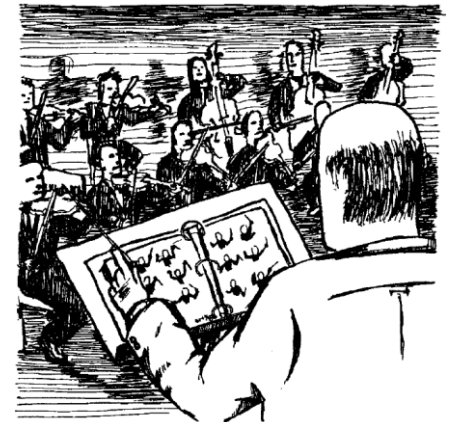


Tecnologia e Aplicações de Semicondutores 1o semestre/2024

Semicondutores – Teoria I

Dr. Adenilson José Chiquito

Departamento de Física
Universidade Federal de São Carlos

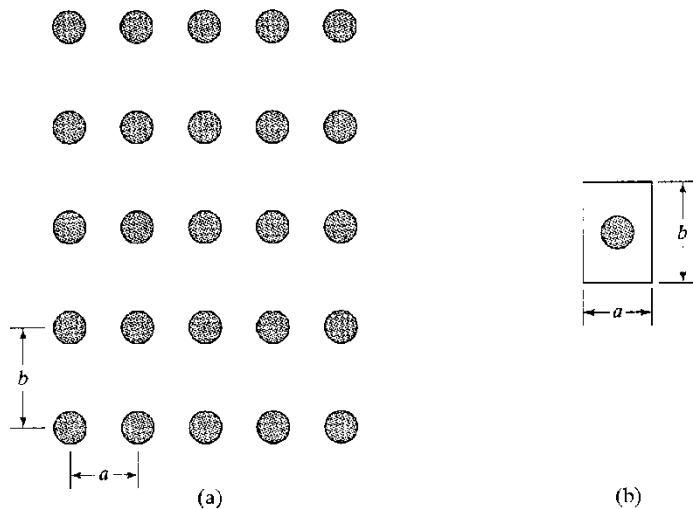


A SEMI-CONDUCTOR

Semicondutores e alguns pontos de Física de Estado Sólido

Algumas propriedades importantes sobre cristais...

1. Todos os cristais são caracterizados por uma estrutura regular bem definida e **periódica!**
2. A menor parte do cristal que quando repetida forma o cristal todo é a chamada célula unitária primitiva. Para descrever a célula unitária precisamos de uma base de vetores – vetores primitivos!

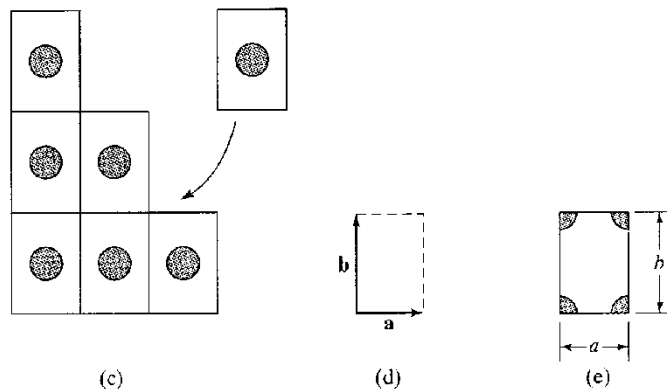


$$\mathbf{R} = h\mathbf{a} + k\mathbf{b}$$

A rede cristalina será construída repetindo-se a célula unitária e transladando-a por quantidades a , b , $r = a+b$, etc...

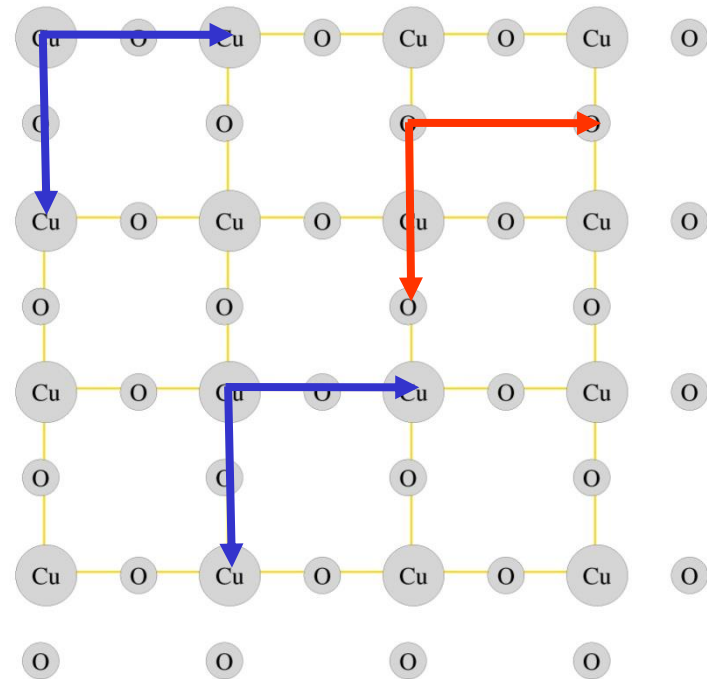
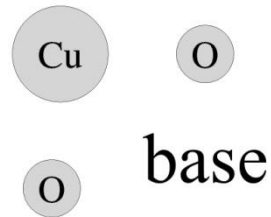
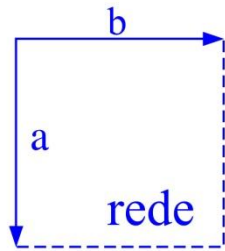
Importante:

