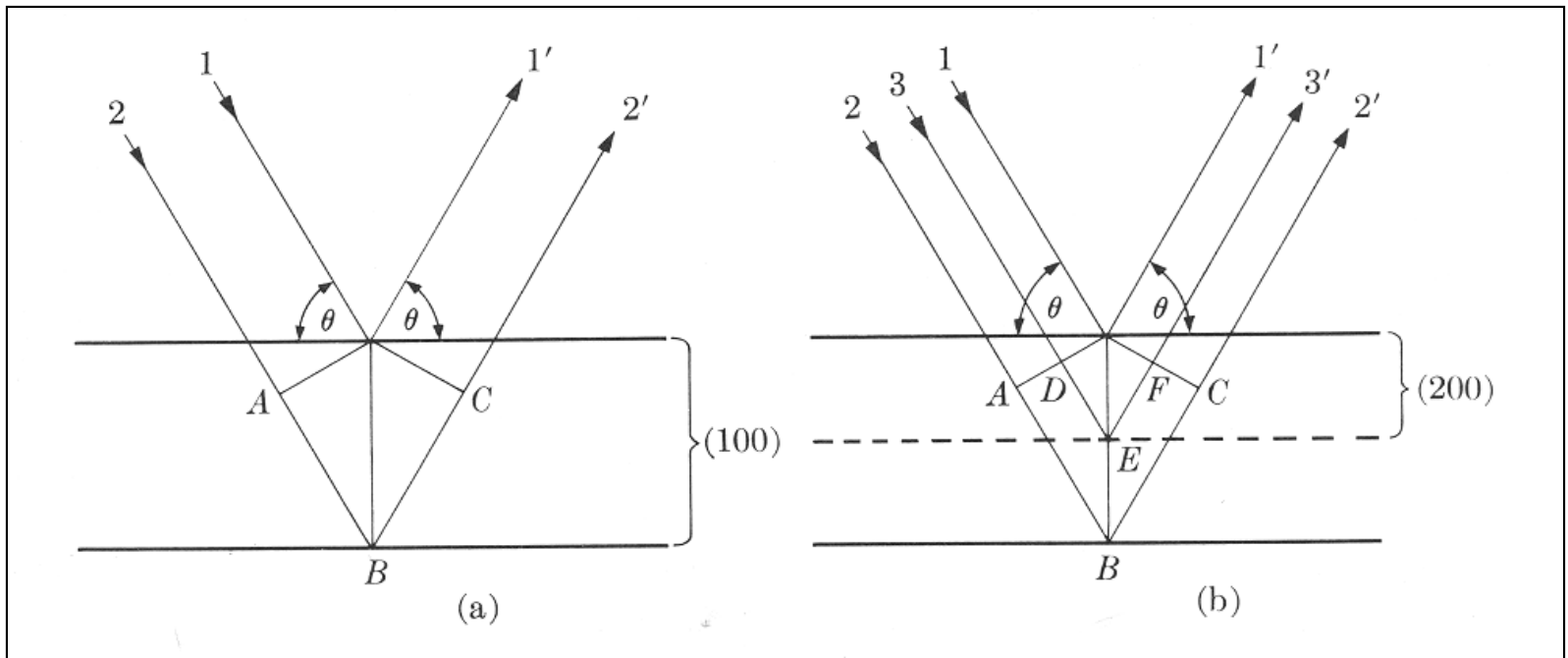
$$OK - PR = PK \cos \theta - PK \cos \theta = 0.$$

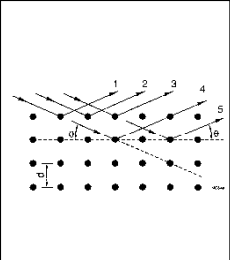
$$ML + LN = d' \sin \theta + d' \sin \theta.$$

$$n\lambda = 2d' \sin \theta.$$

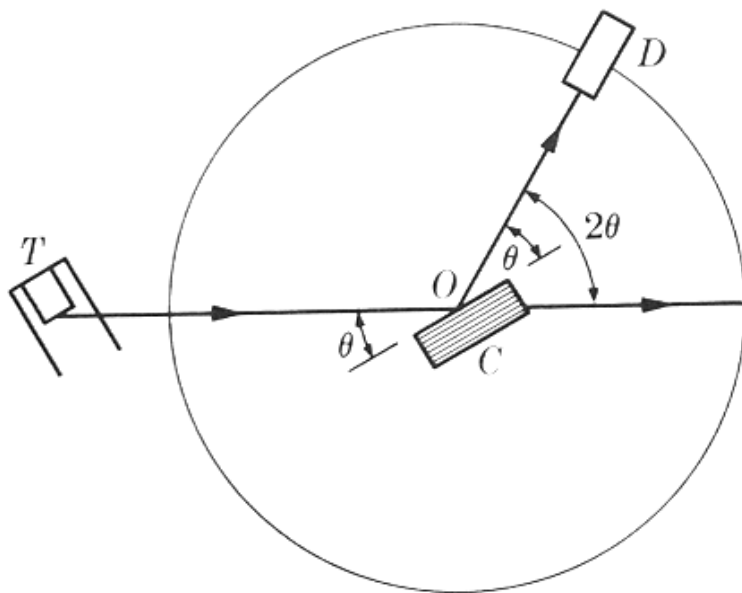


# LEI DE BRAGG





# DIFRATÔMETROS



Configuração Bragg-Brentano  $\theta - 2\theta$

A lei de Bragg pode ser usada de duas maneiras:

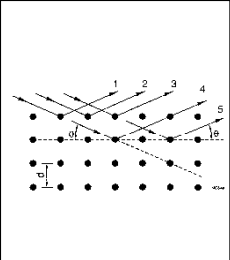
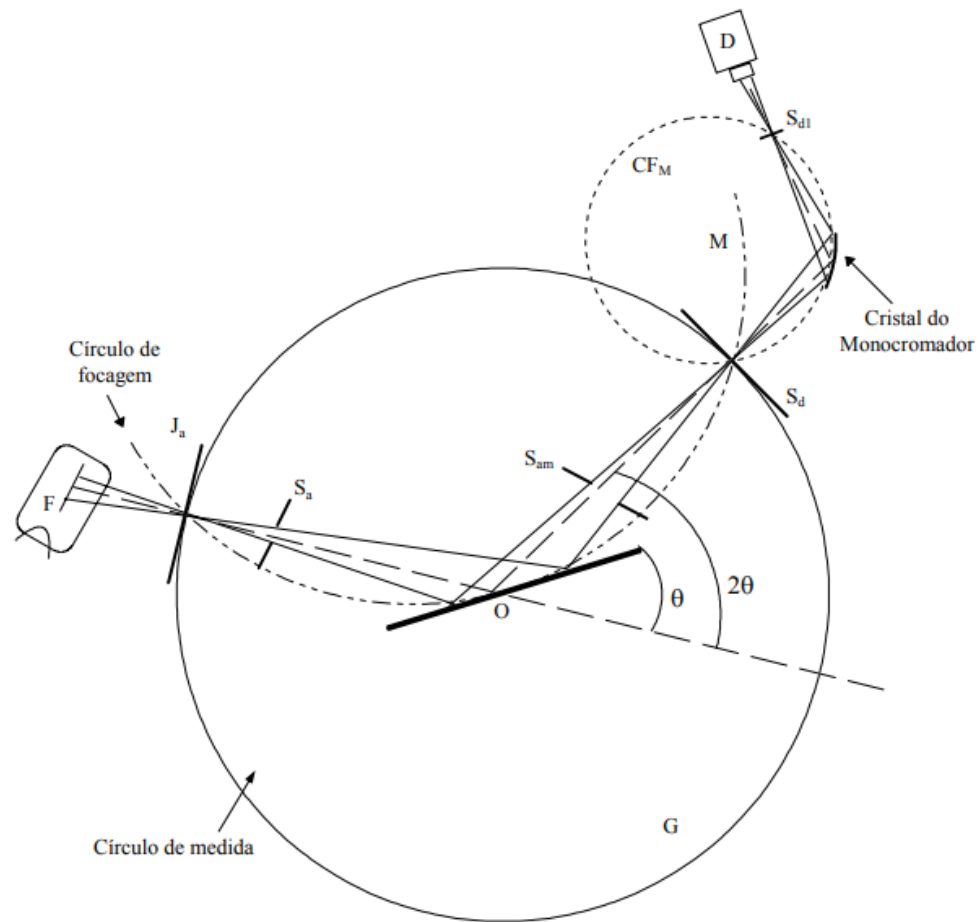
a) Análise estrutural

