

Estrutura dos sólidos cristalinos:

- **Raio atômico**
- **Modelo de empacotamento compacto em sólidos metálicos**
- **Sítios cristalinos octaédricos e tetraédricos**

Ciência dos Materiais

2. Estrutura dos sólidos cristalinos

ligações químicas

rede cristalina

célula unitária

raio atômico

modelo de empacotamento compacto em sólidos metálicos

sítios cristalinos octaédricos e tetraédricos

superfícies de baixo índice de Miller

estruturas polifásicas e polimorfismo em metais

Ciência dos Materiais

2. Estrutura dos sólidos cristalinos

raio atômico

modelo de empacotamento compacto em sólidos metálicos

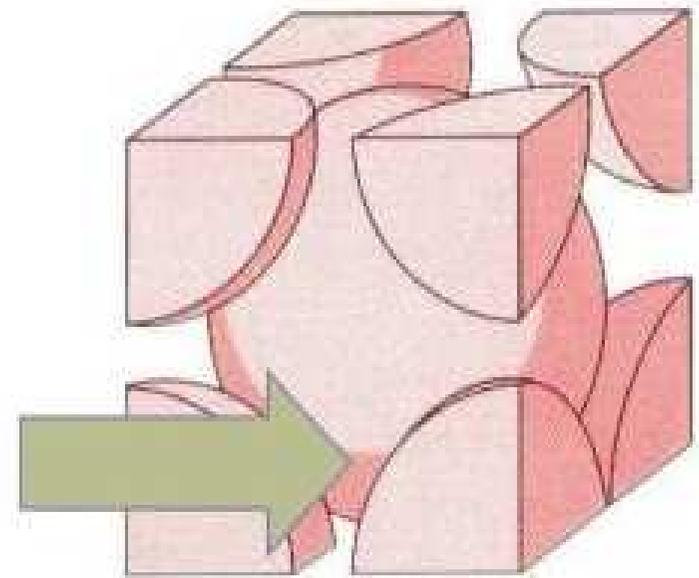
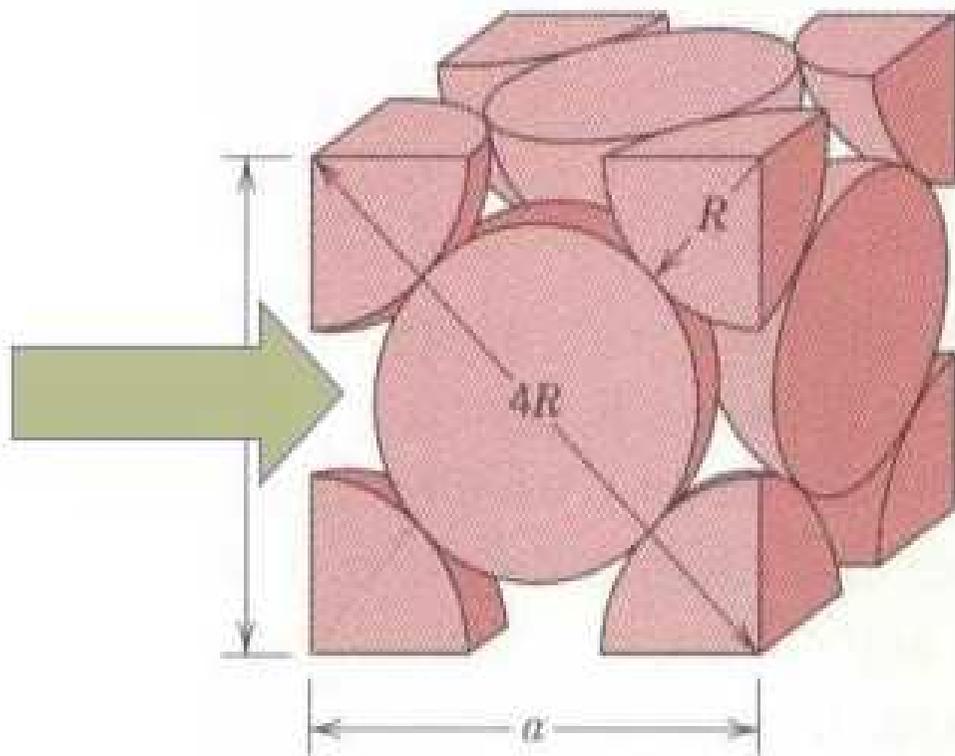
sítios cristalinos octaédricos e tetraédricos

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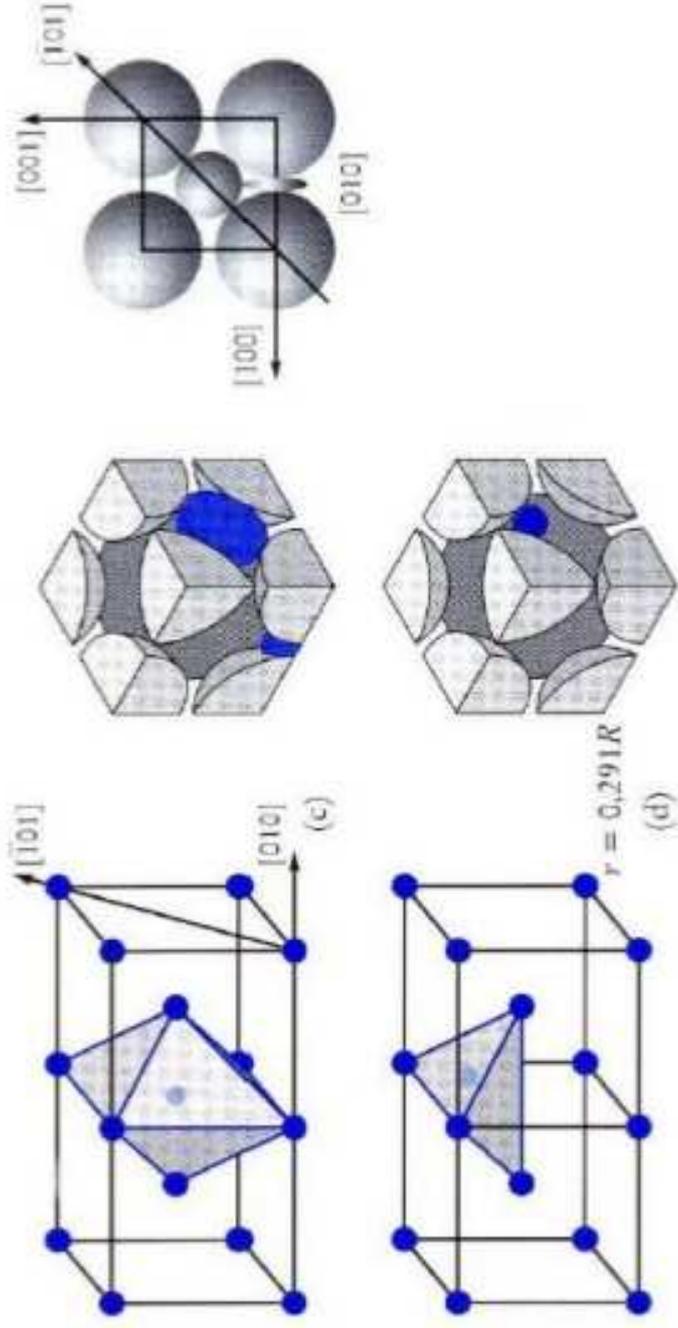
Estrutura dos sólidos cristalinos:

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- **Sítios cristalinos octaédricos e tetraédricos**

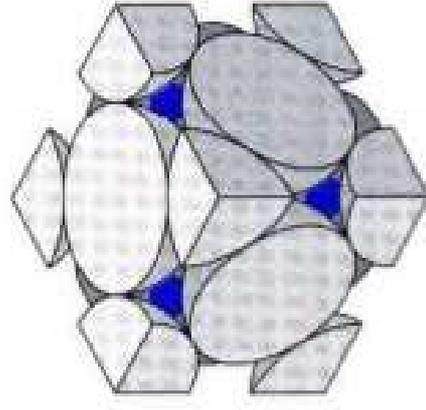
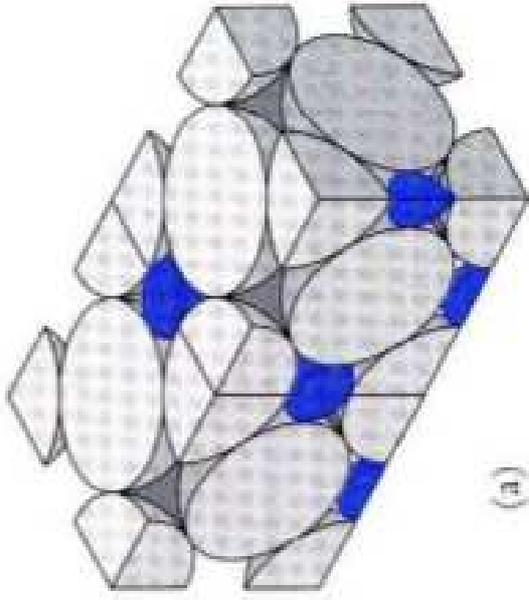
Raio Atômico



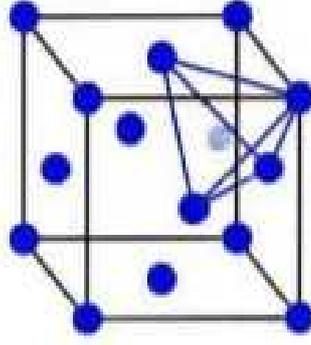
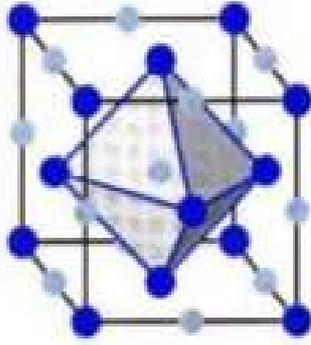
Sítios intersticiais



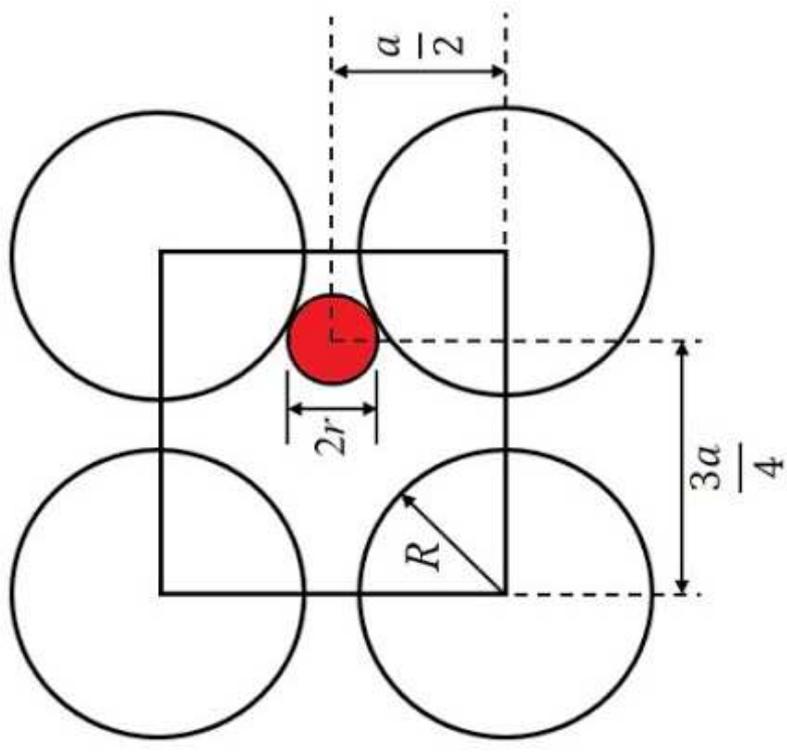
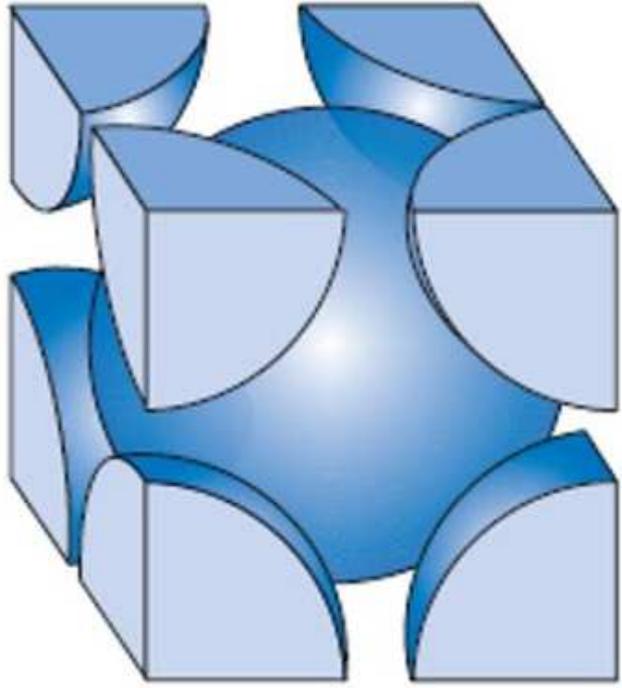
Sítios intersticiais da estrutura CCC: (a) octaédricos; (b) tetraédricos.



$$r_s = 0,225R_A$$

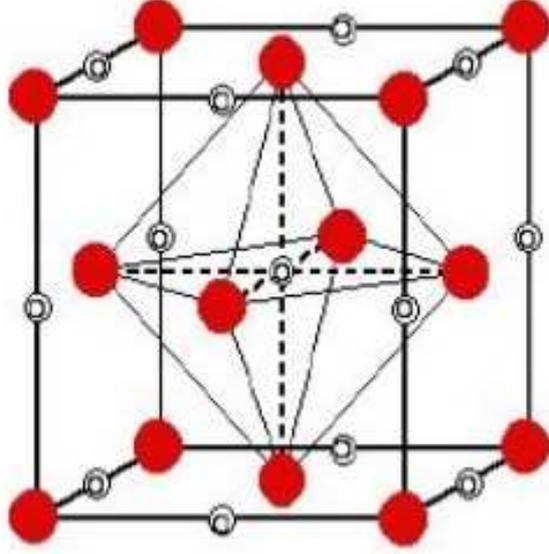


Sítios intersticiais da estrutura CFC:
 (a) octaédricos; (b) tetraédricos

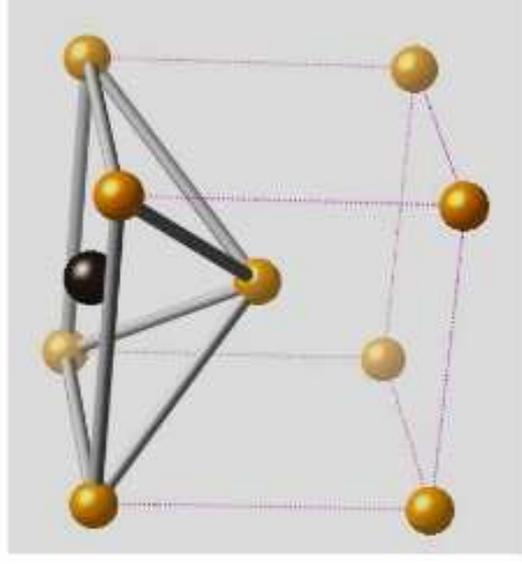


Sítio Intersticial Tetraédrico para Célula CCC

Dimensões dos interstícios



4 interstícios octaédricos
 $r_i = 0,414R$
8 interstícios tetraédricos
 $r_i = 0,225R$

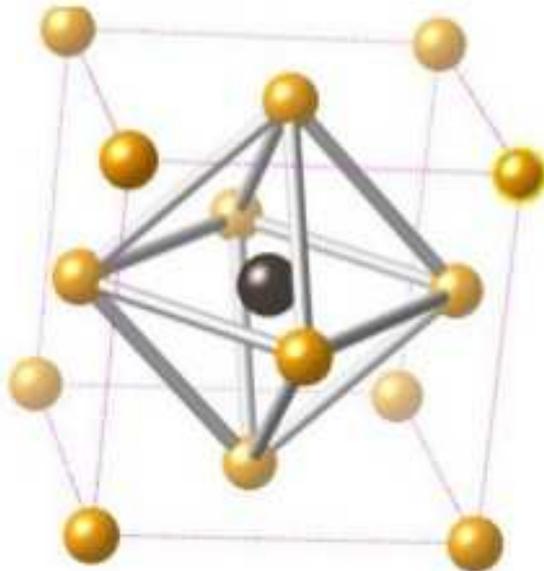


6 interstícios octaédricos
 $r_i = 0,155R$
12 interstícios tetraédricos
 $r_i = 0,291R$