- células unitárias não são únicas!
- Uma célula unitária não necessita ser primitiva (a menor possível)

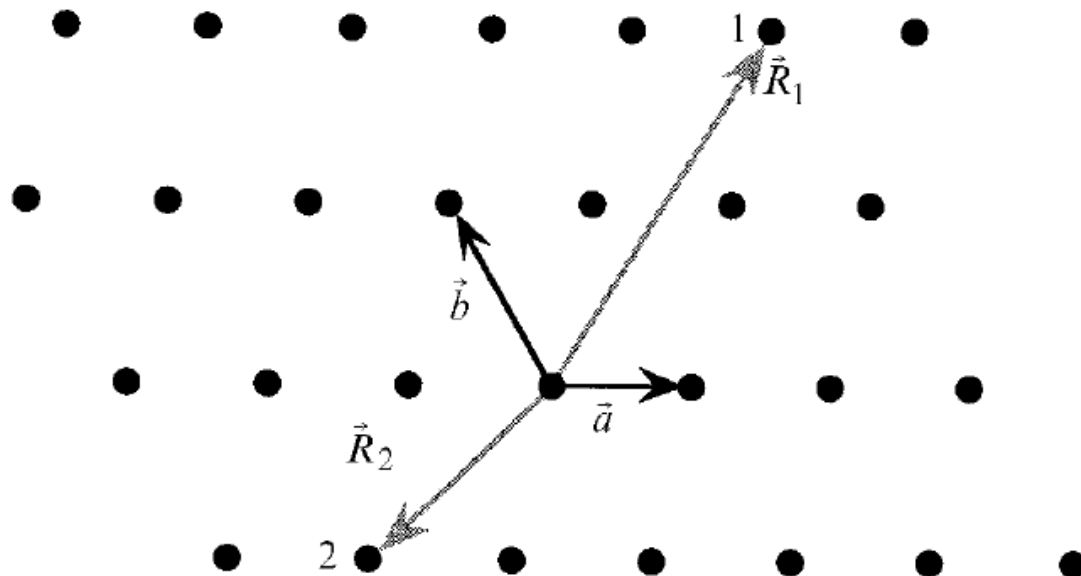


Redes cristalinas – cristais

Rede + Base = Cristal



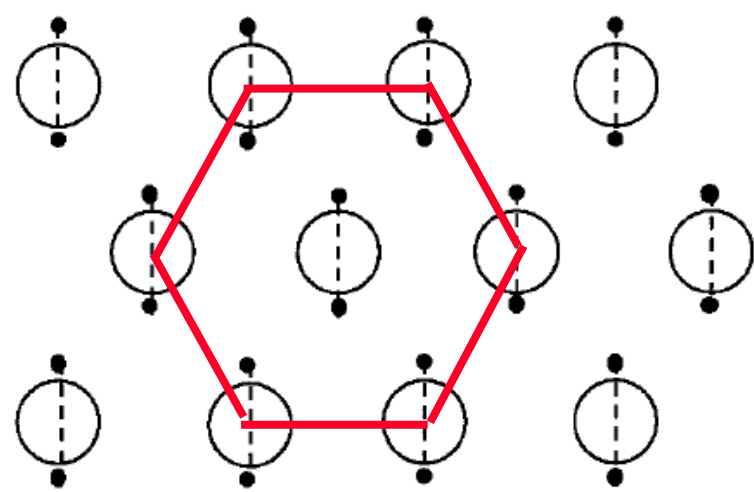
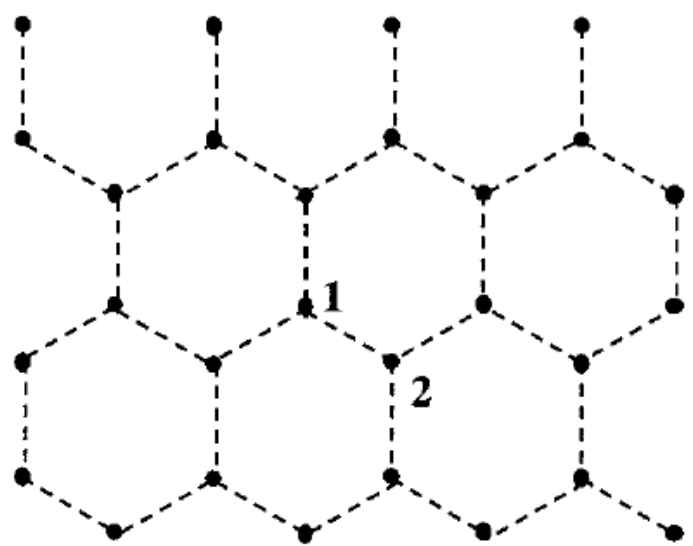
Exemplos