- Raios-X de comprimento de onda  $\lambda$  conhecido (monocromático) permitem medir o ângulo  $\theta$  de difração e determinar o espaçamento  $d$  entre planos cristalinos.

b) Espectroscopia de raios-X

- Usar um cristal de com espaçamento interplanar  $d$  conhecido e medir o ângulo  $\theta$  de difração e assim determinar o comprimento de onda da radiação emitida.

# CONFIGURAÇÃO BRAGG-BRENTANO $\theta - 2\theta$



# DIFRATOMETRIA

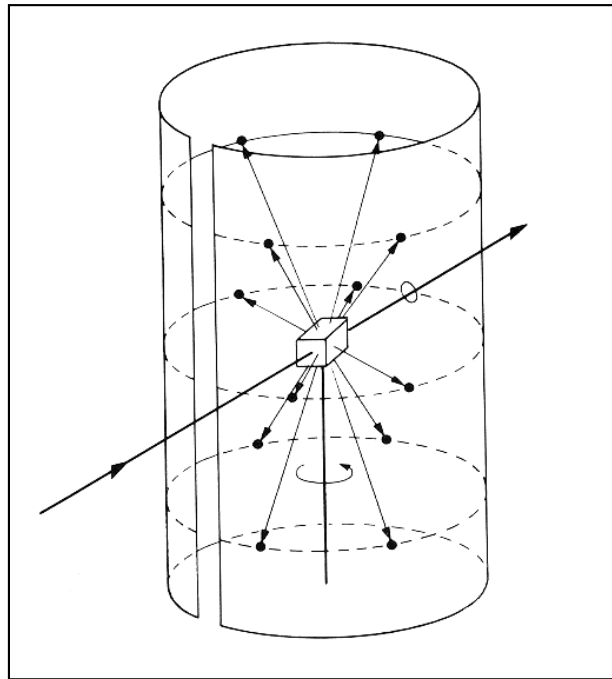
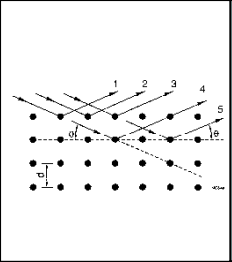


FIG. 3-9. Rotating-crystal method.

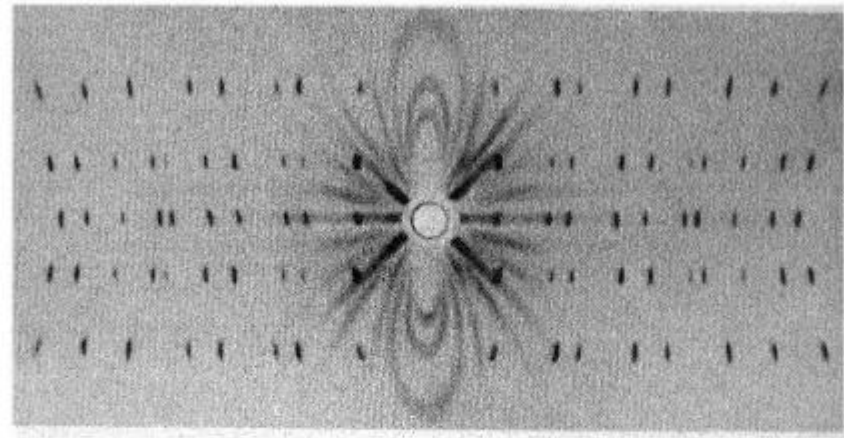


FIG. 3-10. Rotating-crystal pattern of a quartz crystal (hexagonal) rotated about its  $c$  axis. Filtered copper radiation. (The streaks are due to the white radiation not removed by the filter.) (Courtesy of B. E. Warren.)



# MÉTODO DE LAUE PARA MONOCRISTAIS

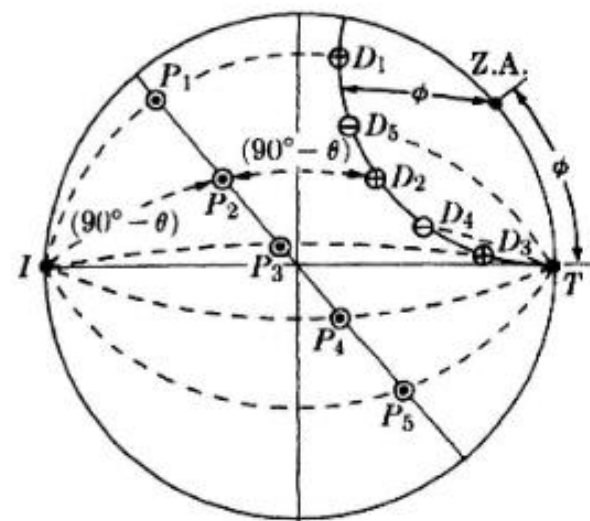
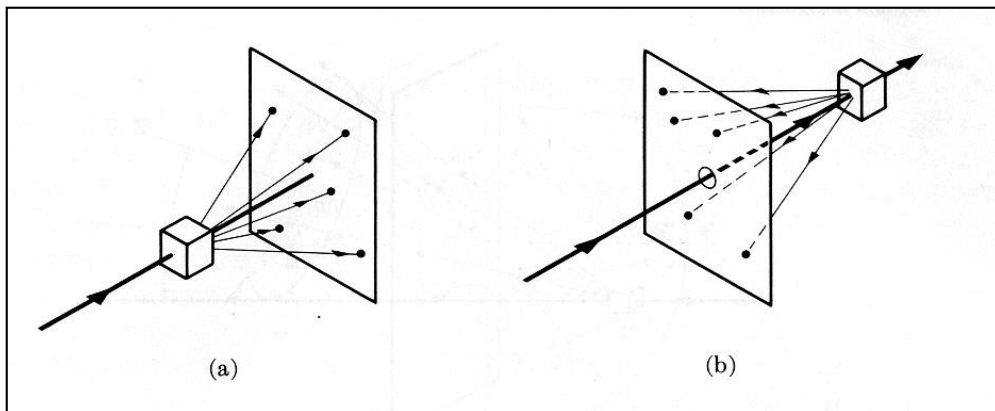
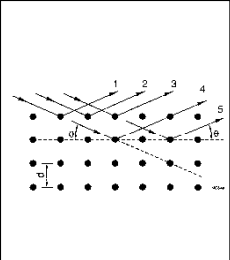
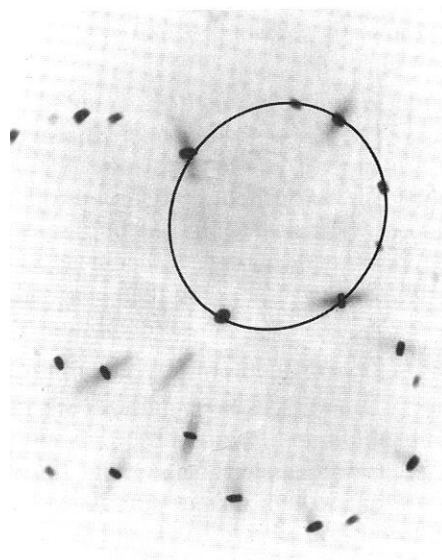
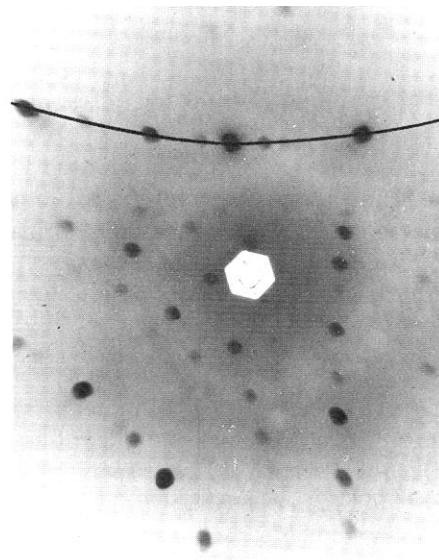