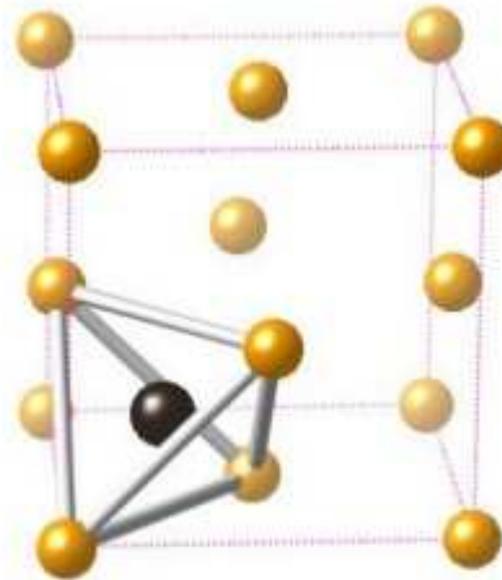
Dimensões dos interstícios *CFC*

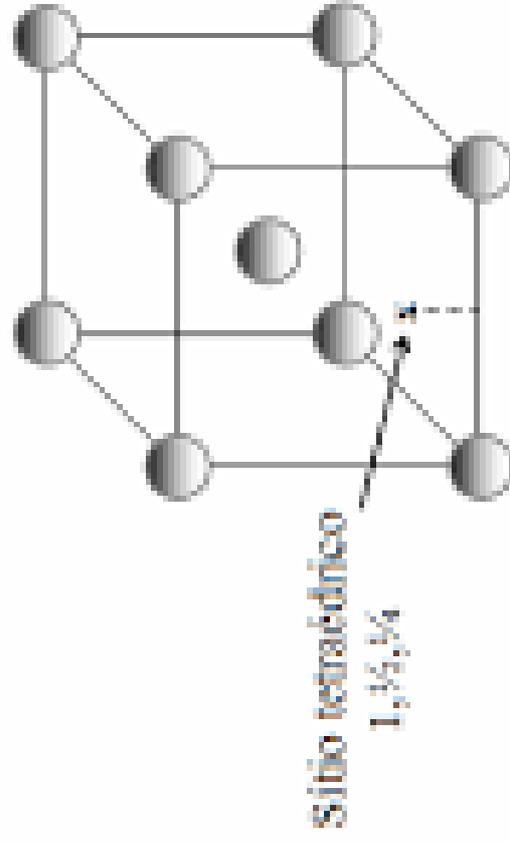
► Tipos

Octaédricos

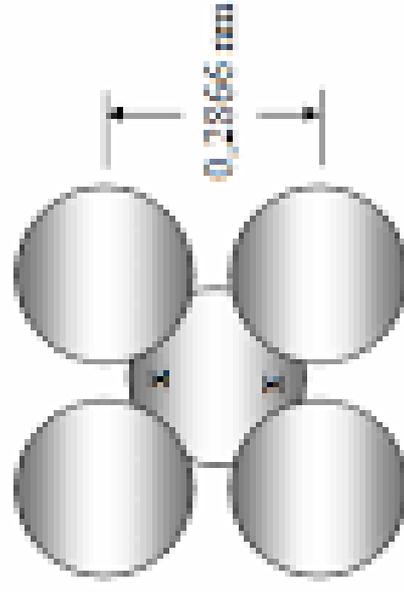


Tetraédricos

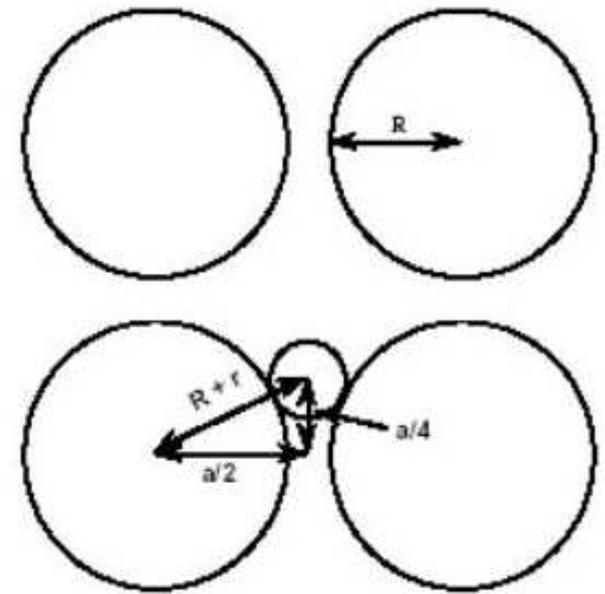
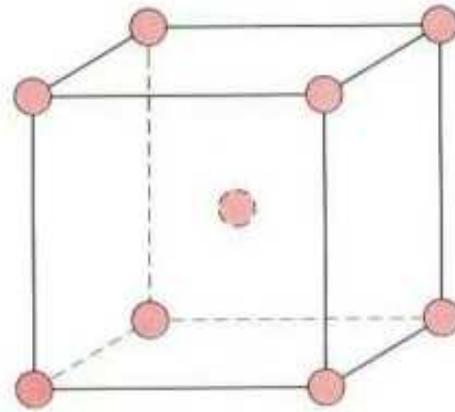
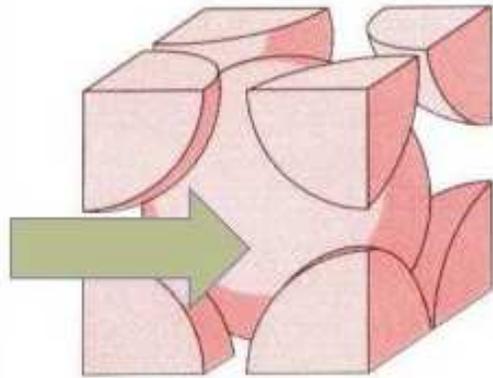




CCC



- Átomo de carbono – Raio = 0,0710 nm
- x Sítios tetraédricos – espaço = 0,0361 nm

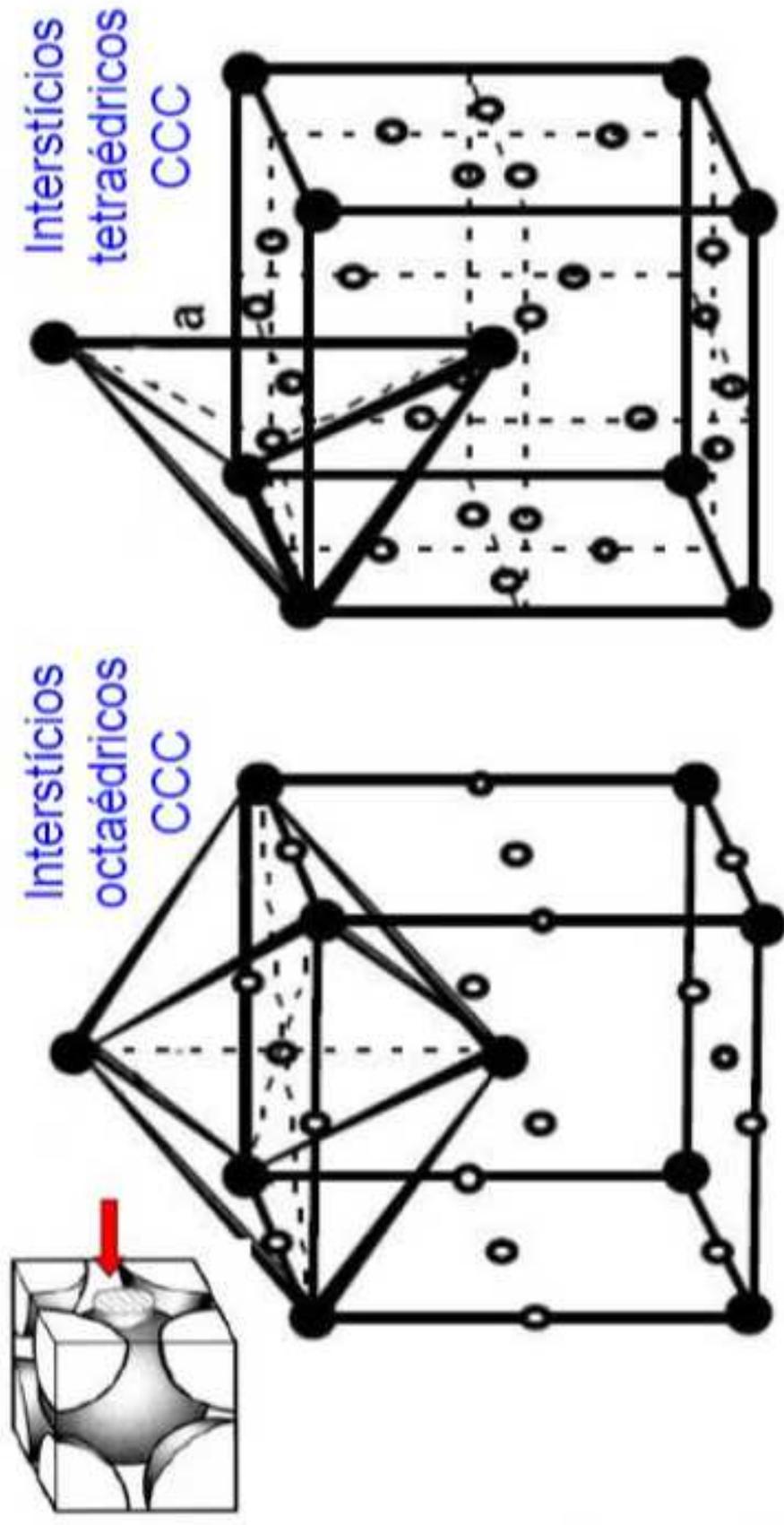


$$a = \frac{4R}{\sqrt{3}}$$

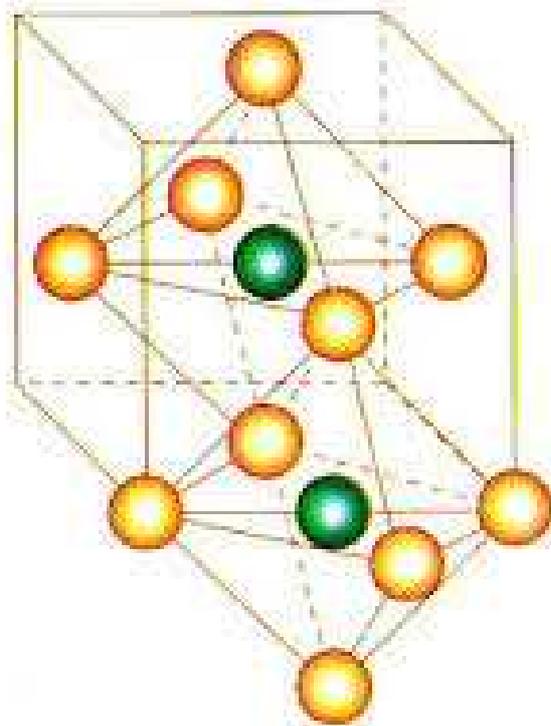
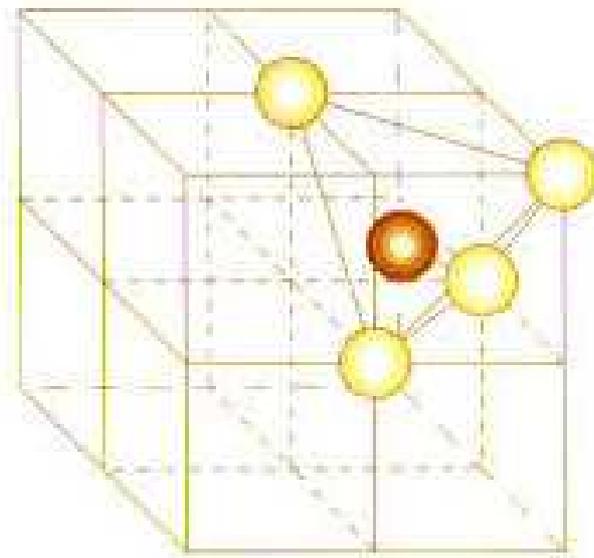
$$\left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2 = (R+r)^2$$

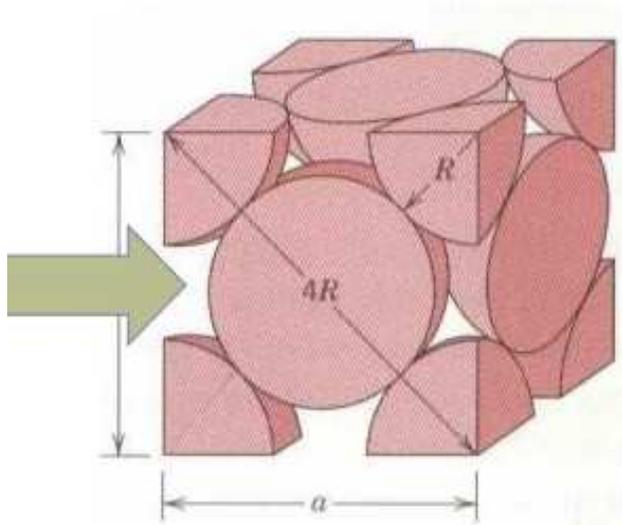
$$r = 0,29R$$

Exemplo: átomos de carbono em ferro

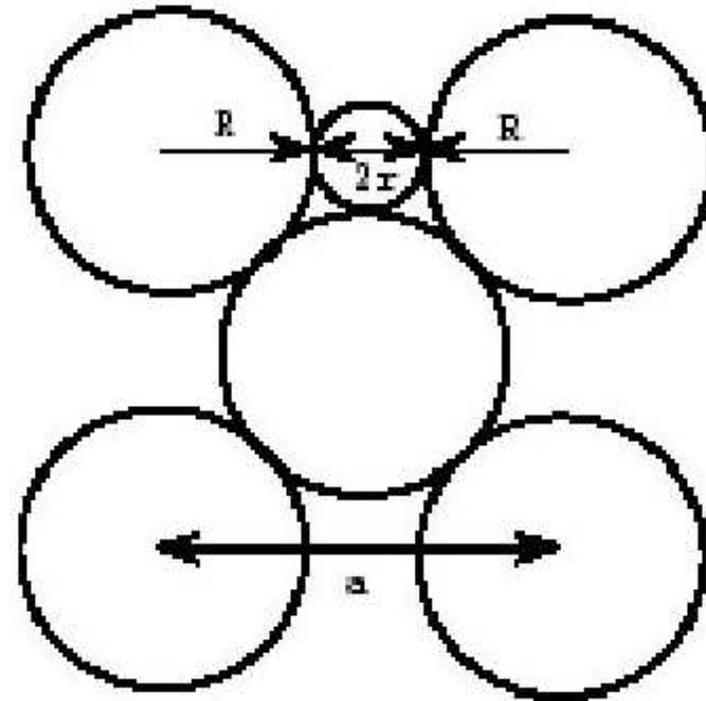


➤ Solubilidade máxima C na ferrita a 723°C: **0,02%p**



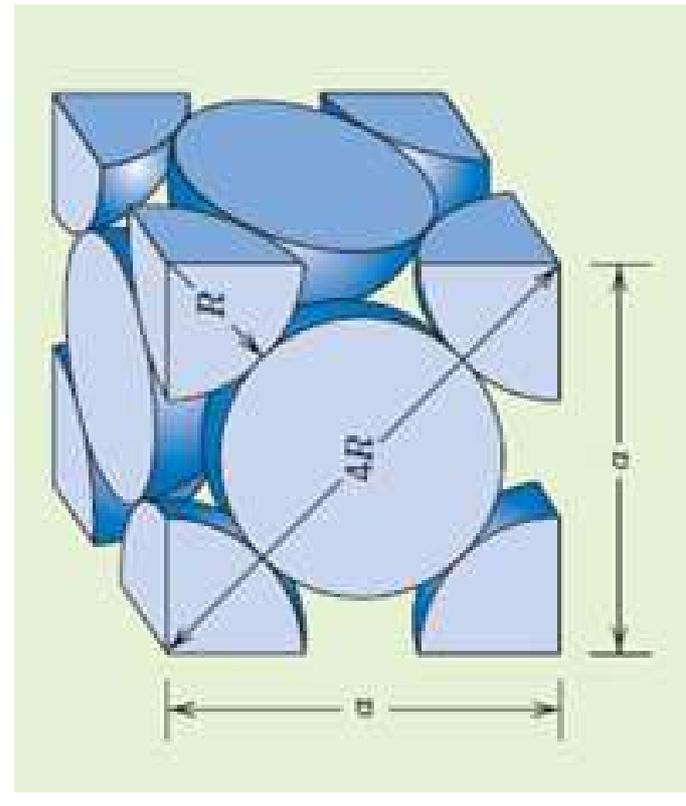
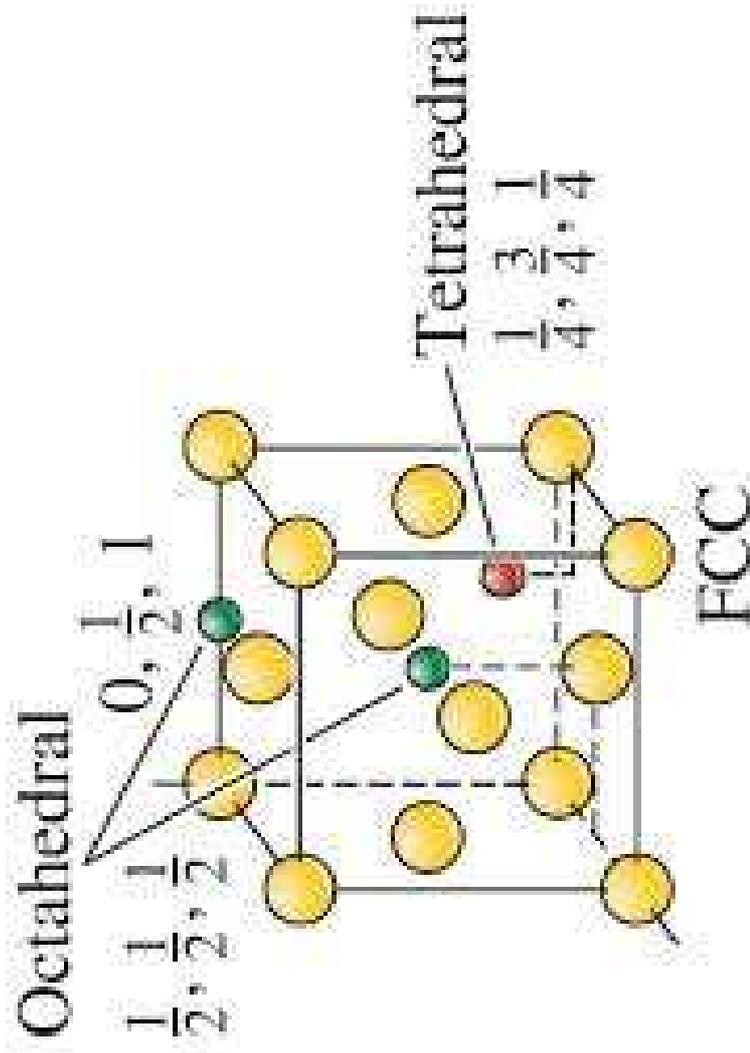