$$\vec{R} = u\vec{a} + v\vec{b}$$

$$\vec{R}_1 = 3\vec{a} + 2\vec{b}$$

$$\vec{R}_2 = -2\vec{a} - \vec{b}$$



Conceitos importantes

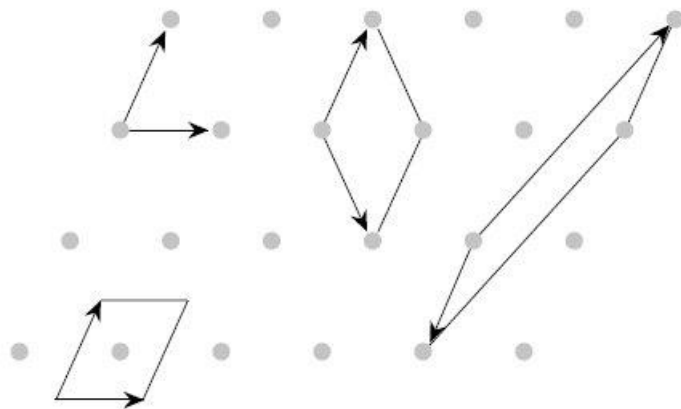
Rede de Bravais: coleção de pontos que preenchem o espaço e dessa forma todo ponto tem o mesmo “ambiente” ao seu redor

Vetores de translação: a translação do cristal por um vetor T que liga um ponto R da rede a um ponto $R+T$ e deixa o cristal como um todo invariante

Vetores primitivos: a partir de qualquer ponto da rede, pode-se construir 3 vetores que ligam-se aos três pontos vizinhos mais próximos e não coplanares: estes são os vetores primitivos a_1 , a_2 , a_3

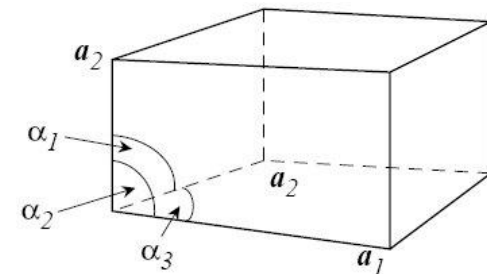
Base: um cristal pode ser descrito atribuindo-se uma base para cada ponto da rede e pode ter um ou mais átomos

Célula primitiva: os vetores primitivos definem paralelepípedo de volume $a_1(a_2 \times a_3)$ que é chamado de célula primitiva