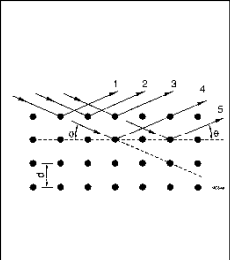
FIG. 3-8. Stereographic projection of transmission Laue method.



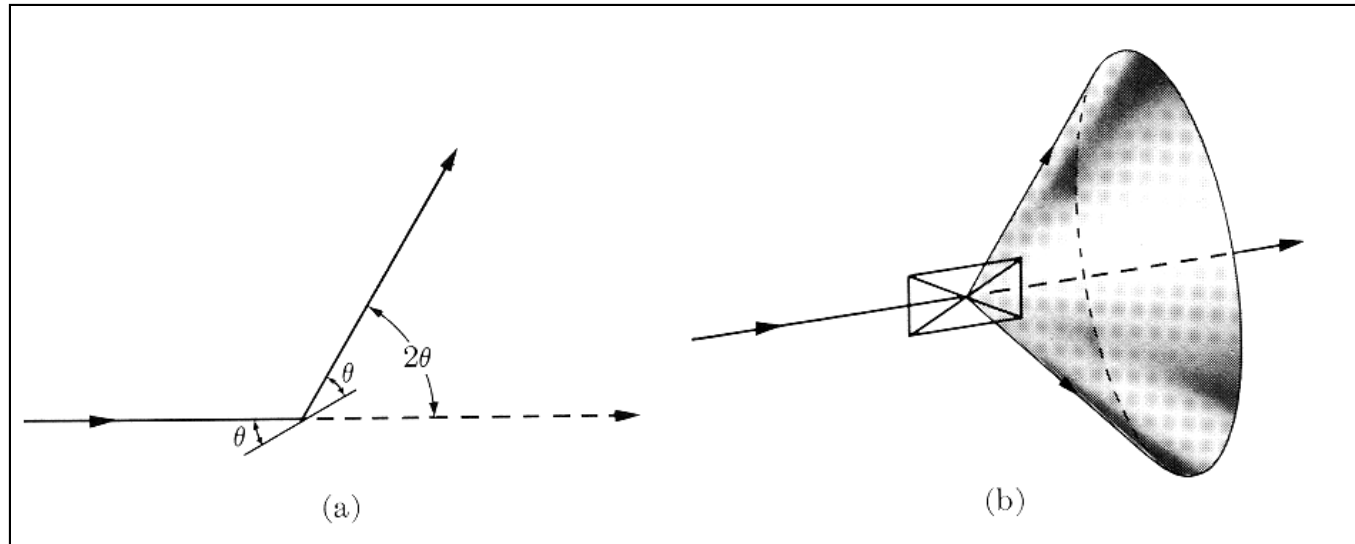
(a)



(b)



# CONES DE DIFRAÇÃO



# CONES DE DIFRAÇÃO

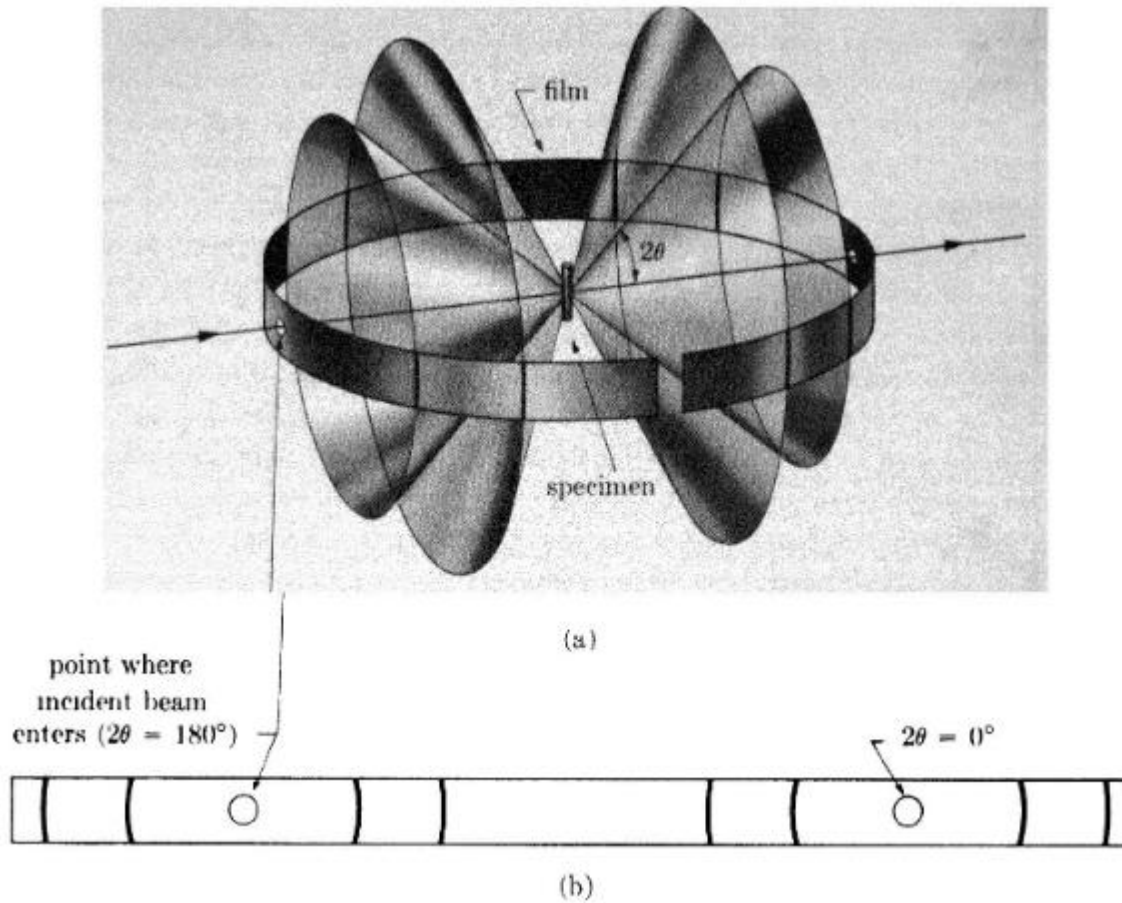
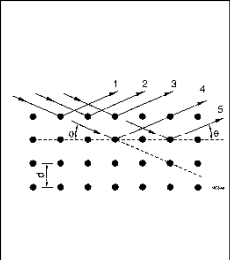