$$a = 2\sqrt{2}R = 2R + 2r$$



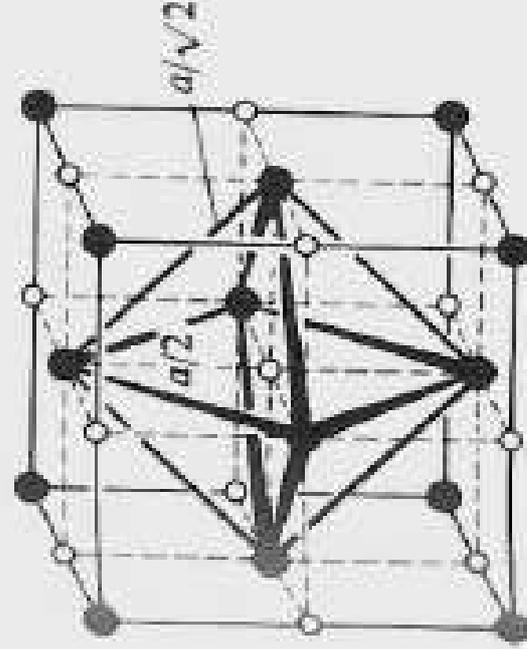
$$2r = a - 2R$$

$$r = 0,41R$$

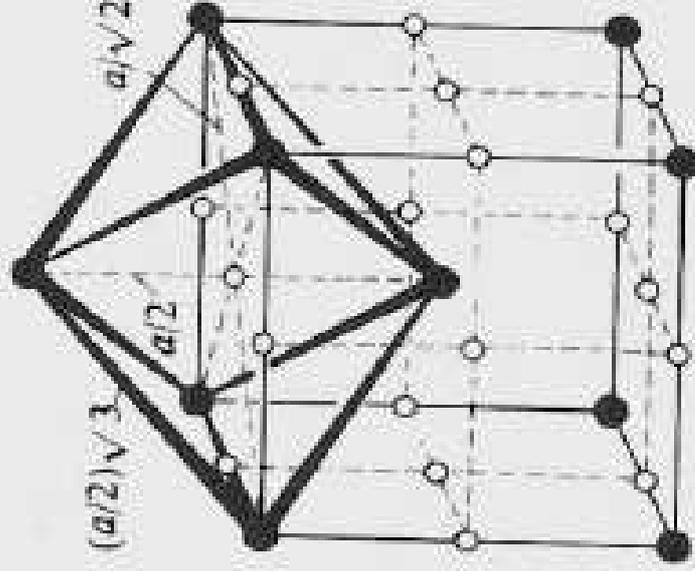


Intersticios de C na rede de Fe

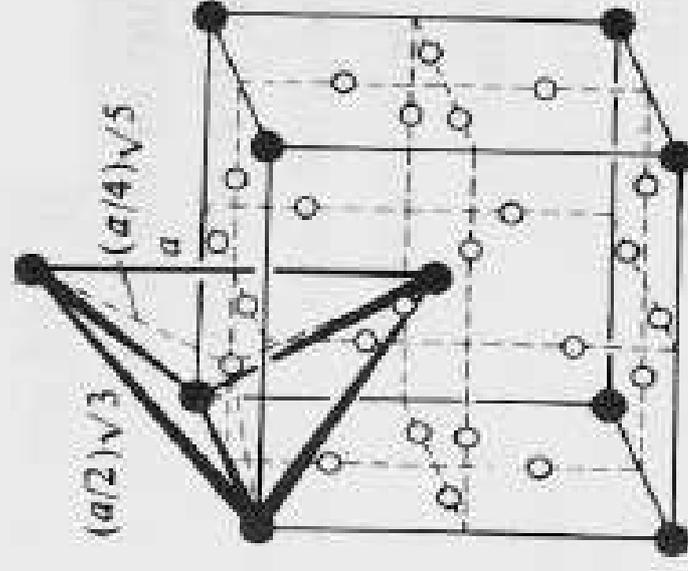
● Fe ○ C



interstício octaédrico
Fe FCC

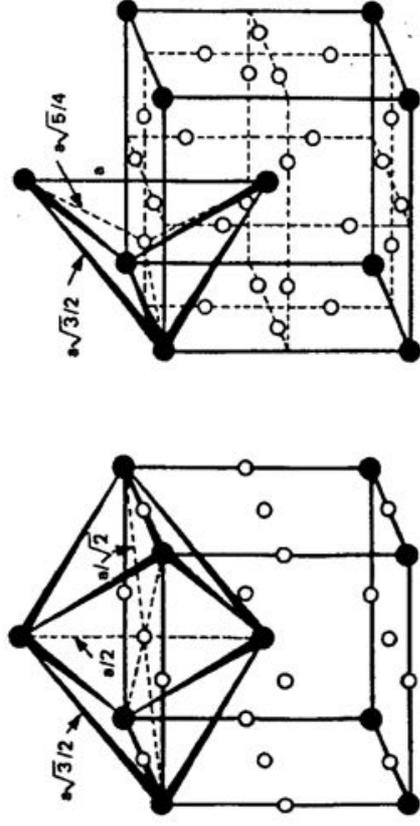


interstício octaédrico
Fe CCC

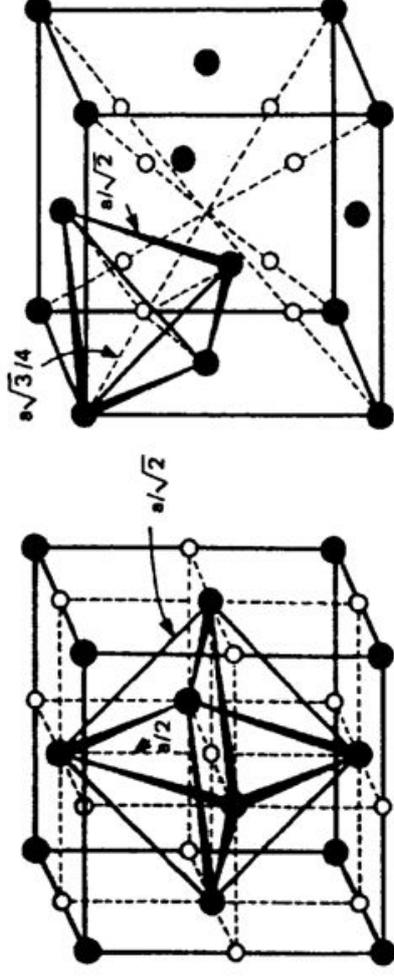


interstício tetraédrico
Fe CCC

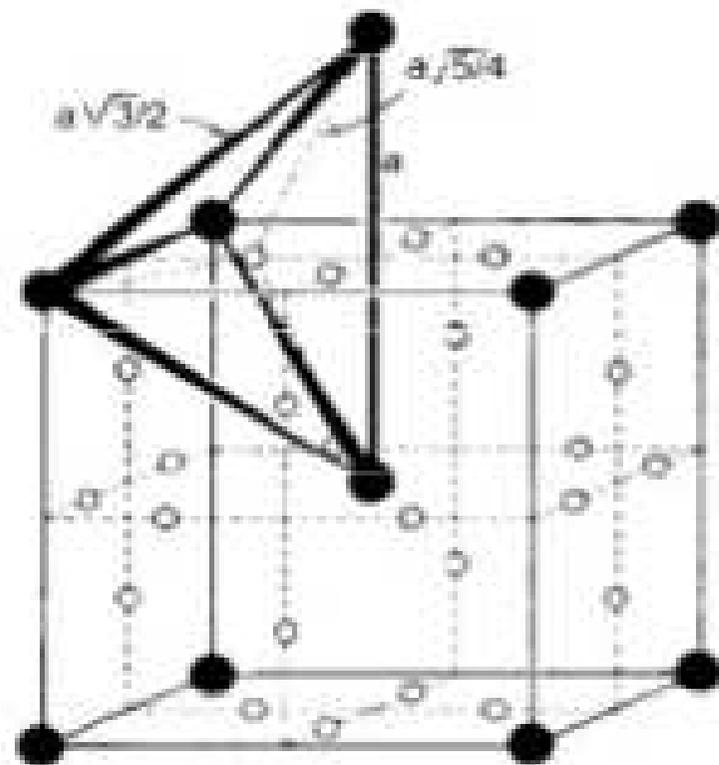
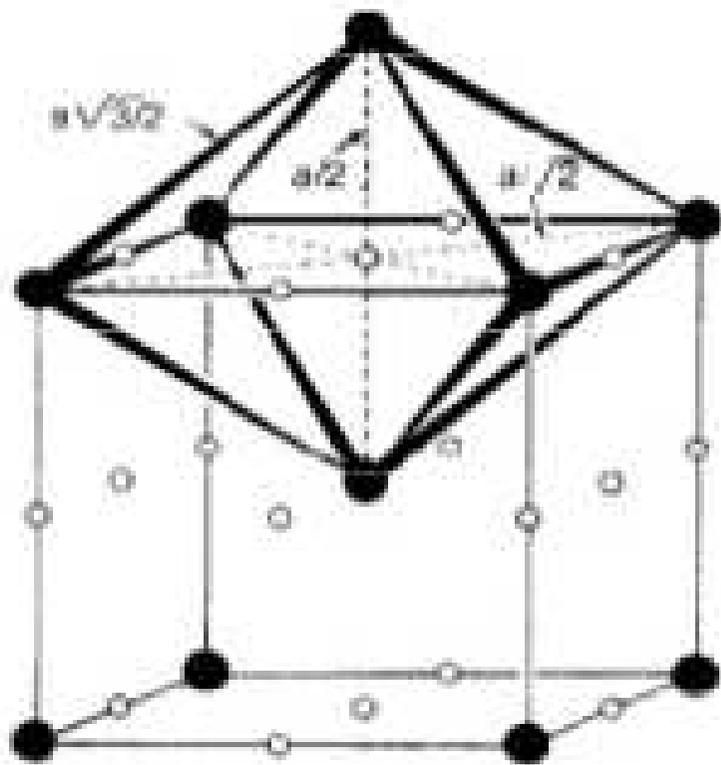
INTERSTÍCIOS EM CÉLULAS CÚBICAS



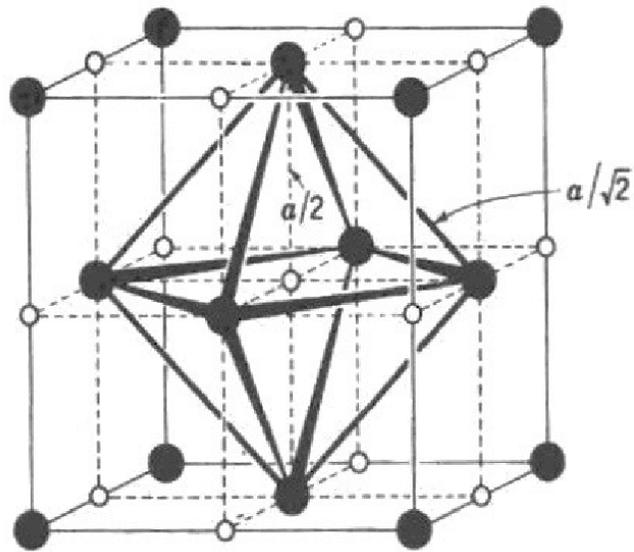
Interstícios octaédricos (a) e interstícios tetraédricos (b) em uma estrutura cúbica de corpo centrado.



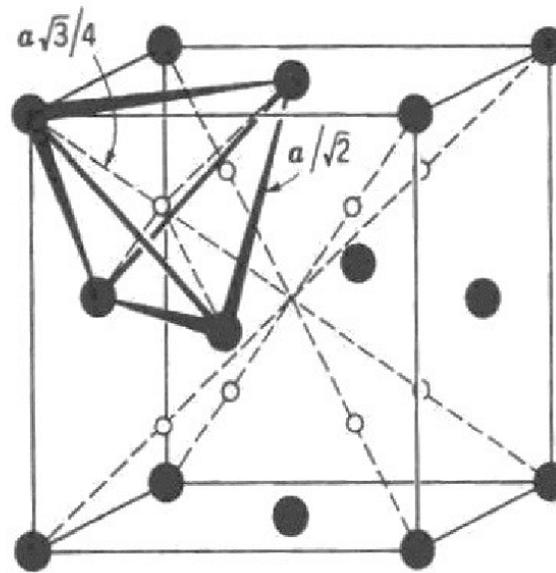
Interstícios octaédricos (a) e interstícios tetraédricos (b) em uma estrutura de faces centradas.



CCC

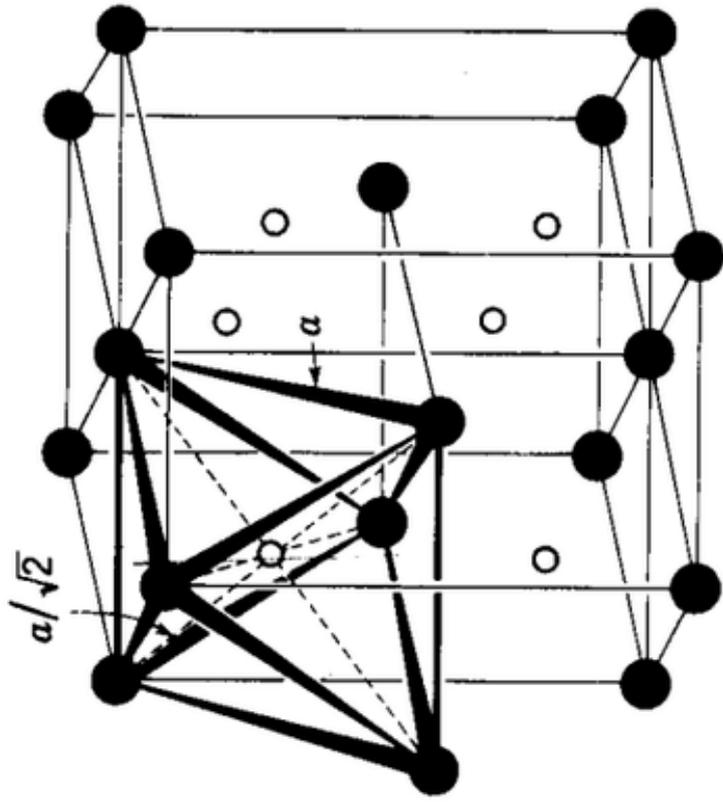


- Metal atoms
- Octahedral interstices



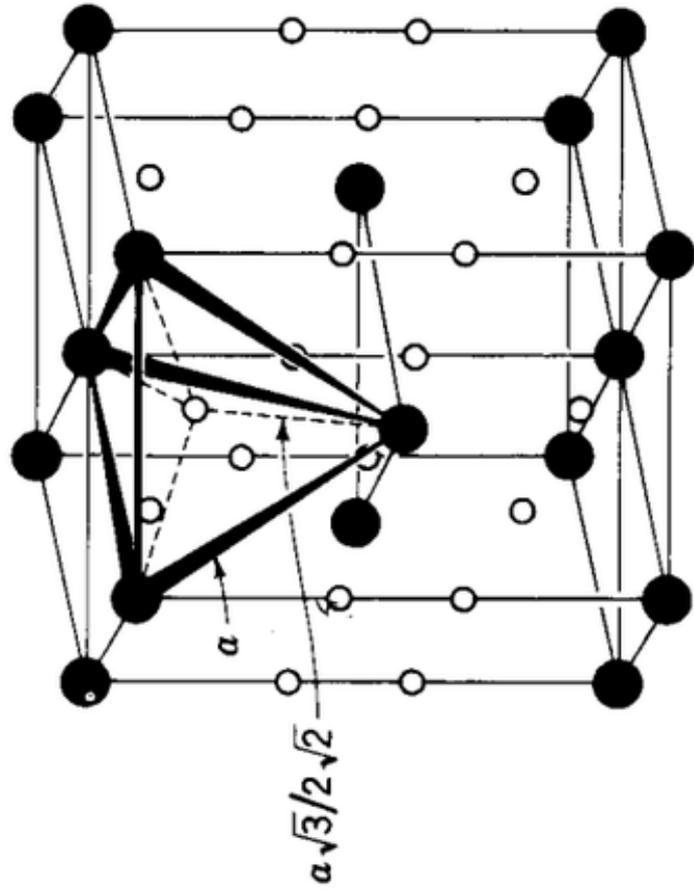
- Metal atoms
- Tetrahedral interstices

CFC



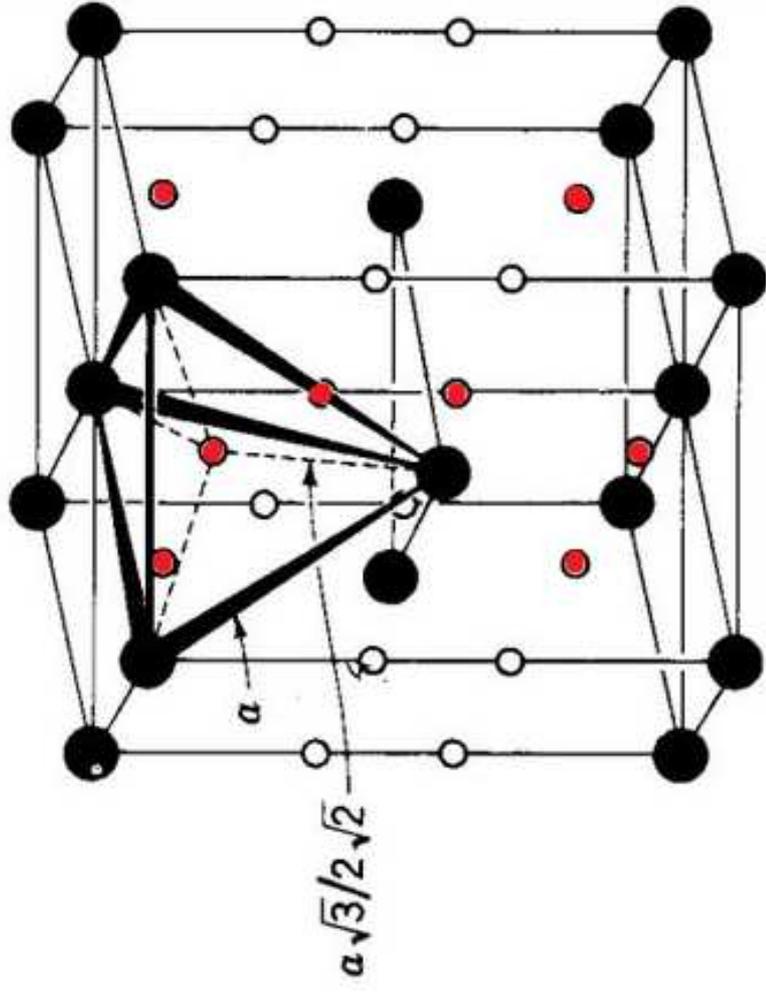
- Metal atoms
- Octahedral interstices

(a)