FIG. 3-12. Debye-Scherrer powder method: (a) relation of film to specimen and incident beam; (b) appearance of film when laid out flat.

# CONES DE DIFRAÇÃO

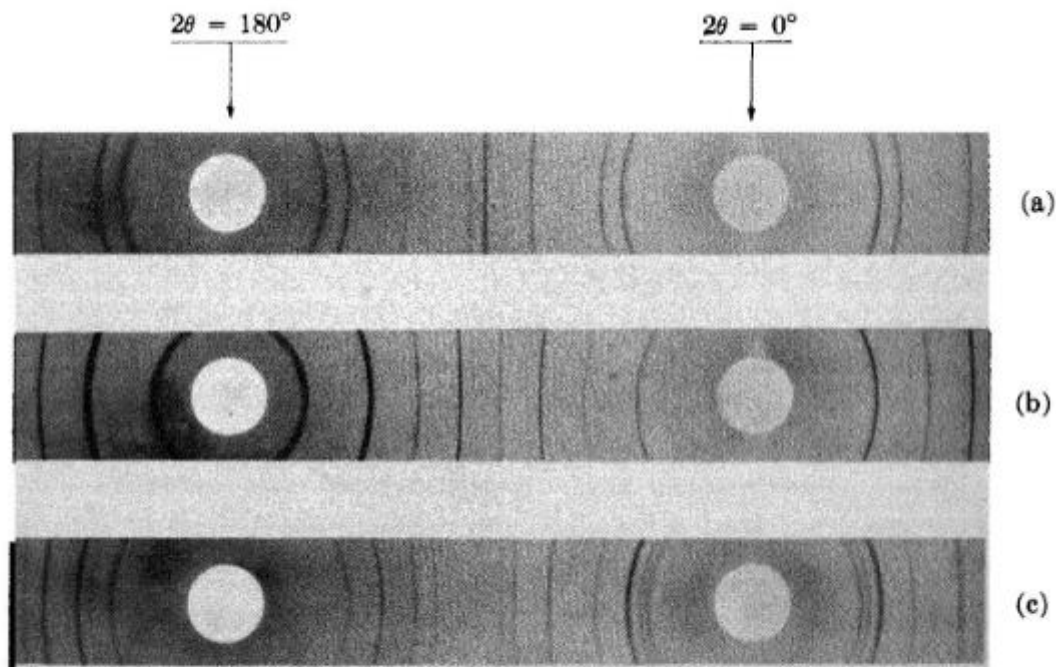
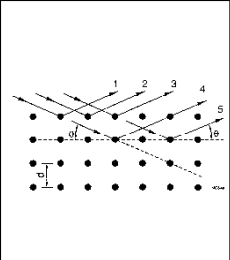
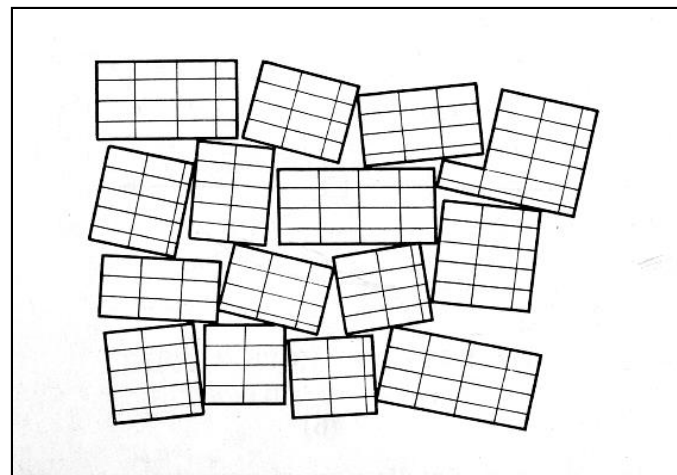
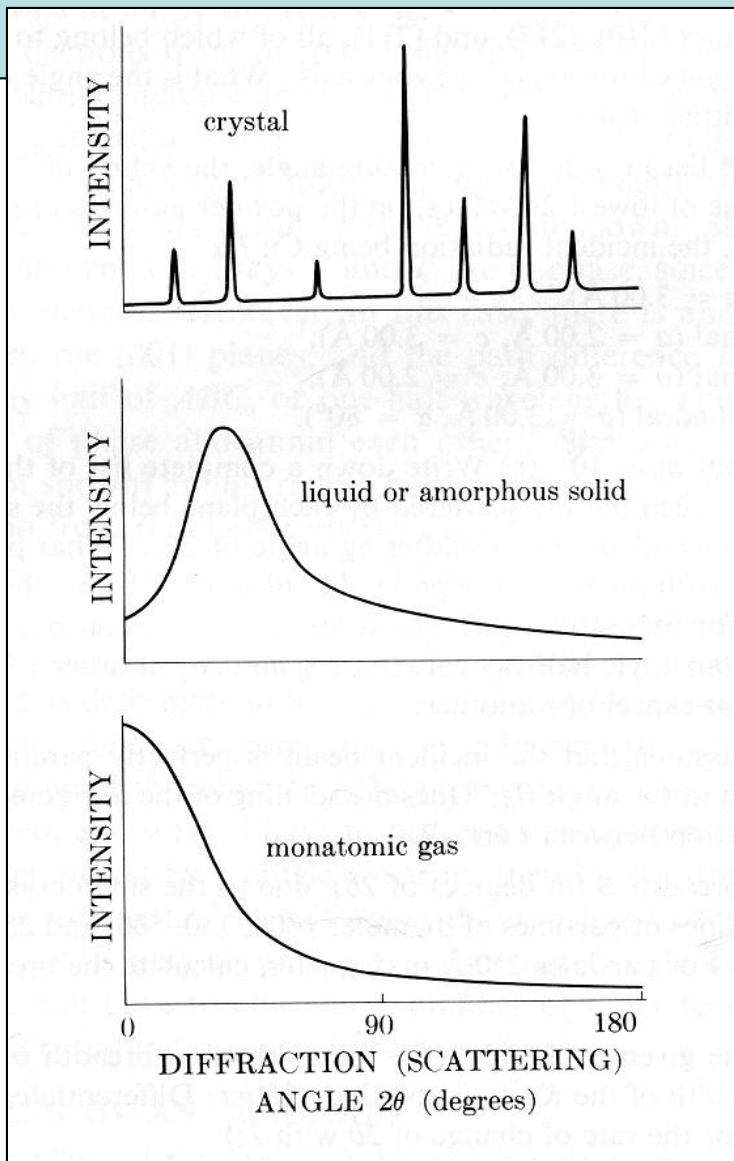
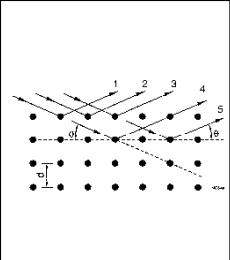
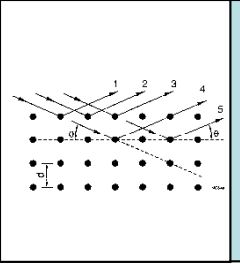


FIG. 3-13. Debye-Scherrer powder patterns of (a) copper (FCC), (b) tungsten (BCC), and (c) zinc (HCP). Filtered copper radiation, camera diameter = 5.73 cm.

# TIPOS DE MATERIAIS





### A3-1 PLANE SPACINGS

The value of  $d$ , the distance between adjacent planes in the set  $(hkl)$ , may be found from the following equations.

*Cubic:* 
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

*Tetragonal:* 
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

*Hexagonal:* 
$$\frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

*Rhombohedral:*

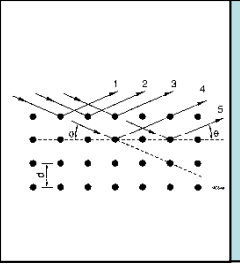
$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha)}$$

*Orthorhombic:* 
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

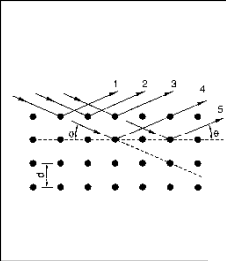
*Monoclinic:* 
$$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

# APPENDIX 10

## QUADRATIC FORMS OF MILLER INDICES



Cubic					Hexagonal	
$h^2 + k^2 + l^2$	$hkl$				$h^2 + hk + k^2$	$hk$
	Simple	Face-centered	Body-centered	Diamond		
1	100				1	10
2	110	. . .	110		2	
3	111	111	. . .	111	3	11
4	200	200	200		4	20
5	210				5	
6	211	. . .	211		6	
7					7	21
8	220	220	220	220	8	
9	300, 221				9	30
10	310	. . .	310		10	
11	311	311	. . .	311	11	
12	222	222	222		12	22
13	320				13	31
14	321	. . .	321		14	
15					15	
16	400	400	400	400	16	40
17	410, 322				17	
18	411, 330	. . .	411, 330		18	
19	331	331	. . .	331	19	32



## Difração

PICOS	$2*\theta$	$\theta$	$\Pi/180$	$\Pi * \theta$	$\sin \theta$	$(\sin^2 \theta)$	X1	X2	X3	X4
pico 1	44,5	22,25	0,0175	0,3883	0,3786	0,1434	1,0	2,0	3,0	4,0
pico 2	51,8	25,9	0,0175	0,4520	0,4368	0,1908	1,3	2,7	4,0	5,3
pico 3	76,4	38,2	0,0175	0,6667	0,6184	0,3824	2,7	5,3	8,0	10,7
pico 4	92,9	46,45	0,0175	0,8107	0,7248	0,5253	3,7	7,3	11,0	14,7
pico 5	98,4	49,2	0,0175	0,8587	0,7570	0,5730	4,0	8,0	12,0	16,0
pico 6	121,9	60,95	0,0175	1,0638	0,8742	0,7642	5,3	10,7	16,0	21,3

$$n\lambda = 2d \sin \theta$$

$$n=1 \quad \lambda^2 = 4d^2 \sin^2 \theta$$

$$\lambda^2 / (4 \sin^2 \theta) = d^2$$

$$n^2 \lambda^2 = 4d^2 \sin^2 \theta$$

$$n^2 \lambda^2 = 4a^2 / (h^2 + k^2 + l^2) \sin^2 \theta$$

$$\sin^2 \theta = (\lambda^2 / 4a^2) (h^2 + k^2 + l^2)$$

$$d^2 = a^2 / (h^2 + k^2 + l^2)$$

mas  $(h^2 + k^2 + l^2)$  é sempre inteiro

e  $\lambda^2 / 4a^2$  é constante para cada padrão

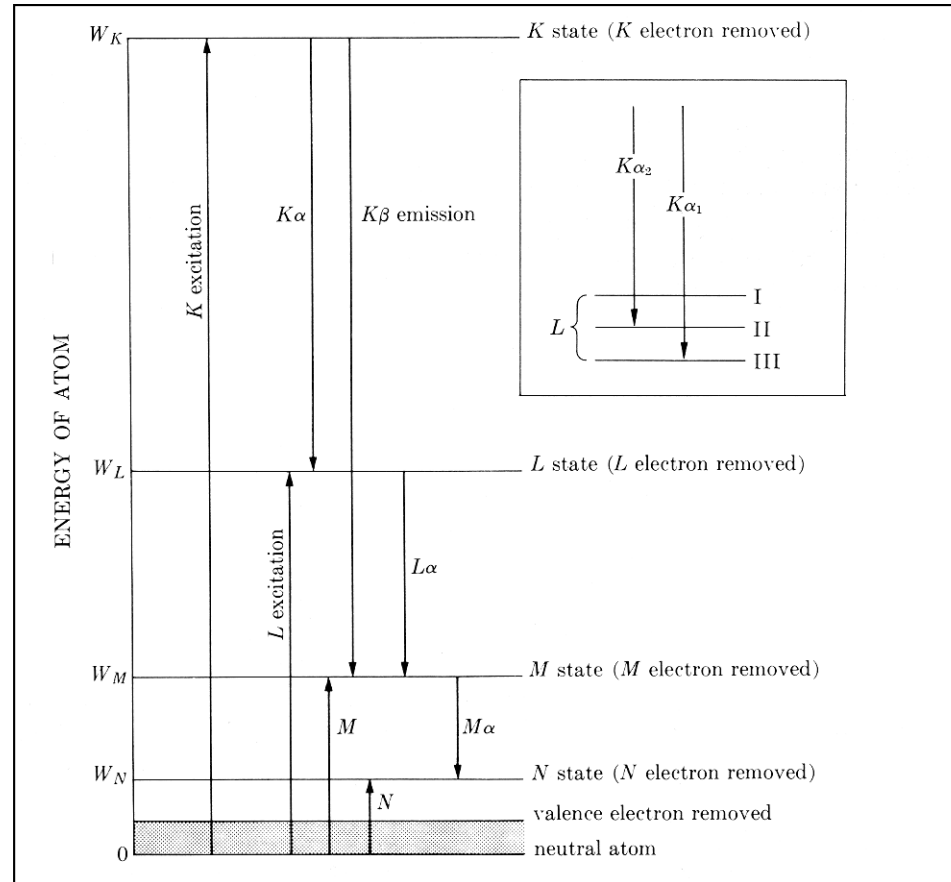
CS 1,2,3,4,5,6,8,9,10,11,12,13,14,16.....