- Metal atoms
- Tetrahedral interstices

(b)



● Metal atoms

○ Tetrahedral interstices

(b)

Estrutura dos sólidos cristalinos:

- **Modelo de empacotamento compacto em sólidos metálicos**

- Maioria dos elementos metálicos (90%) cristaliza-se com estruturas altamente densas:

- Cúbica de Corpo Centrado (CCC),
- Cúbica de Face Centrada (CFC)
- Hexagonal Compacta (HC)

- Dimensões das células cristalinas metálicas são pequenas:

- Aresta de uma célula unitária de Fe (CCC) à temperatura ambiente é igual a 0,287 nm

- Sólidos Cristalinos constituídos de 1 único elemento:

- 52 % - estrutura cúbica
- 28 % - estrutura hexagonal
- 20 % - outros 5 tipos estruturais ()

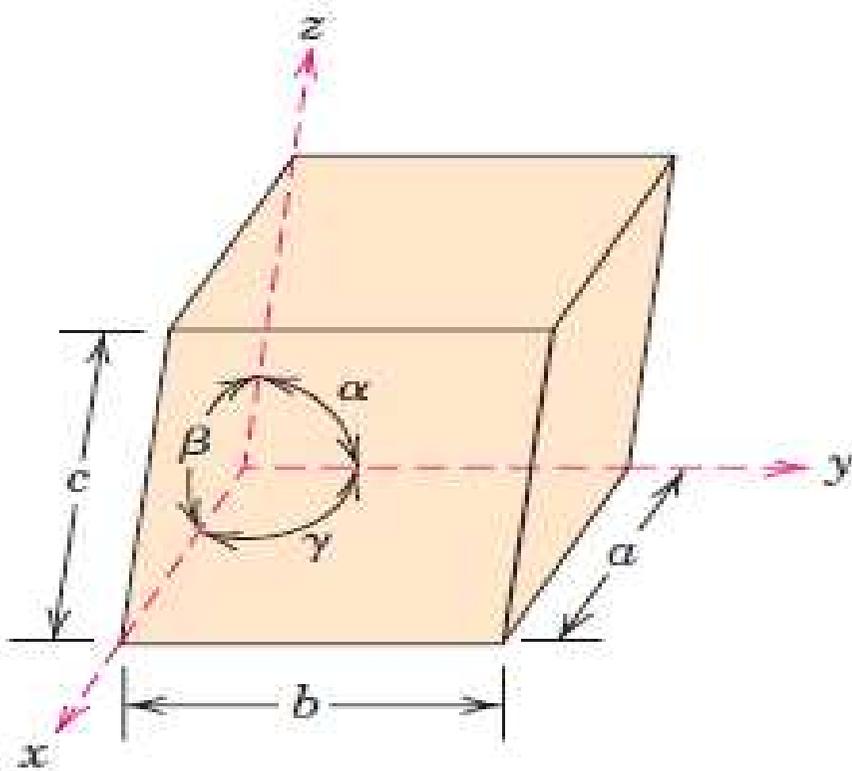
Existem 7 sistemas cristalinos básicos que englobam todas as substâncias cristalinas conhecidas

SISTEMAS	EIXOS	ÂNGULOS ENTRE OS EIXOS
CÚBICO	$a = b = c$	Todos os ângulos = 90°
TETRAGONAL	$a = b \neq c$	Todos os ângulos = 90°
ORTORRÔMBICO	$a \neq b \neq c$	Todos os ângulos = 90°
MONOCLÍNICO	$a \neq b \neq c$	2 ângulos = 90° e 1 ângulo $\neq 90^\circ$
TRICLÍNICO	$a \neq b \neq c$	Todos ângulos diferentes e nenhum igual a 90°
HEXAGONAL	$a_1 = a_2 = a_3 \neq c$	2 ângulos = 90° e 1 ângulo = 120°
ROMBOÉDRICO	$a = b = c$	Todos os ângulos iguais, mas diferentes de 90°

Estrutura dos sólidos cristalinos:

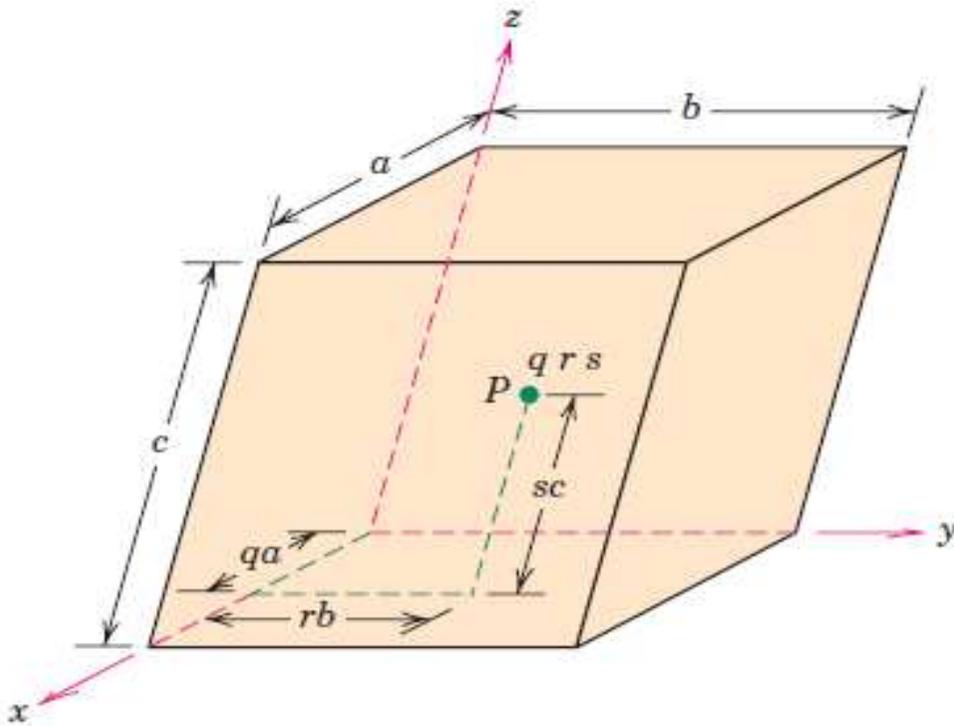
- **Superfícies de baixo índice de Miller**

Pontos, Direções e Planos Cristalográficos



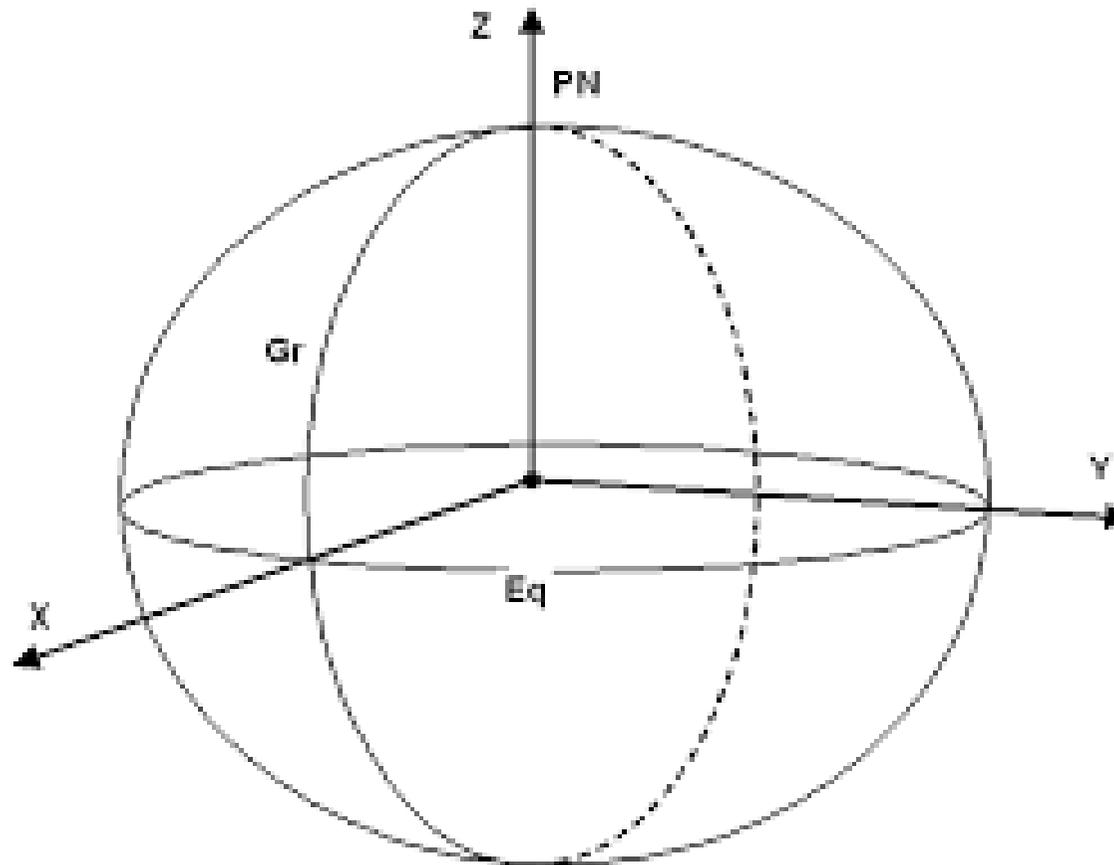
Célula unitária genérica com eixos de coordenadas x , y e z , mostrando as arestas a , b e c e os ângulos α , β e γ

Determinação das coordenadas do ponto P

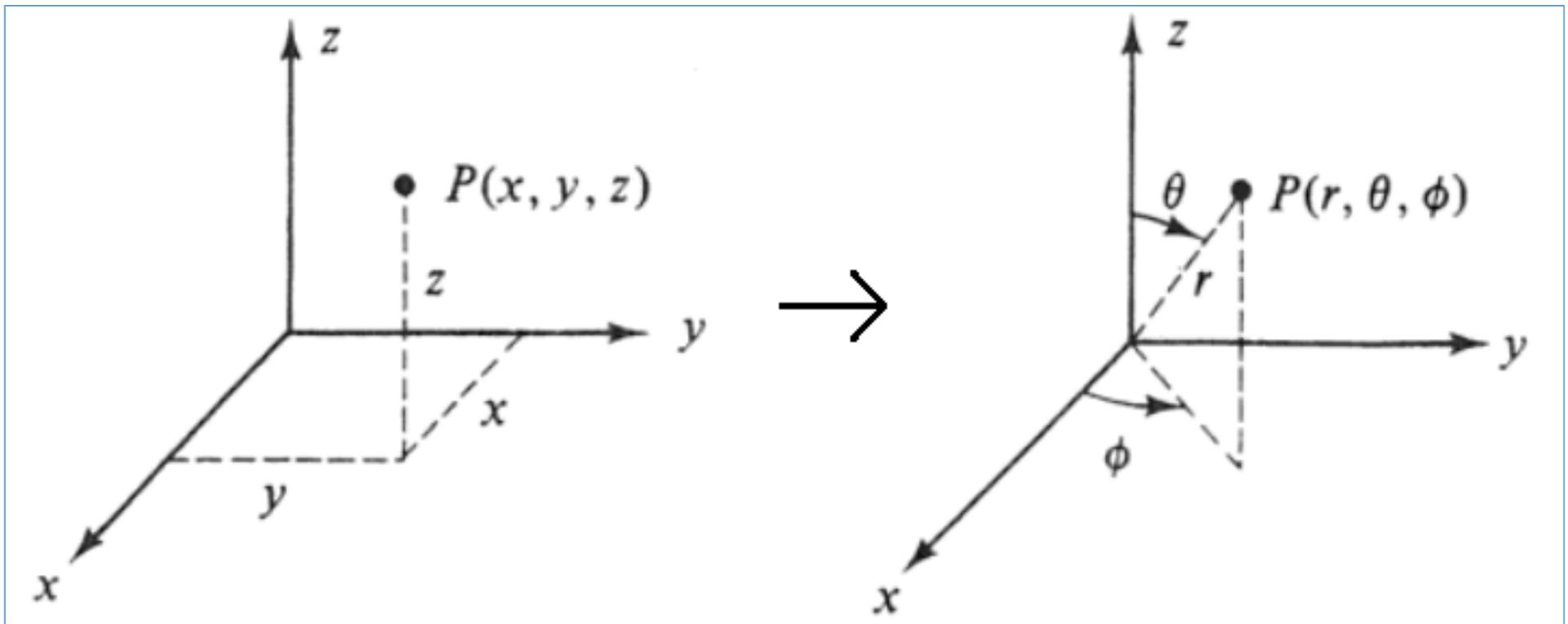


a , b e c são os comprimentos das arestas da célula unitária.
As coordenadas q , r e s correspondem às frações qa , rb e sc .

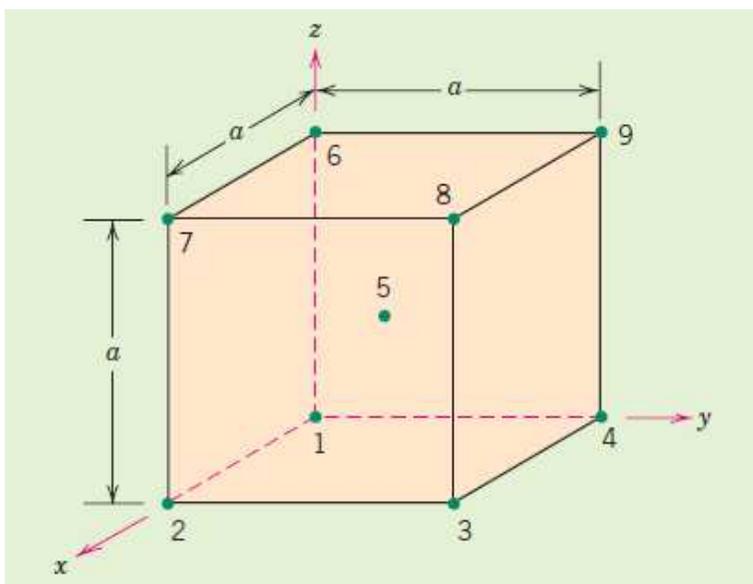
Coordenadas no sistema cristalino cúbico