CCC 2,4,6,8,10,12,14,16.....

CFC 3,4,8,11,12,16.....



# ESPECTROMETRIA DE RAIOS-X

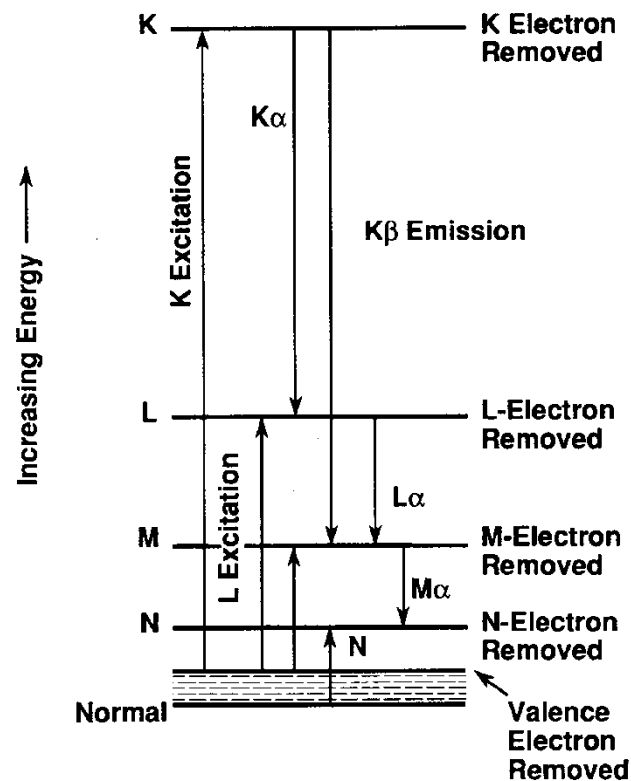
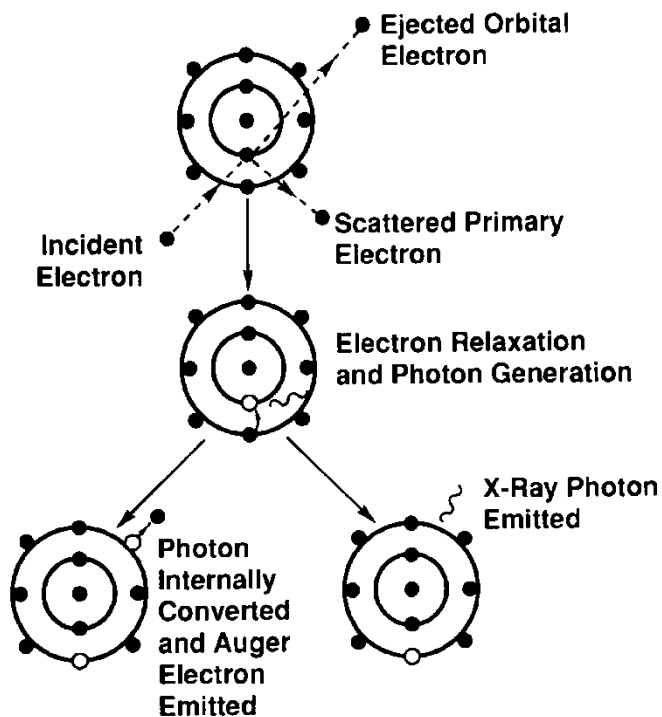


Bombardeamento de amostras com feixe de elétrons haverá emissão de raios-X característicos dos elementos constituintes da amostra

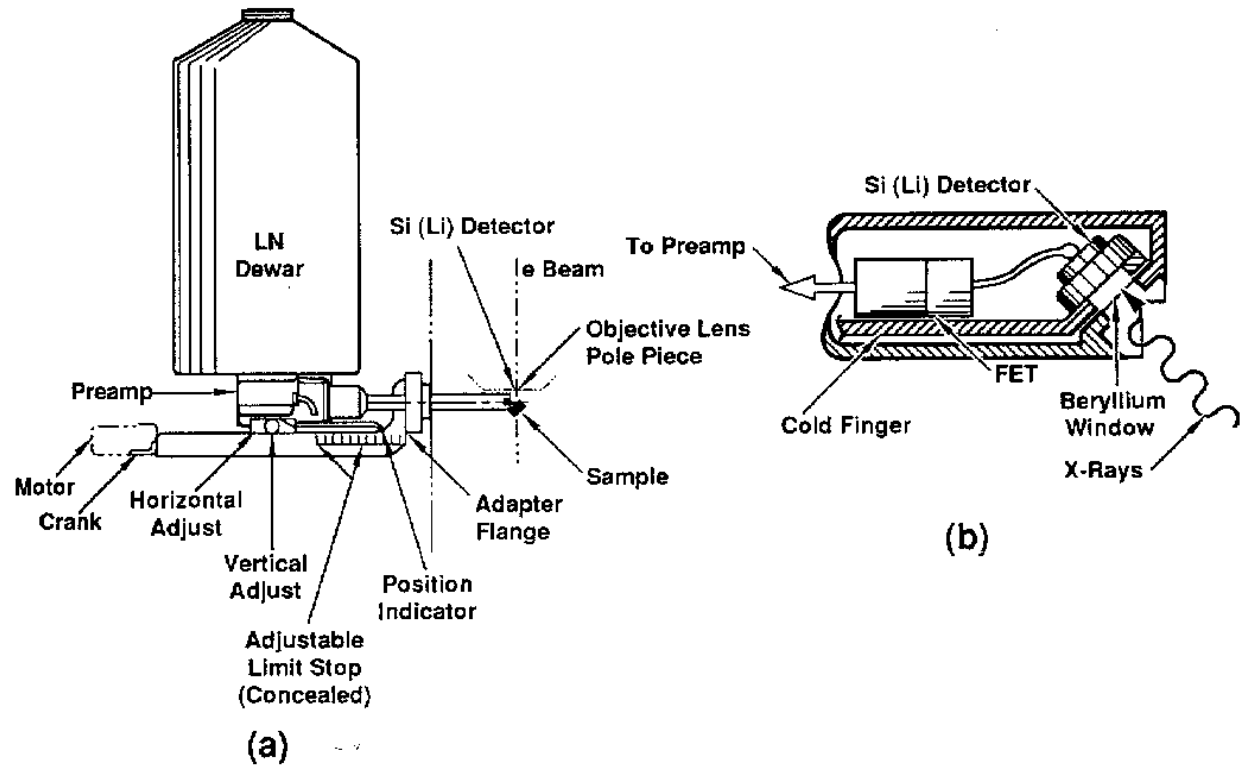
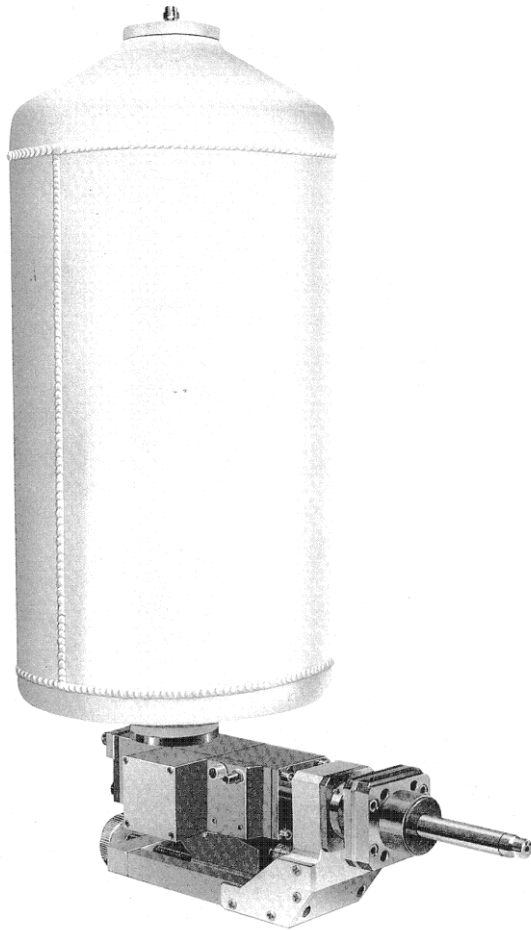
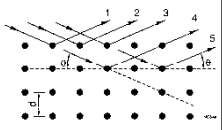


# ESPECTROMETRIA DE RAIOS-X

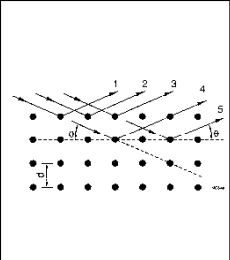
As emissões características de cada elemento têm uma energia associada. É possível identificar os elementos pela separação dos canais de energia.



# ESPECTROMETRIA EDS DE RAIOS-X

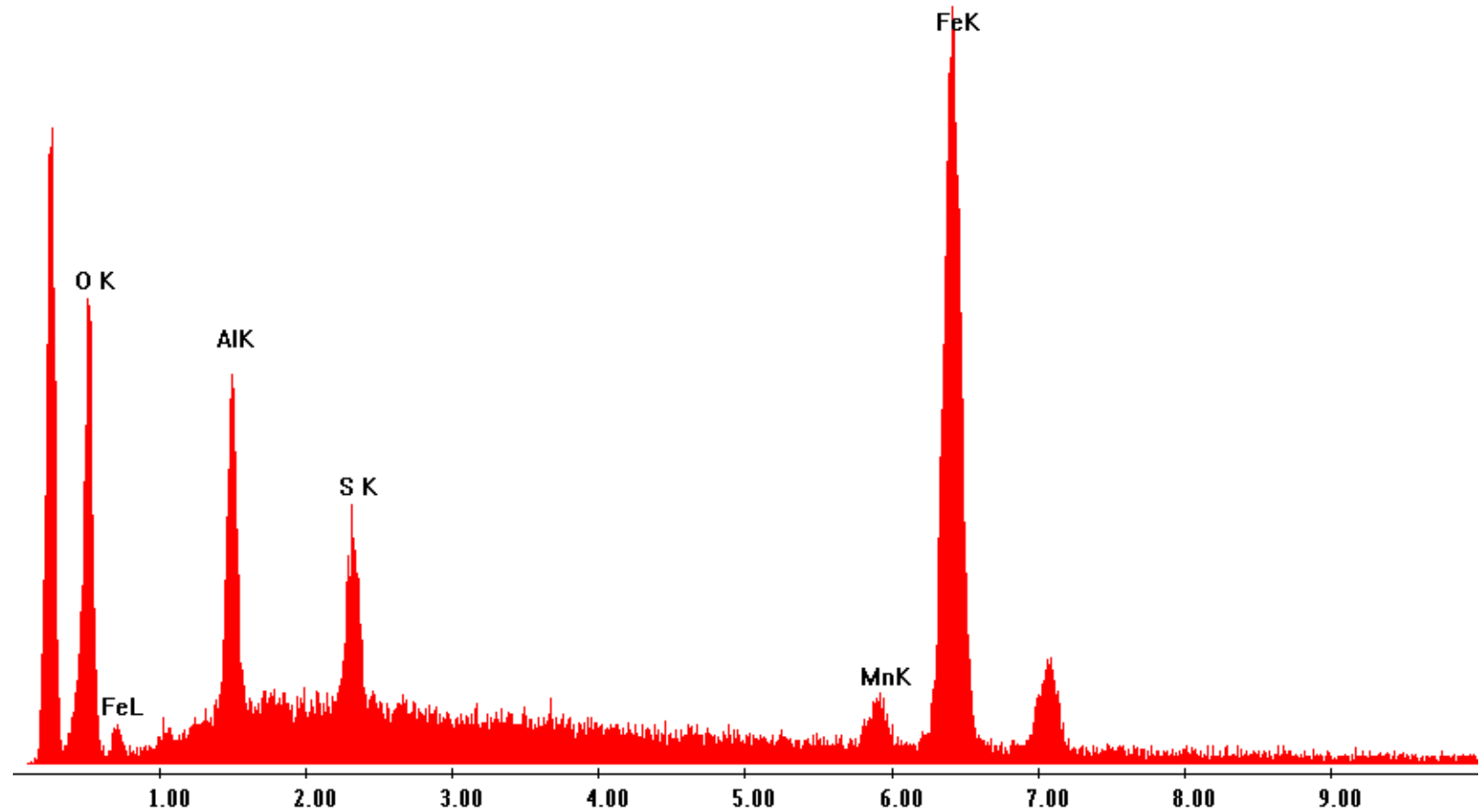


Dispersão de energia



# ESPECTROMETRIA EDS DE RAIOS-X

Label A: Inclusao proxima a trinca



# ESPECTROMETRIA WDS DE RAIOS-X

**Lei de Moseley:**

$$\lambda = B / (Z - C)^2, \text{ onde}$$

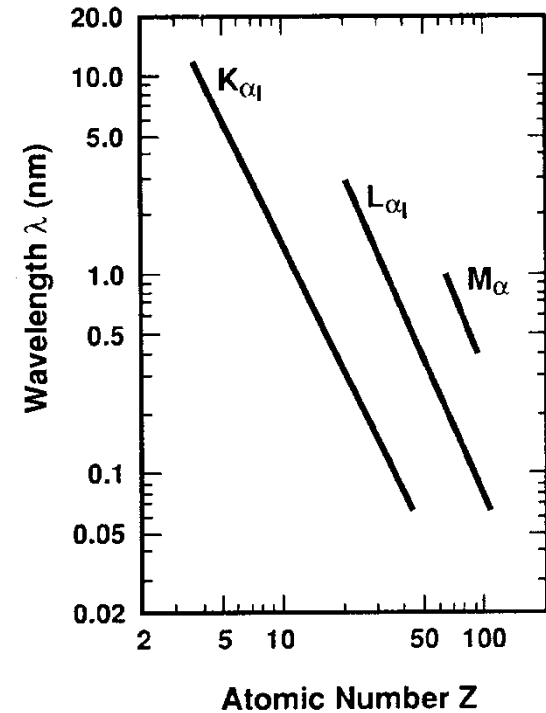
$\lambda$  - comprimento de onda

**B, C** - constantes diferentes para K,  
L, M

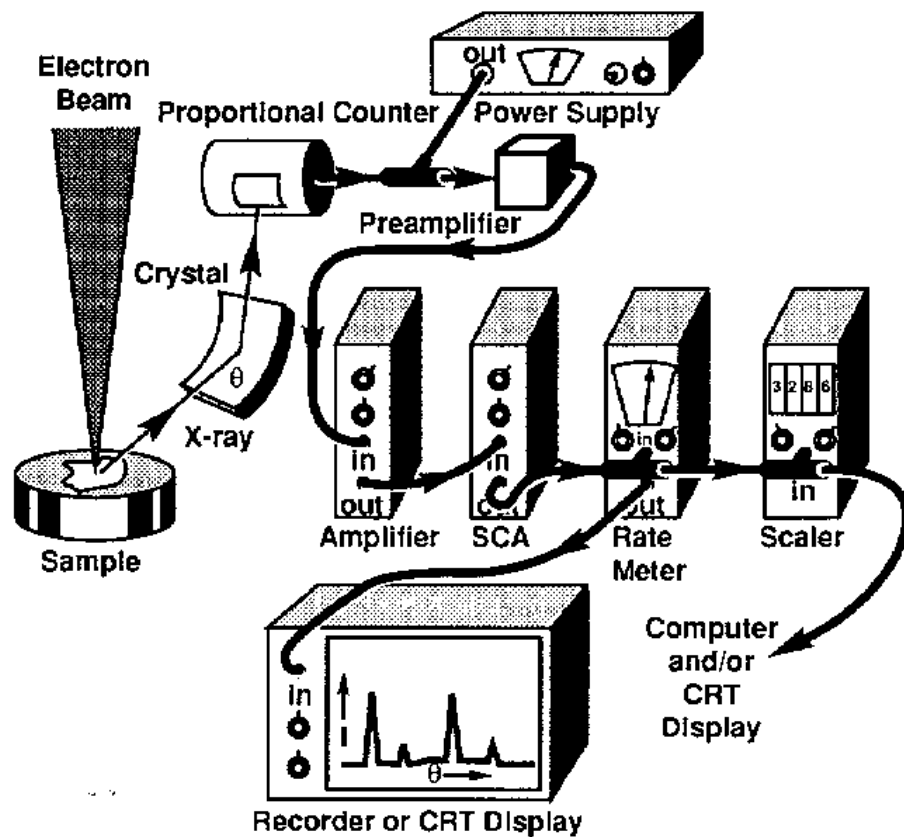
**Z** - número atômico

$$\lambda = 1,2396 / E$$