Coordenadas cartesianas vs. coordenadas polares

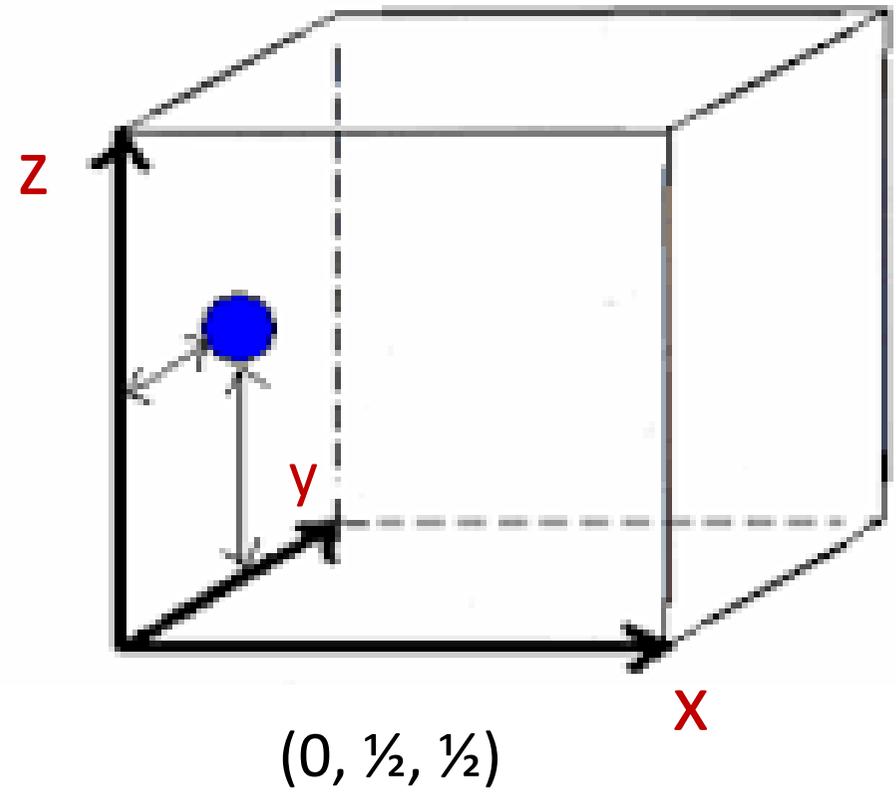
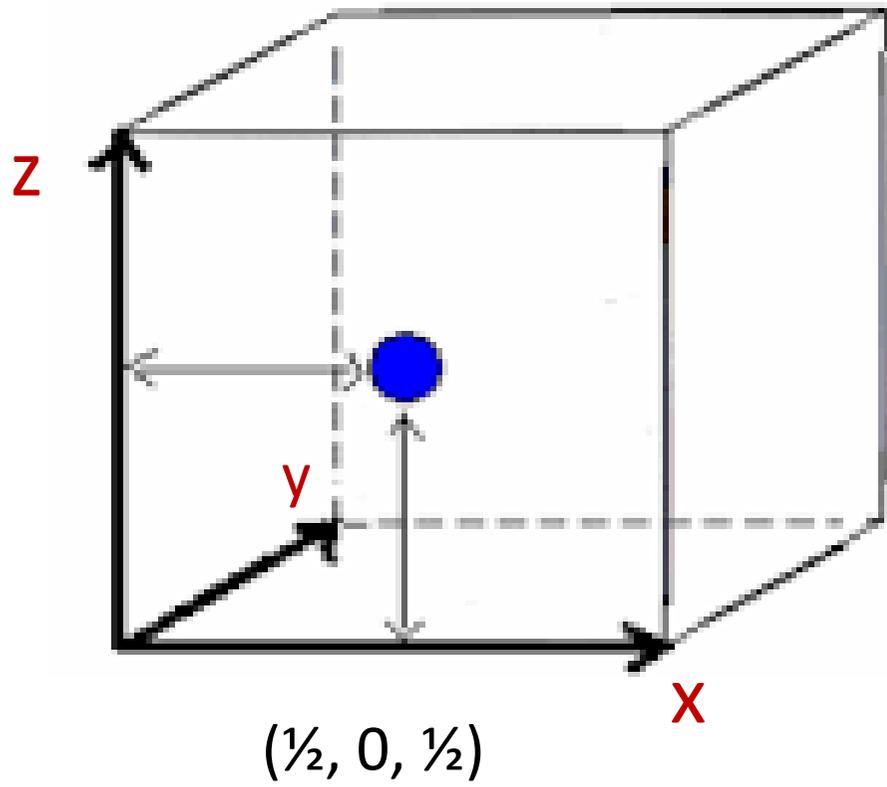


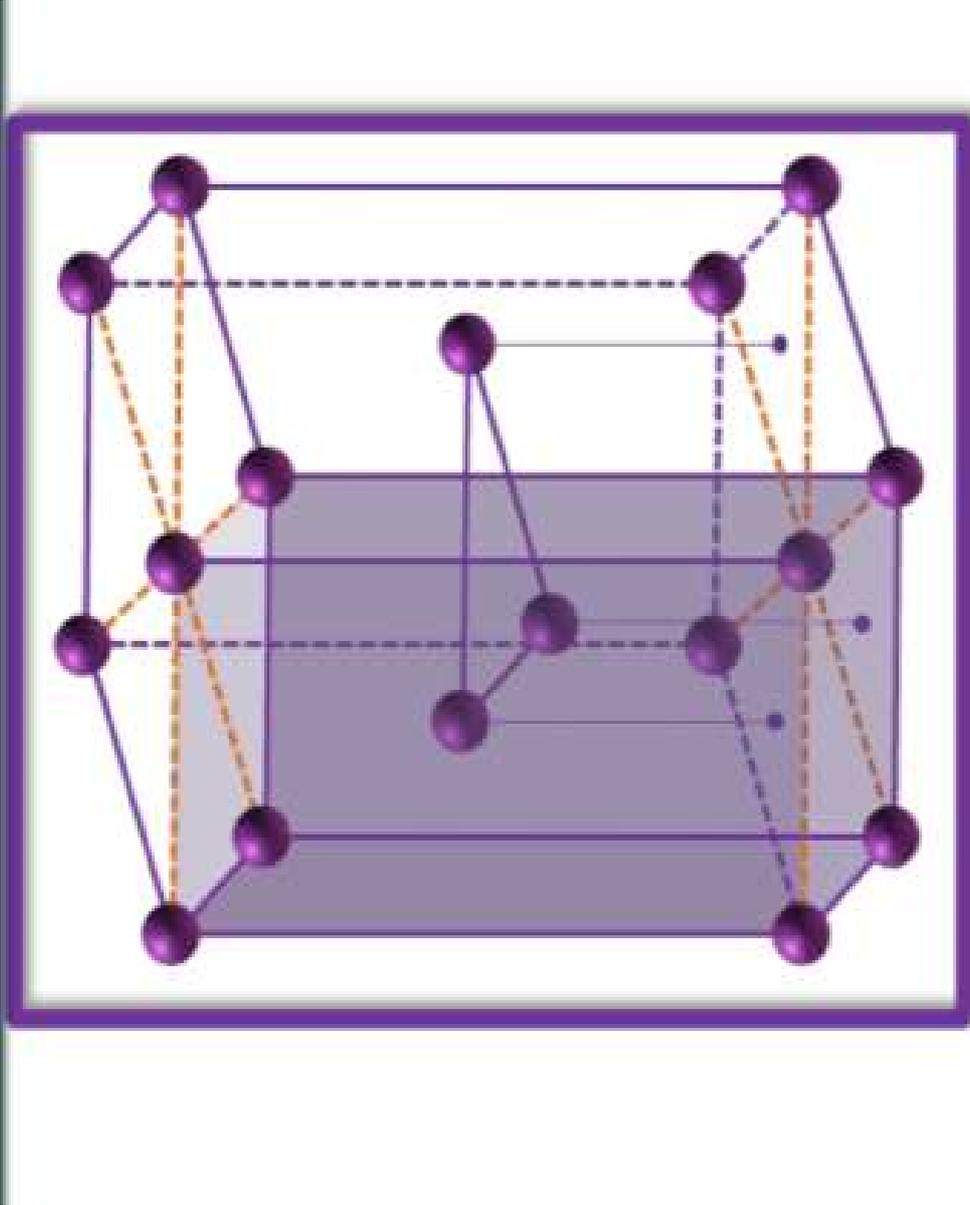
Coordenadas no sistema cúbico: coordenadas dos pontos numerados (posições atômicas) em uma célula unitária CCC.



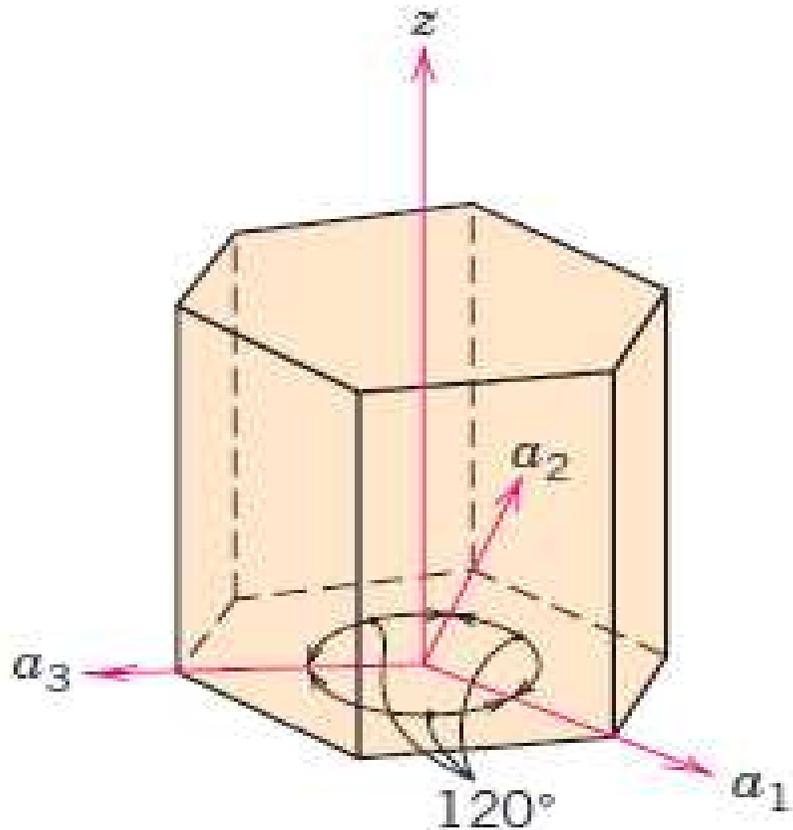
<i>Point Number</i>	<i>Fractional Lengths</i>			<i>Point Coordinates</i>
	<i>x axis</i>	<i>y axis</i>	<i>z axis</i>	
1	0	0	0	0 0 0
2	1	0	0	1 0 0
3	1	1	0	1 1 0
4	0	1	0	0 1 0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2} \frac{1}{2} \frac{1}{2}$
6	0	0	1	0 0 1
7	1	0	1	1 0 1
8	1	1	1	1 1 1
9	0	1	1	0 1 1

Sistema CFC



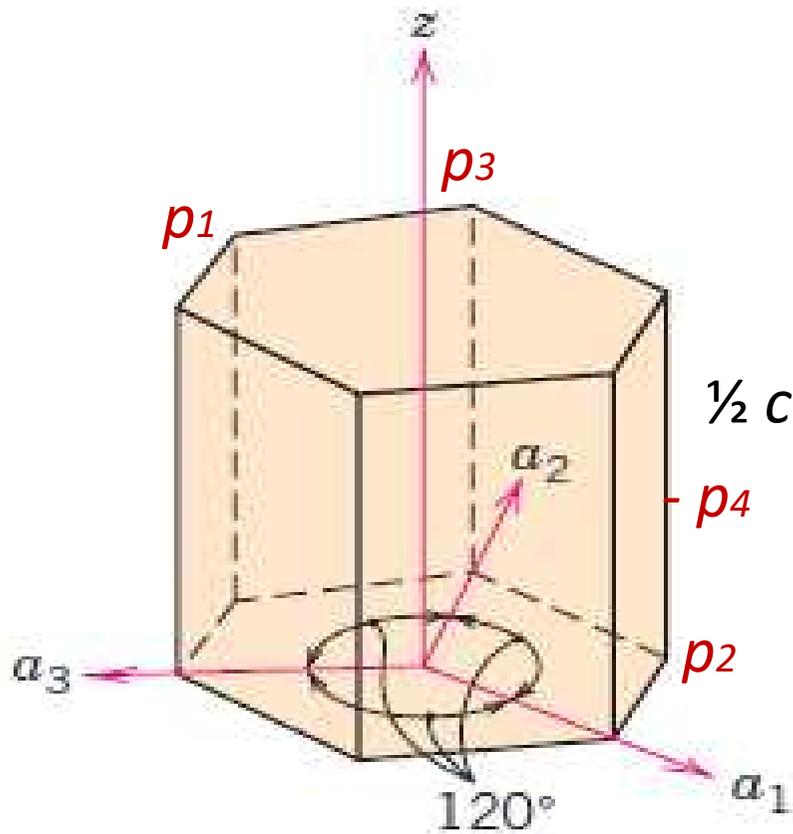


Coordenadas no sistema hexagonal



Sistema de coordenada com quatro eixos: três dos eixos estão contidos no mesmo plano a_1 , a_2 e a_3 (*plano basal*) e formam ângulos de 120° entre si. O eixo z é perpendicular ao plano basal. As coordenadas de um ponto no sistema hexagonal são representadas por quatro pontos.

Coordenadas dos pontos



$$P_1 = (-1, 0, 0, 1)$$

$$P_2 = (0, 0, -1, 0)$$

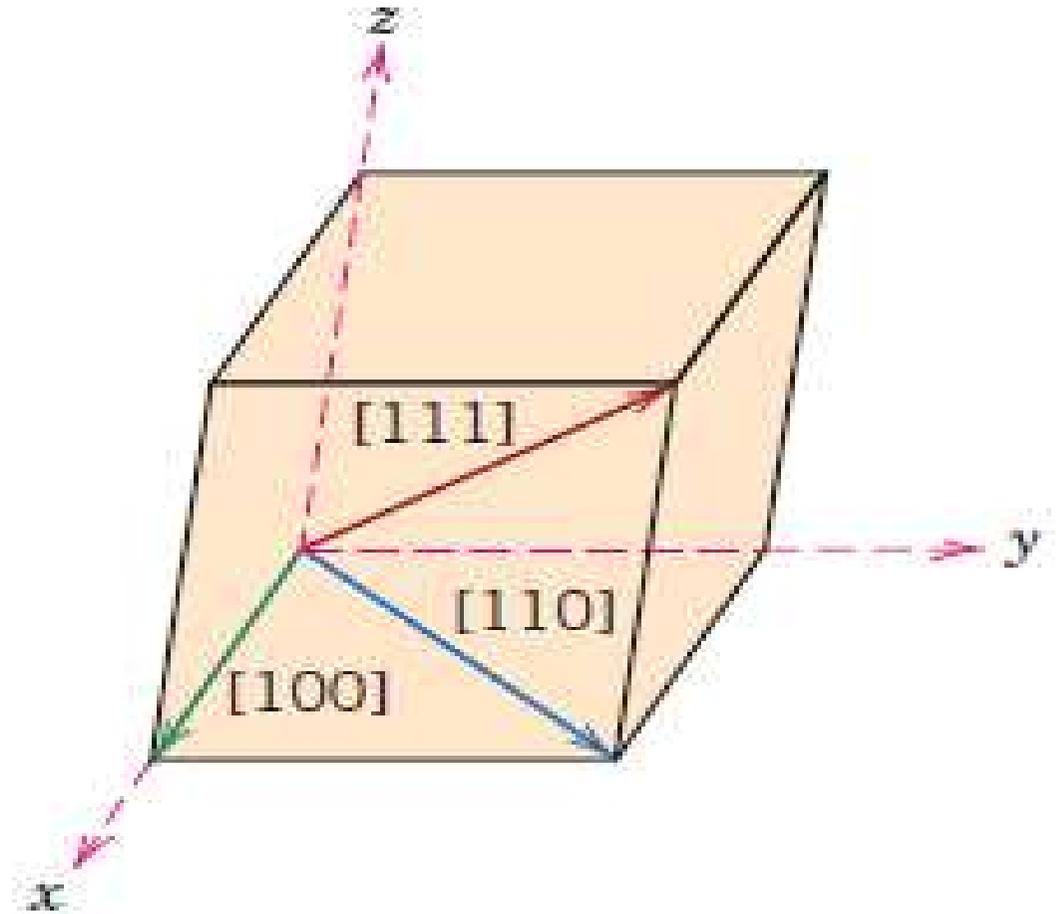
$$P_3 = (0, 1, 0, 1)$$

$$P_4 = (0, 0, -1, \frac{1}{2})$$

Direções Cristalográficas – Índice de Miller-Bravais

DIREÇÕES SÃO IDENTIFICADAS
PELOS ÍNDICES DE MILLER

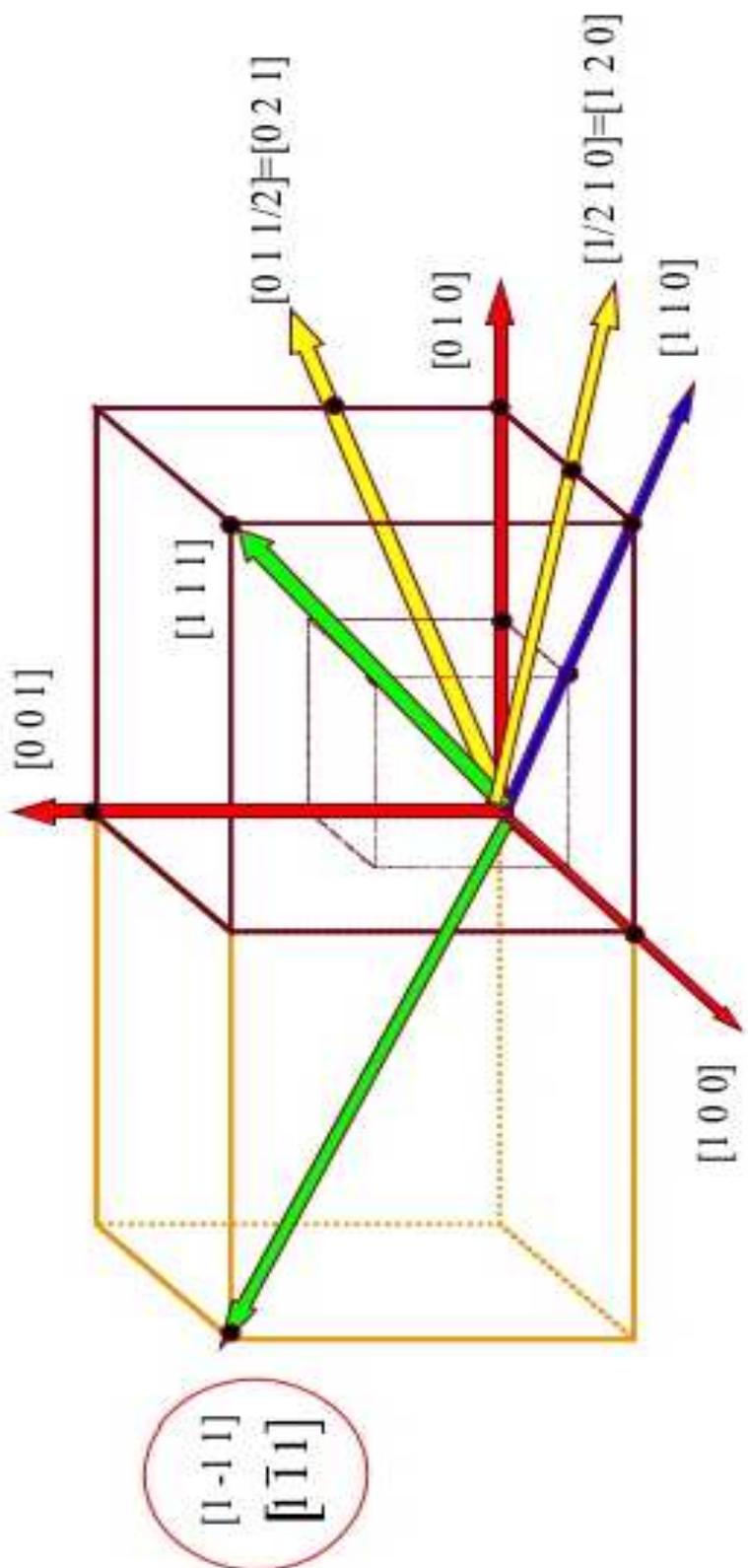
Direções $[1\ 0\ 0]$, $[1\ 1\ 0]$ e $[1\ 1\ 1]$
dentro da célula unitária

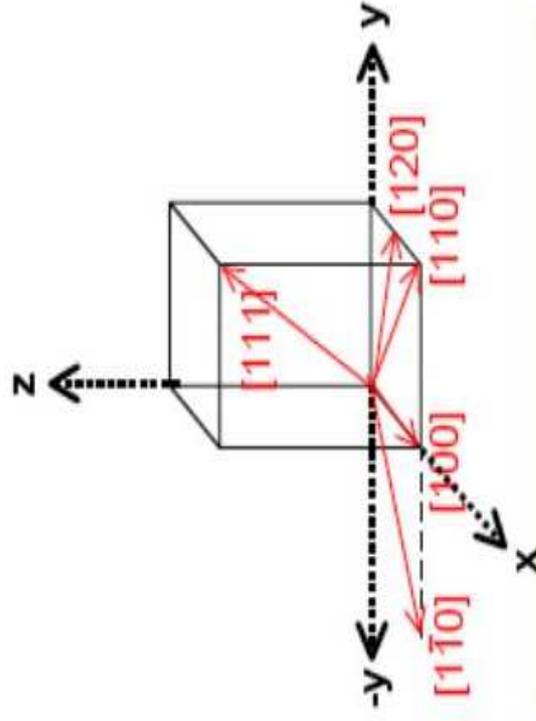


Direções Cristalográficas no Sistema Cúbico

As seguintes etapas devem ser consideradas para determinação dos índices direcionais:

- 1- O vetor deve ser posicionado passando através da origem do sistema de coordenadas, mantendo-se o seu paralelismo;
- 2- Determinar os comprimentos das projeções do vetor sobre cada um dos três eixos;
- 3- Esses três números são multiplicados ou divididos por um fator comum, para reduzi-los aos menores valores inteiros;
- 4- Os três índices são colocados entre colchetes, sem separação por vírgulas: $[u\ v\ w]$.

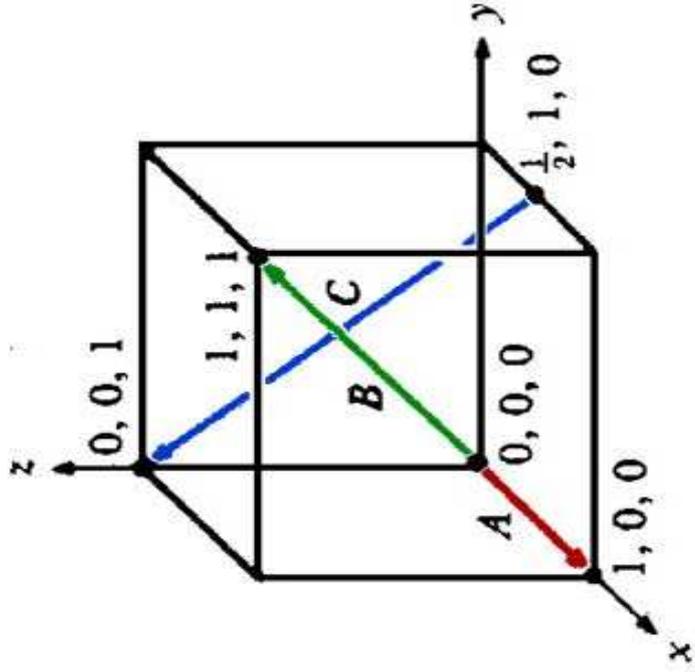




Índices de uma direção [120]

	x	y	z
Projeções	a/2	b	0c
Projeções	1/2	1	0
Reduções	1	2	0

Representação [120]



Direção A:

1. alvo = 1, 0, 0; origem = 0, 0, 0
2. alvo - origem = 1, 0, 0
3. sem frações
4. $[1\ 0\ 0]$

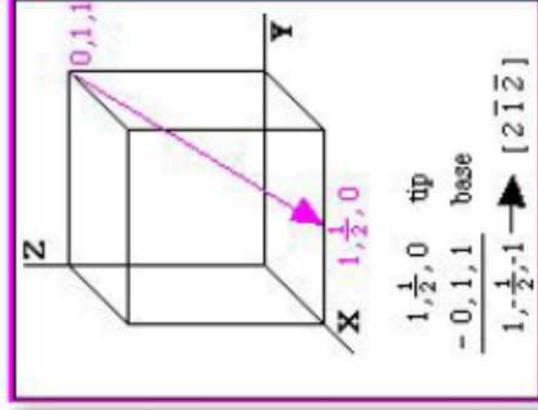
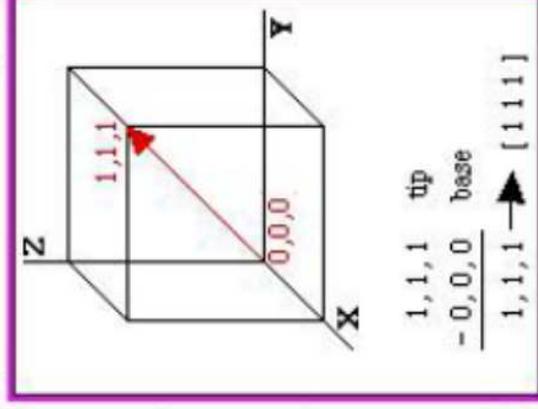
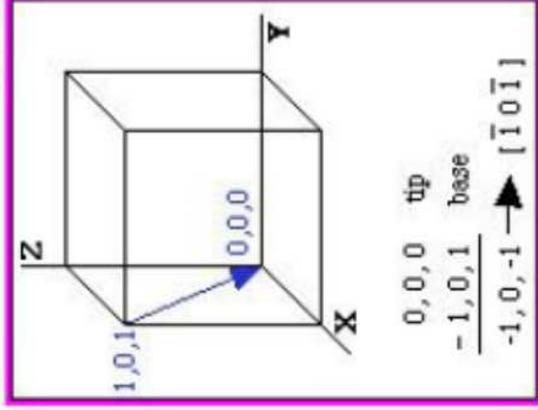
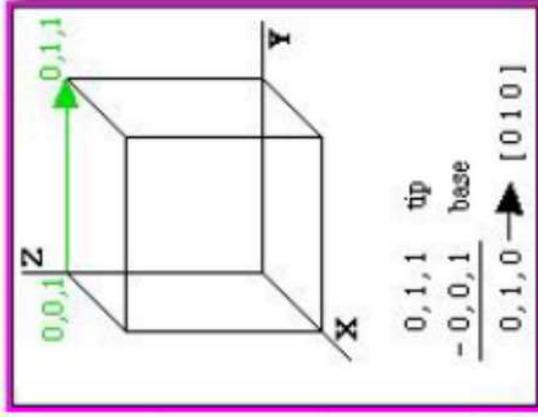
Direção B:

1. alvo = 1, 1, 1; origem = 0, 0, 0
2. alvo - origem = 1, 1, 1
3. sem frações
4. $[1\ 1\ 1]$

Direção C:

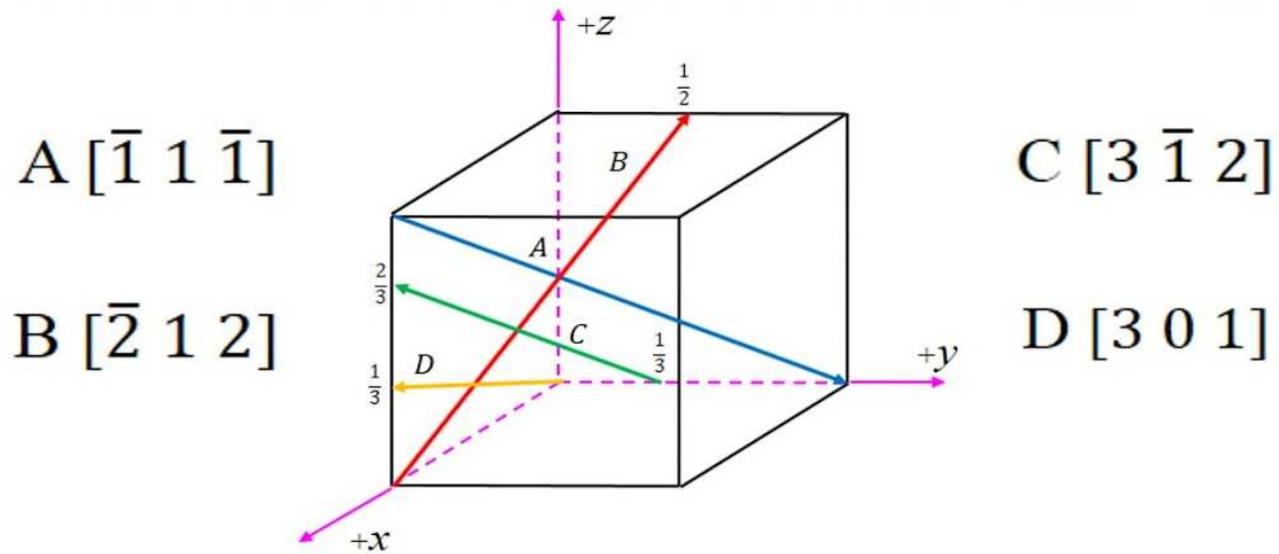
1. alvo = 0, 0, 1; origem = $1/2, 1, 0$
2. alvo - origem = $-1/2, -1, 1$
3. $2(-1/2, -1, 1) = -1, -2, 2$
4. $\overline{[1\ 2\ 2]}$

➤ Direções cristalinas em estruturas cúbicas – $[hkl]$ ou $\langle hkl \rangle$



Regras:

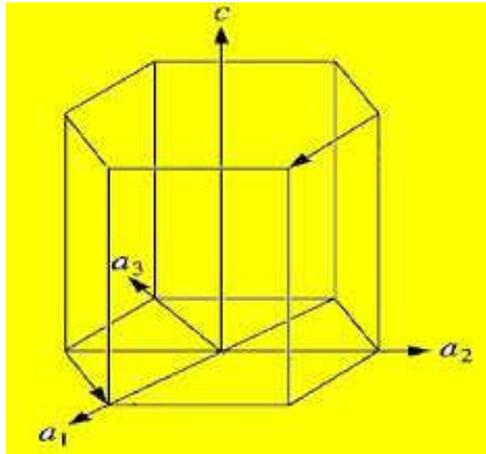
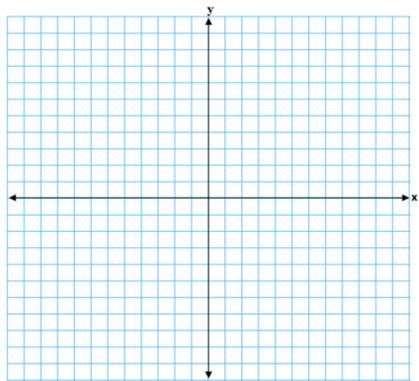
- Estabeleça a origem do sistema de coordenadas
- Determine as coordenadas da base do “vetor”
- Determine as coordenadas da ponta do “vetor”
- Subtraia as coordenadas
- Caso necessário racionalize os índices $[hkl]$ para números inteiros



A	B	C	D
$(0, 1, 0)$	$(0, \frac{1}{2}, 1)$	$(1, 0, \frac{2}{3})$	$(1, 0, \frac{1}{3})$
$-(1, 0, 1)$	$-(1, 0, 0)$	$-(0, \frac{1}{3}, 0)$	$-(0, 0, 0)$
<hr/>	<hr/>	<hr/>	<hr/>
$[\bar{1} \ 1 \ \bar{1}]$	$[\bar{1} \ \frac{1}{2} \ 1] \equiv [\bar{2} \ 1 \ 2]$	$[1 \ \frac{1}{3} \ \frac{2}{3}] \equiv [3 \ \bar{1} \ 2]$	$[1 \ 0 \ \frac{1}{3}] \equiv [3 \ 0 \ 1]$

Direções Cristalográficas no Sistema Hexagonal

Direções em cristais hexagonais



$$[x \ y \ z] \rightarrow [a_1, a_2, a_3, c]$$

Conversão do sistema de três índices
basais para o sistema de quatro índices:

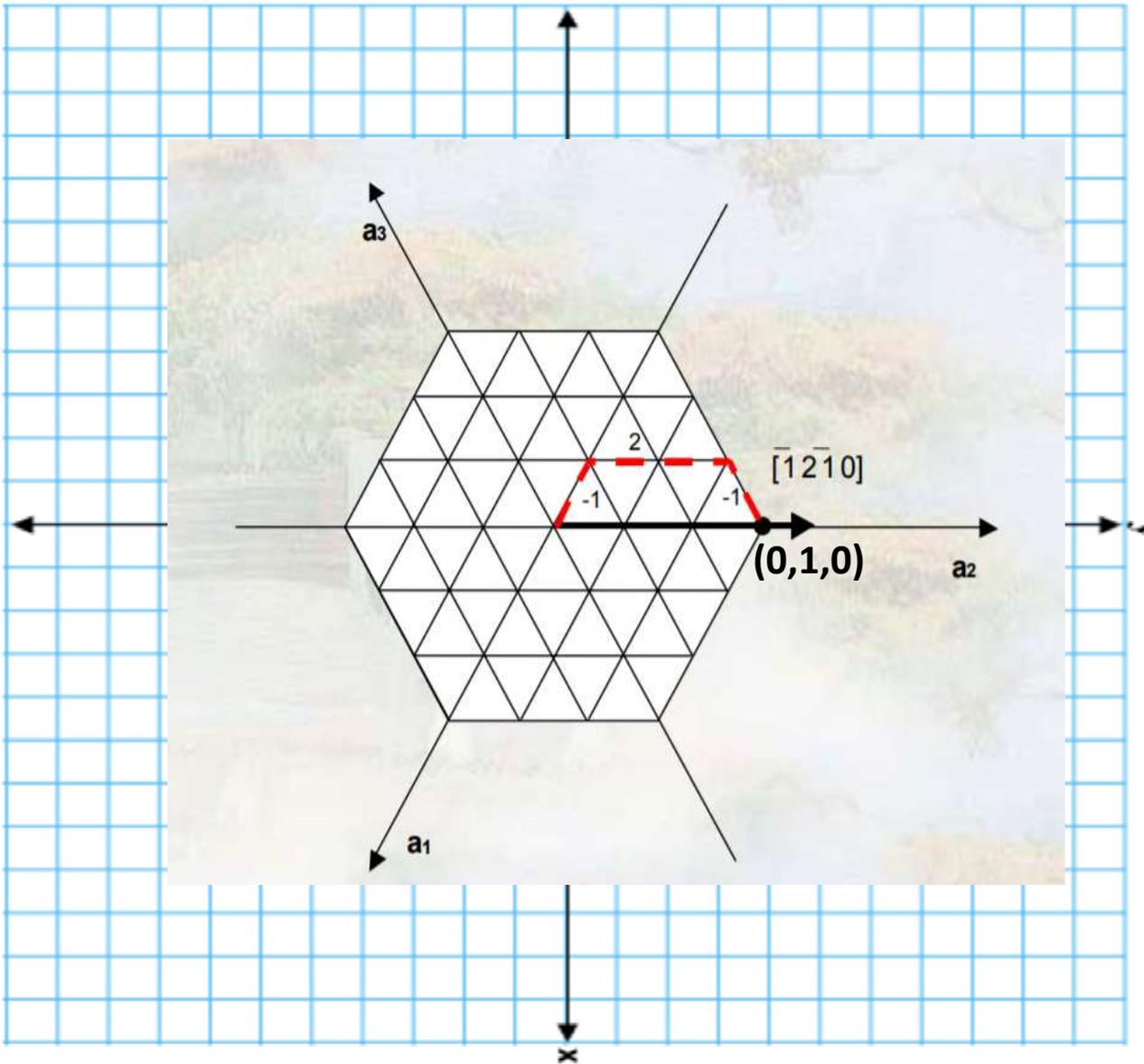
$$[UVW] \rightarrow [uvw]$$

$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

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

$$w = z$$



Para o ponto: $(0,1,0)$, $U=0$, $V=1$ e $W=0$

$$u = \frac{1}{3}(2U - V) \rightarrow u = \frac{1}{3}(2 \times 0 - 1) = -\frac{1}{3}$$