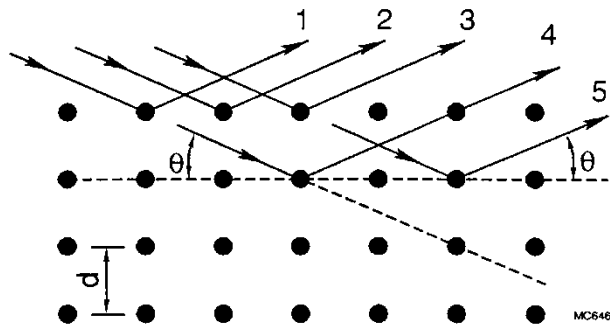
Dispersão de comprimento de onda



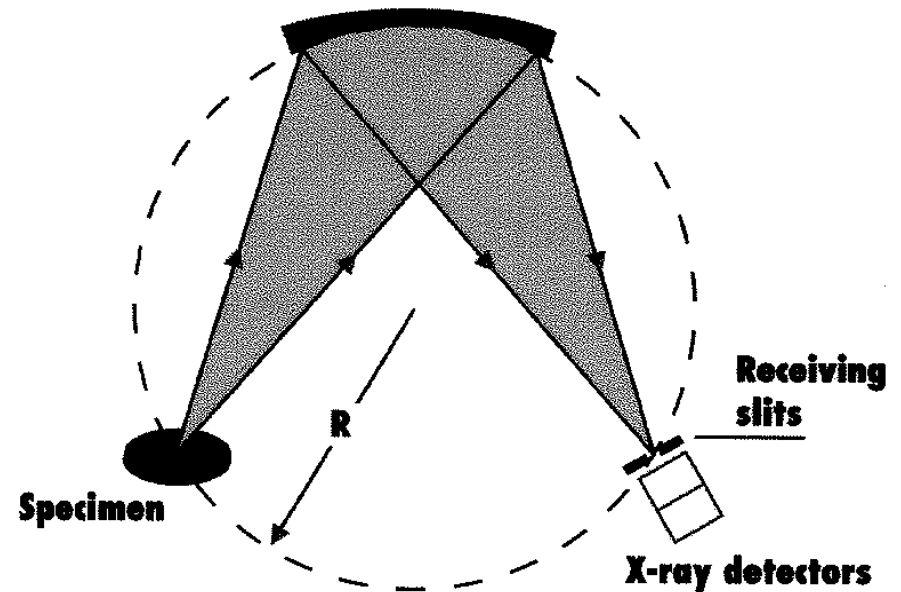
# Espectrômetro por dispersão de comprimento de onda - WDS



# DISPERSÃO DE COMPRIMENTO DE ONDA - DIFRAÇÃO



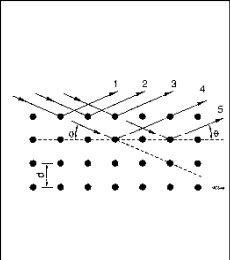
Lei de Bragg  $n\lambda = 2d\text{sen}\theta$



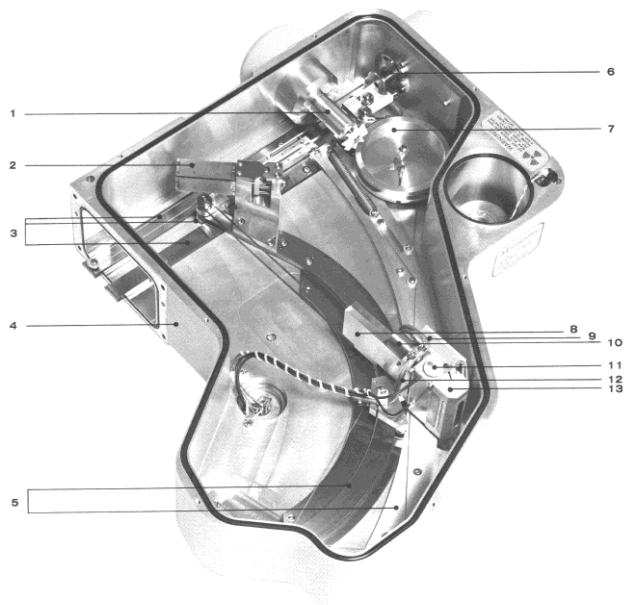
Fully focusing crystal

Geometria do WDS





# ESPECTRÔMETRO WDS



- 1 CRYSTAL CHANGE MECHANISM
- 2 CRYSTAL TURRET
- 3 LINEAR GUIDANCE SYSTEM
- 4 VACUUM HOUSING
- 5 CURVED SEGMENTS
- 6 SLIT POSITIONING MECHANISM

- 7 TAPE DRUM
- 8 DETECTOR COLLIMATOR
- 9 X-RAY PREAMPLIFIER
- 10 SLIT SIZE MECHANISM
- 11 FPC DETECTOR
- 12 RECEIVING SLITS
- 13 SPC DETECTOR