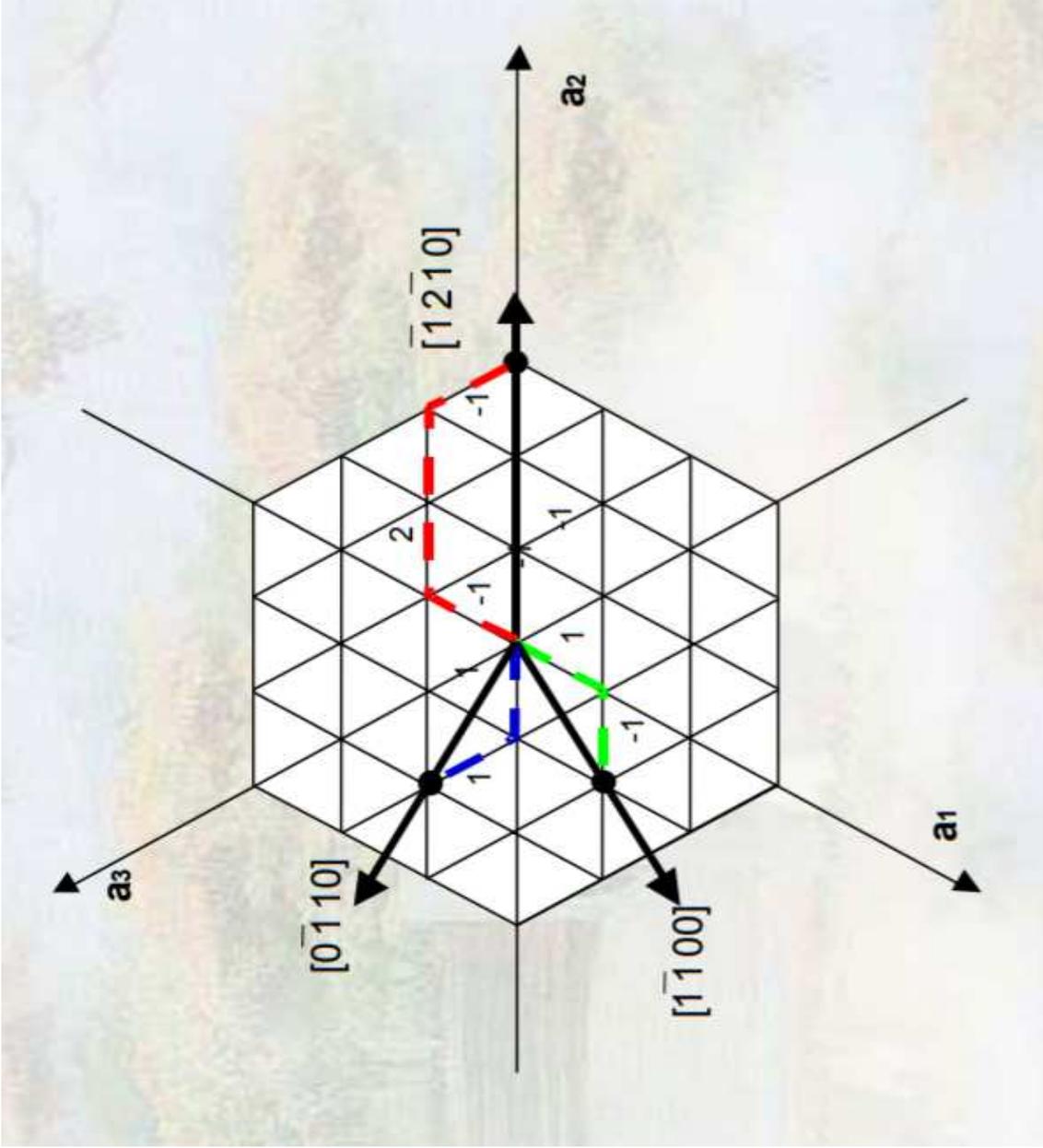
$$v = \frac{1}{3}(2V - U) \rightarrow v = \frac{1}{3}(2 \times 1 - 0) = \frac{2}{3}$$

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

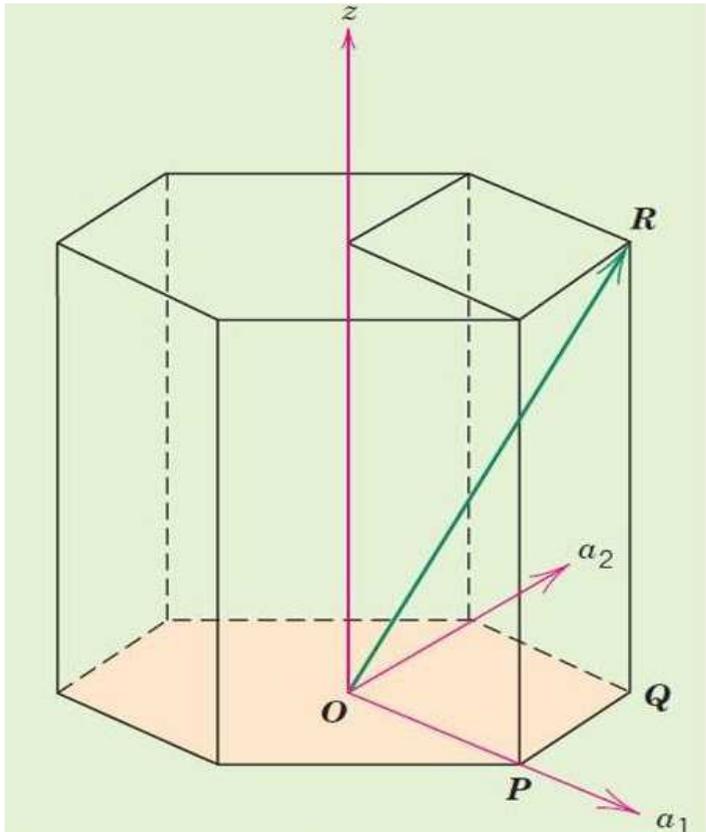
$$w = z = 0$$

Coordenadas de Miller da direção:

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



$$[a_1 a_2 a_3 c] \rightarrow [u v t w]$$



Coordenadas do ponto R: (0,1,1)

$$[U V W] \rightarrow [u v t w]$$

$$[0 \ 1 \ 1] \rightarrow [u v t w]$$

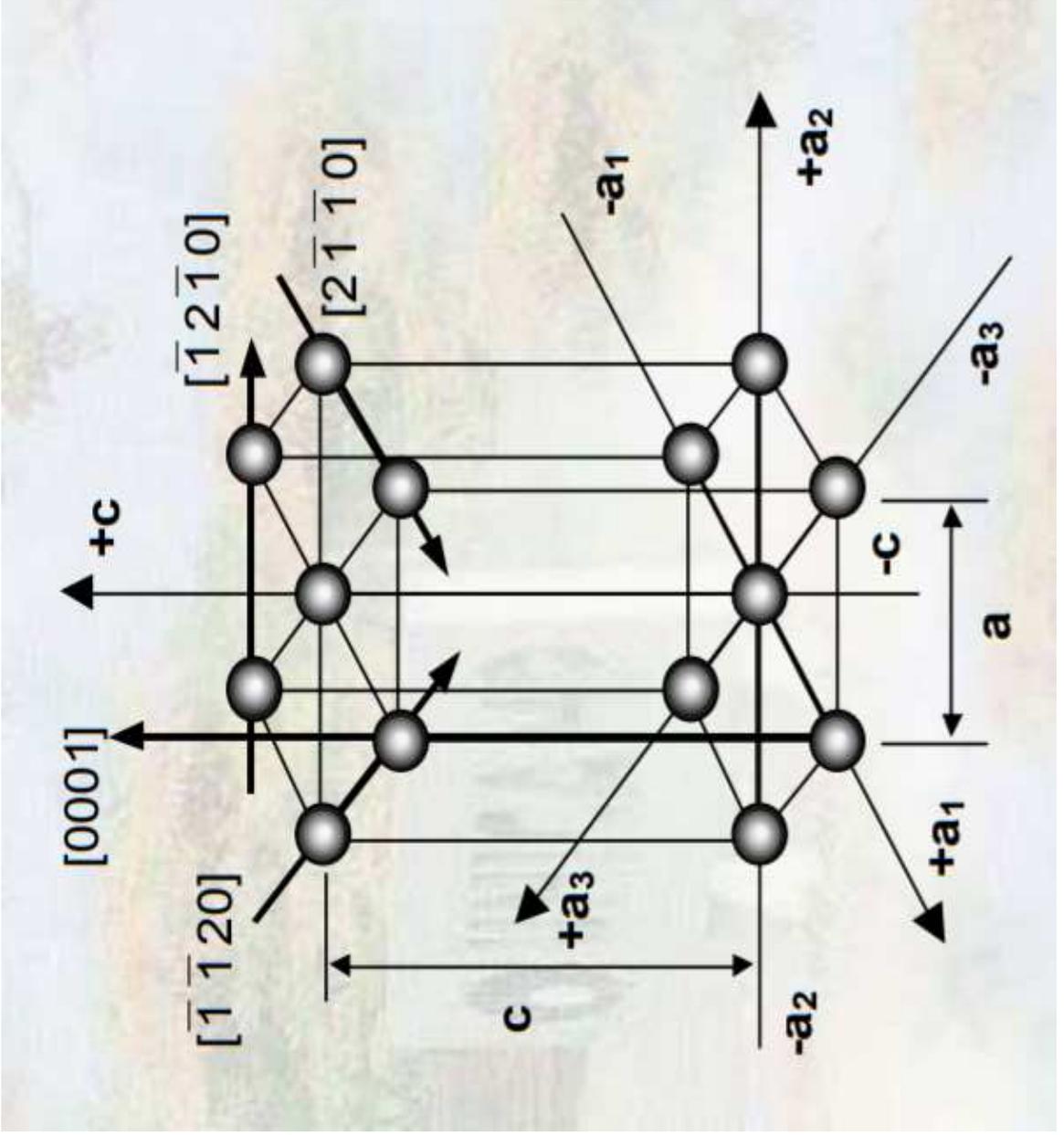
$$u = \frac{1}{3}(2U - V) = \frac{1}{3}(2 \times 0 - 1) = -\frac{1}{3}$$

$$v = \frac{1}{3}(2V - U) = \frac{1}{3}(2 \times 1 - 0) = \frac{2}{3}$$

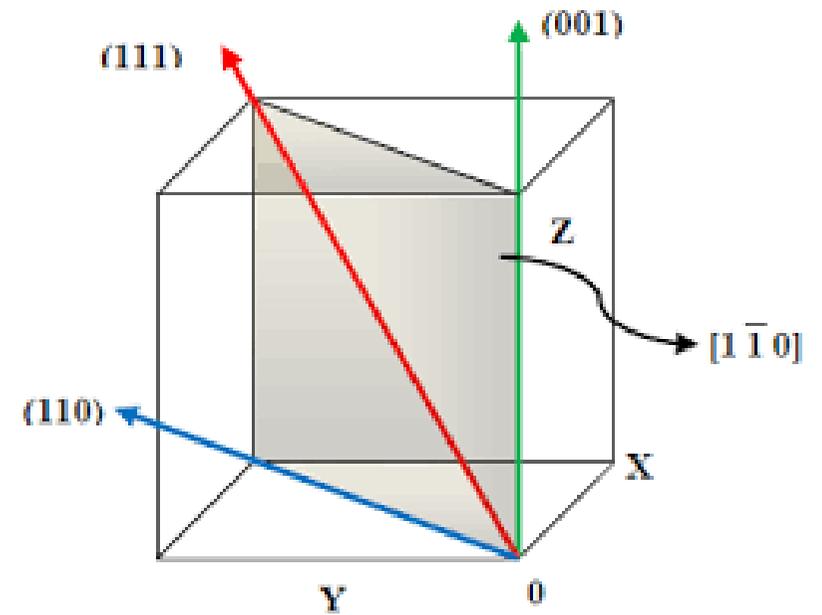
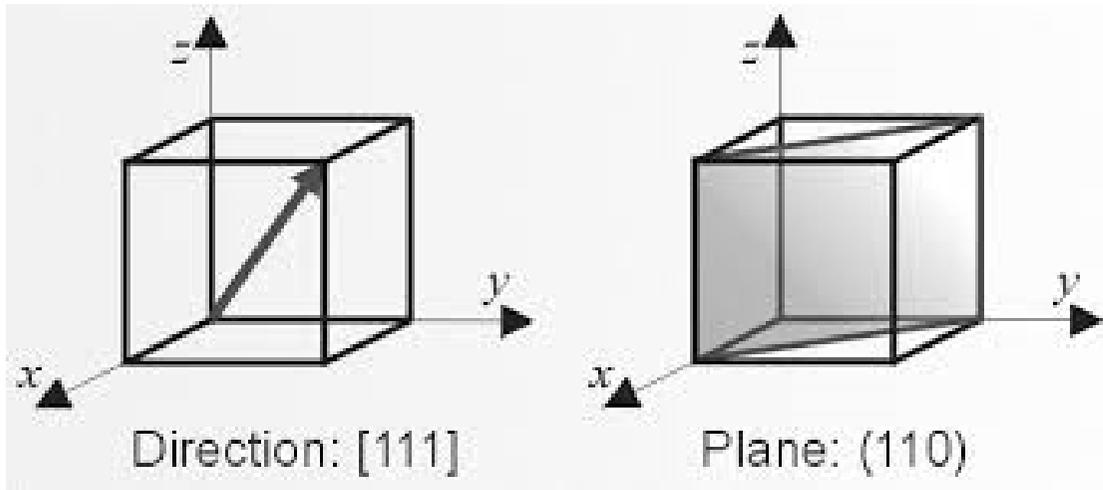
$$t = -(u + v) = -\left(-\frac{1}{3} + \frac{2}{3}\right) = -\frac{1}{3}$$

$$w = 1$$

$$\left[\bar{1} \ \frac{2}{3} \ -\frac{1}{3} \ 1 \right] \equiv [\bar{1} \ 2 \ \bar{1} \ 1]$$



Planos Cristalográficos no Sistema Cúbico



Crystallographic Planes

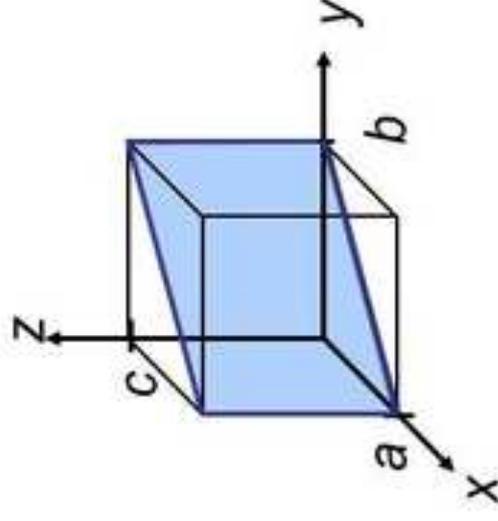
Example 1

1. Intercepts

a	b	c
1	1	∞
2. Reciprocals

a	b	c
$1/1$	$1/1$	$1/\infty$
3. Reduction

a	b	c
1	1	0
1	1	0
4. Miller Indices (110)



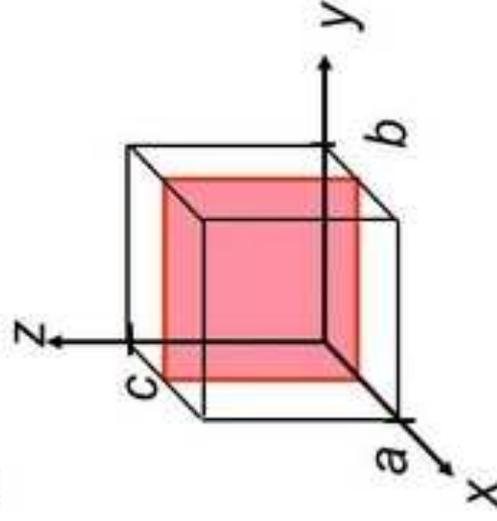
Example 2

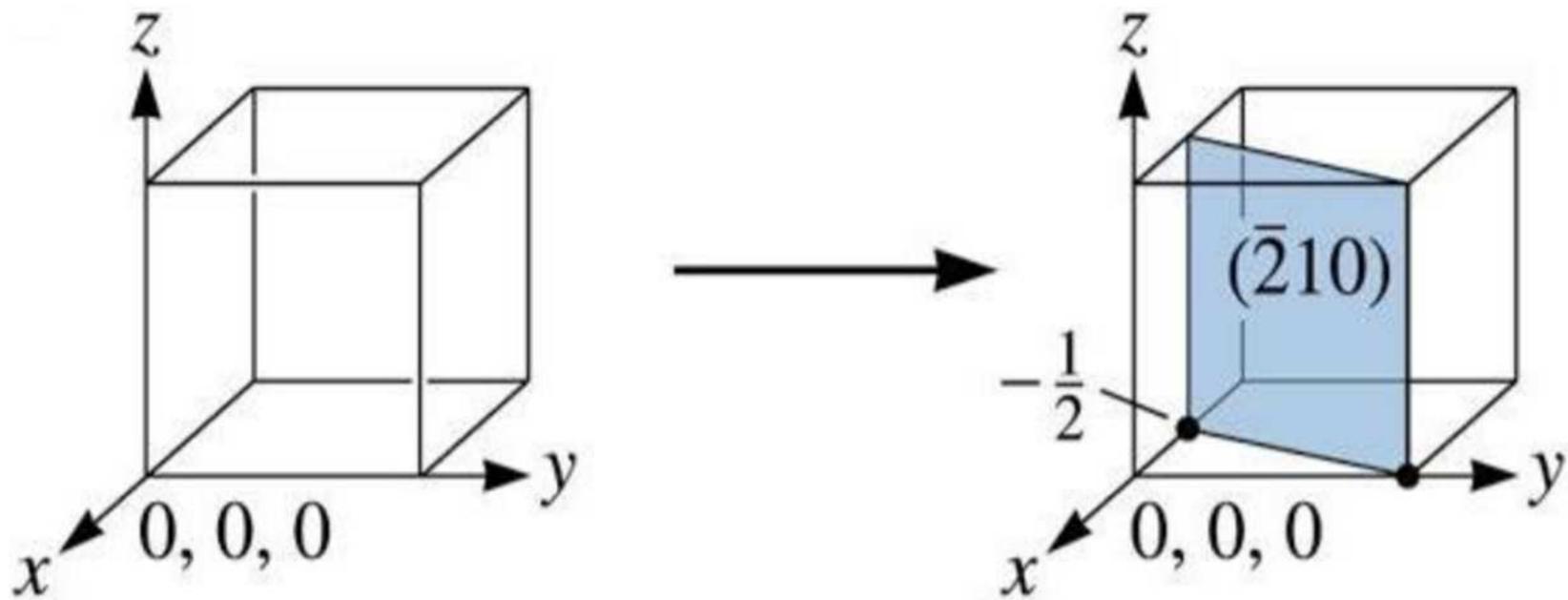
1. Intercepts

a	b	c
$1/2$	∞	∞
2. Reciprocals

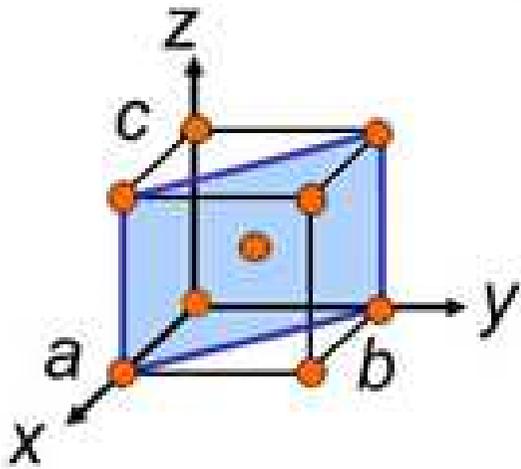
a	b	c
$1/1/2$	$1/\infty$	$1/\infty$
3. Reduction

a	b	c
2	0	0
2	0	0
4. Miller Indices (200)

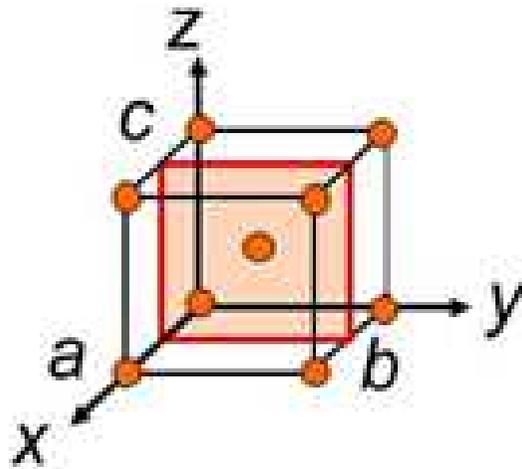




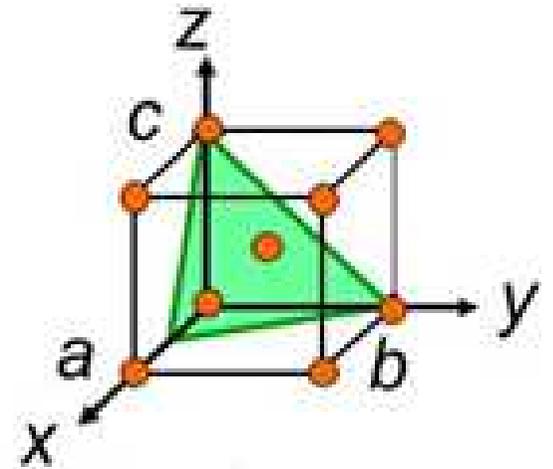
Coordenadas do plano $(\frac{\bar{1}}{2} \ 1 \ \frac{1}{\infty}) \equiv (\bar{2} \ 1 \ 0)$



(1 1 0)



(2 0 0)



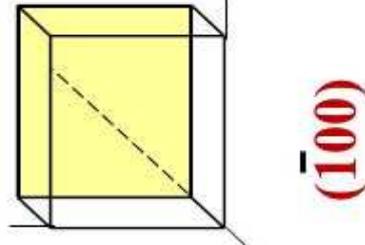
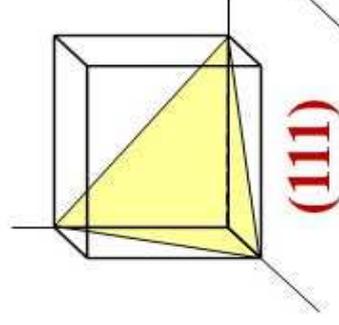
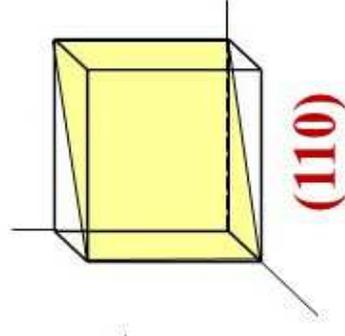
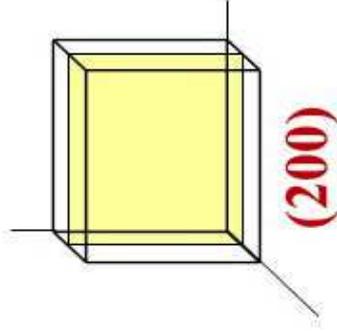
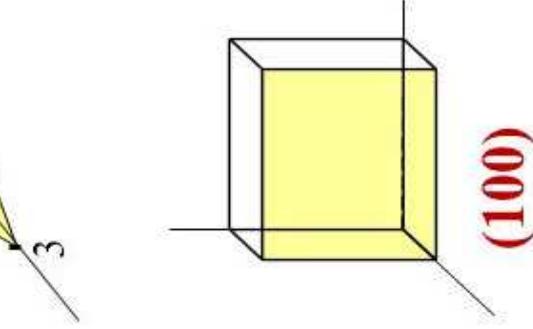
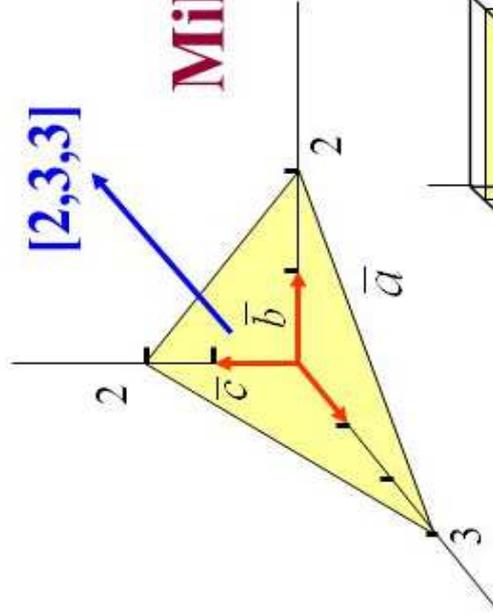
(2 1 1)

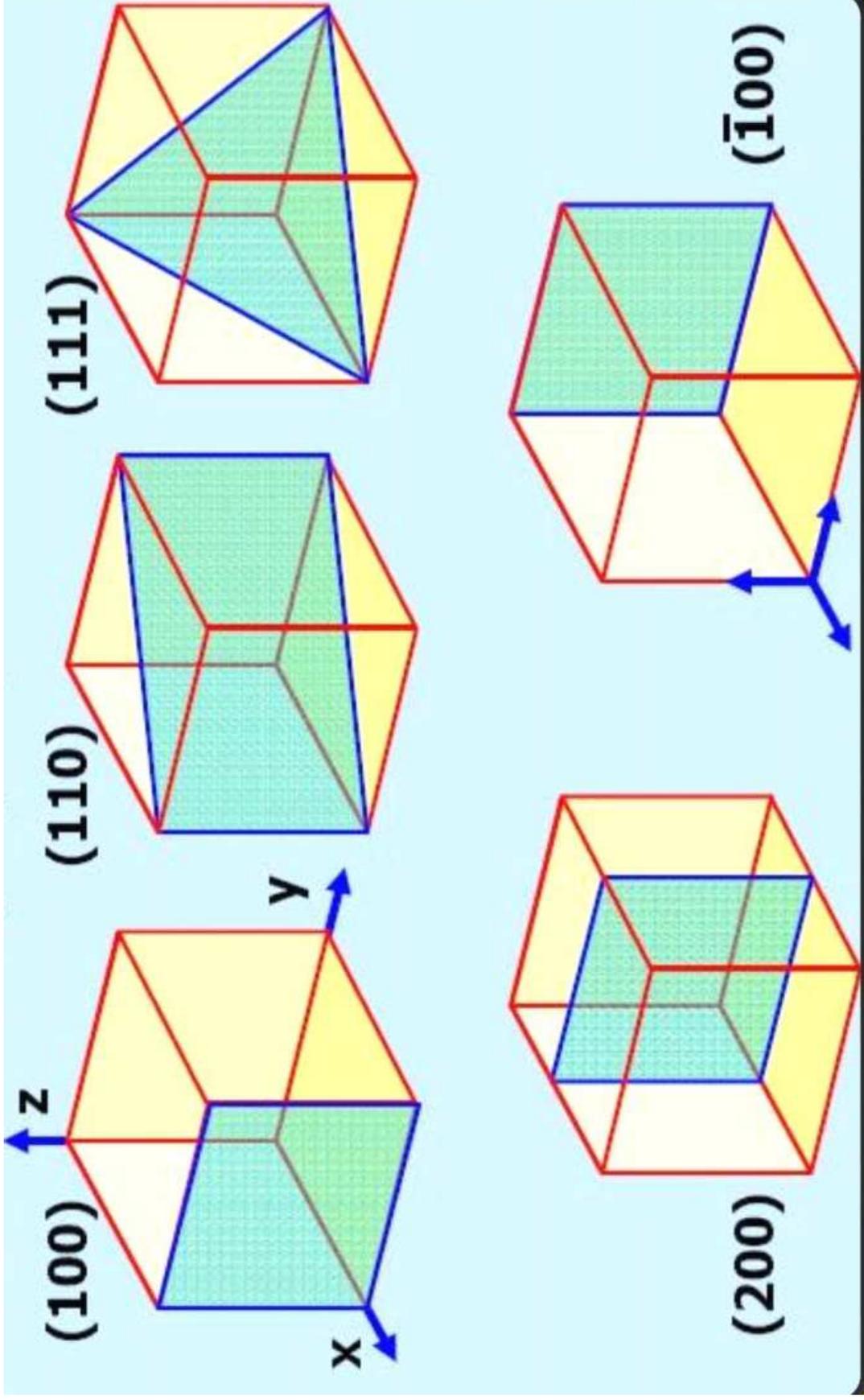
Plane intercepts axes at $3\bar{a}$, $2\bar{b}$, $2\bar{c}$

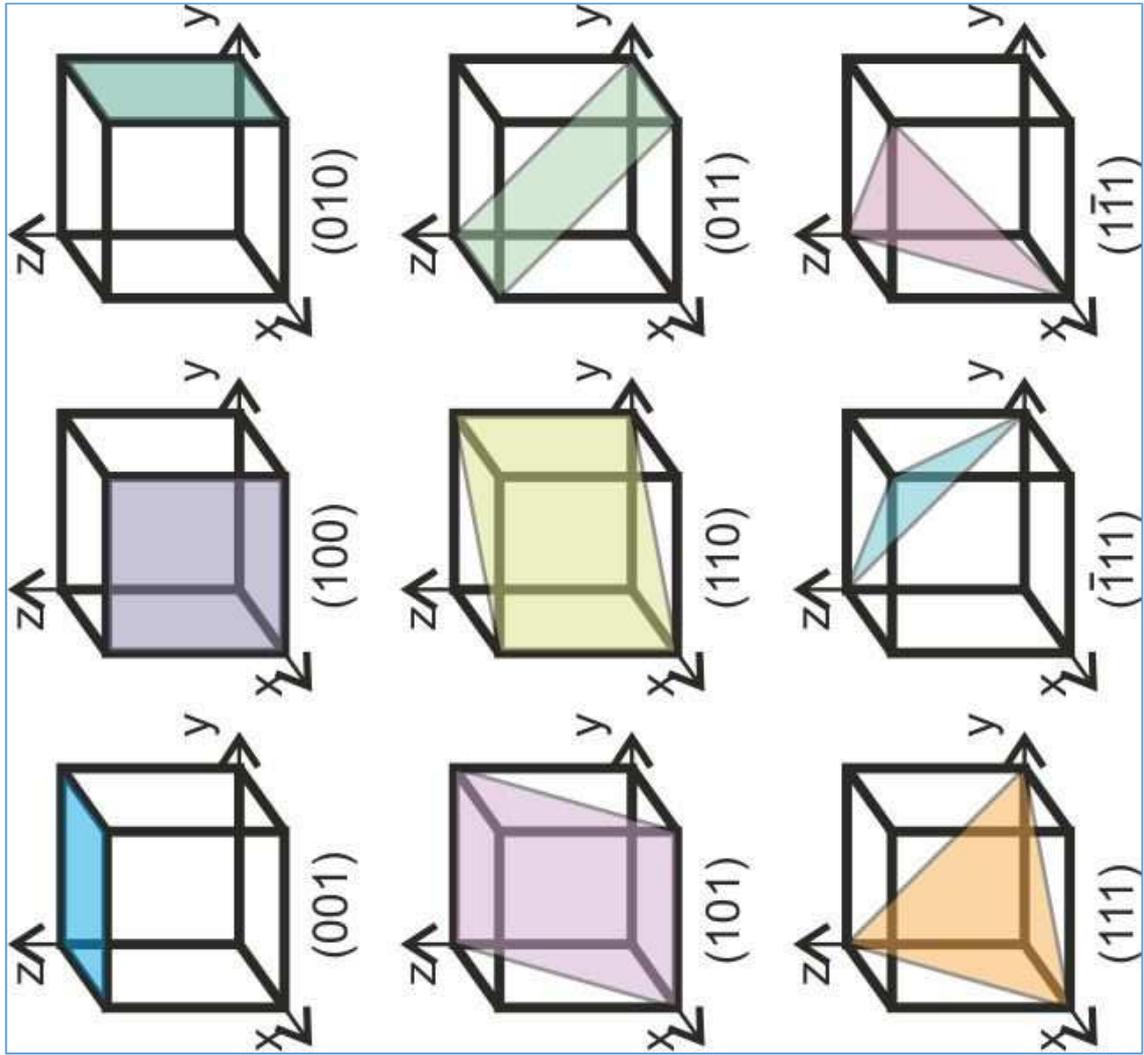
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Miller Indices of the plane: (2,3,3)

Indices of the direction: [2,3,3]







Planos da Rede Hexagonal

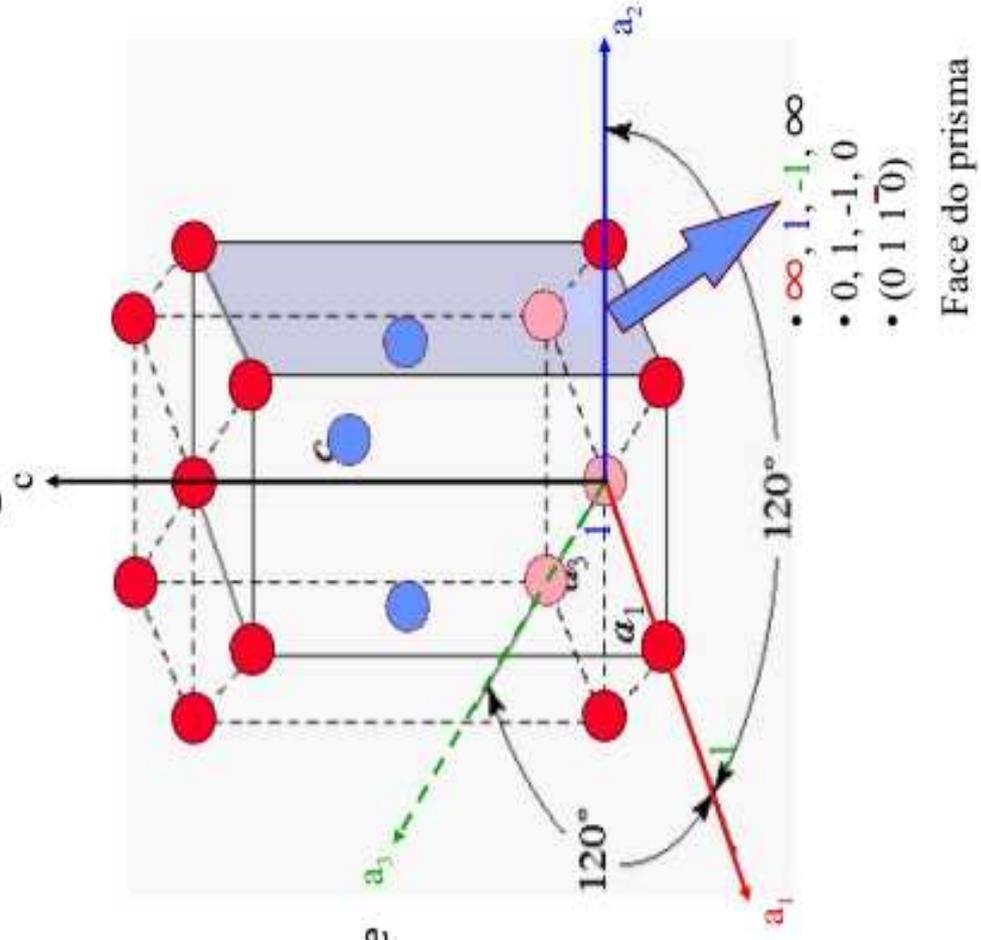
- ✓ Os 3 eixos, a_1 , a_2 e a_3 eixes estão contidos dentro da base planar;
- ✓ O ângulo entre eles é de 120°
- ✓ O eixo Z é perpendicular à base planar.

$$[h'k'l'] \longrightarrow [hkil]$$

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

Índices de Miller-Bravais

- 4 coordenadas
- redundância



Planos Cristalográficos em Metais: Sistema Hexagonal

example

1. Intercepts	a_1	a_2	a_3	c
2. Reciprocals	1	∞	-1	1
	1	$1/\infty$	-1	1
3. Reduction	1	0	-1	1
	1	0	-1	1

4. Miller-Bravais Indices $(10\bar{1}1)$