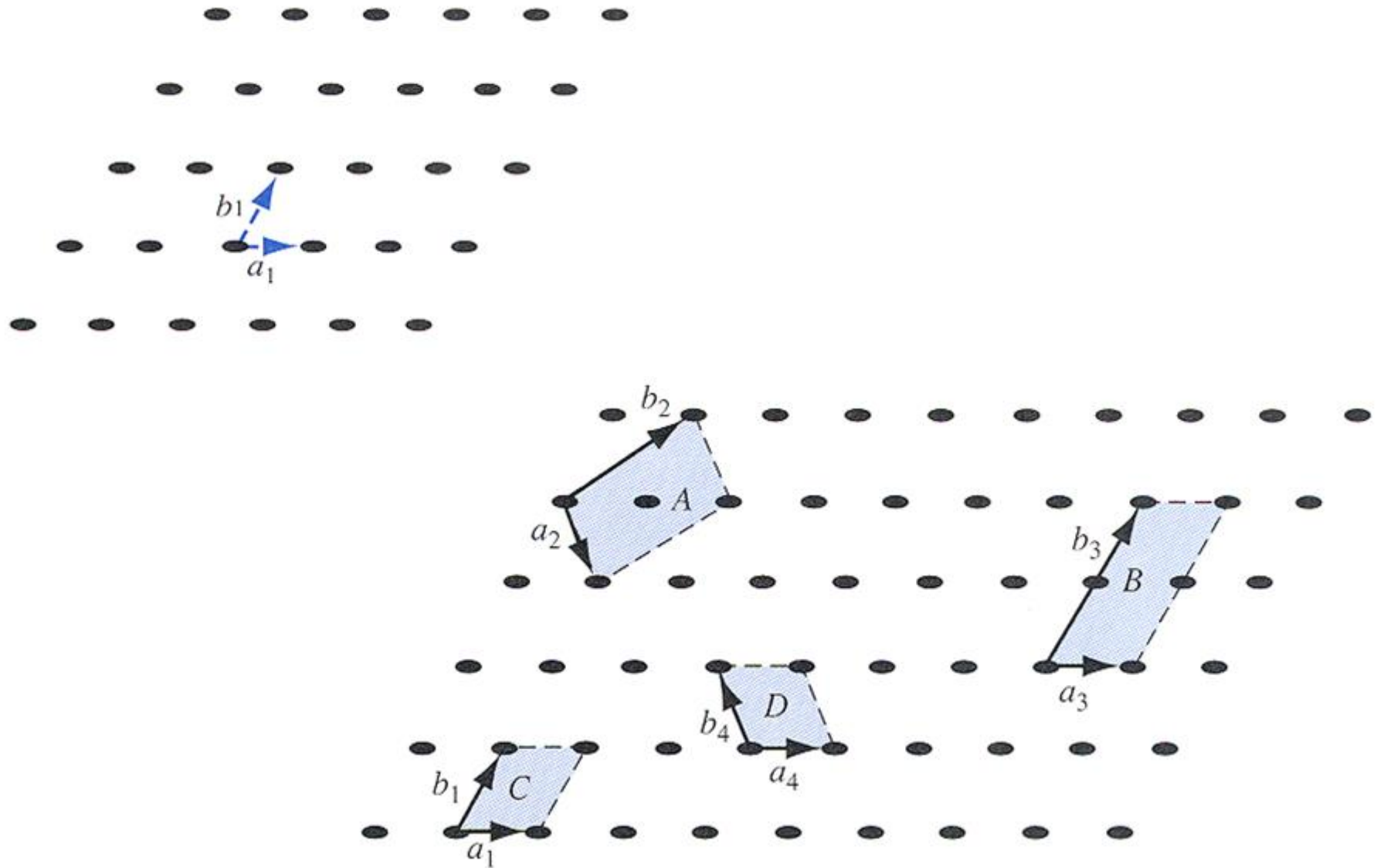


$$a_1 = |a_1|; a_2 = |a_2|; a_3 = |a_3|$$

$$\alpha_1 = \cos^{-1} \frac{a_2 \cdot a_3}{a_2 a_3}; \alpha_2 = \cos^{-1} \frac{a_1 \cdot a_3}{a_1 a_3}; \alpha_3 = \cos^{-1} \frac{a_1 \cdot a_2}{a_1 a_2}$$



Algumas propriedades importantes sobre cristais...



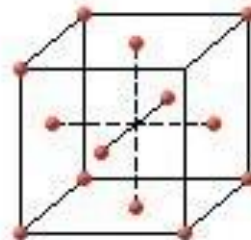
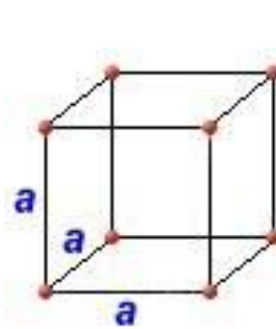
7 sistemas cristalinos

Geometrias das células convencionais

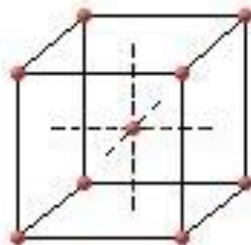
Redes de Bravais e suas particularidades

Sistema Cristalino	Relações Axiais	Ângulos Interaxiais
Cúbico	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ,$ $\gamma = 120^\circ$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Romboédrico	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
Ortorrômbico	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Monoclínico	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$
Triclínico	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$

Redes de Bravais, configurações espaciais

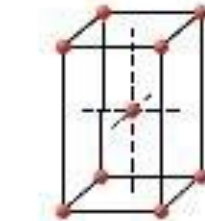
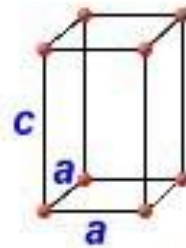


de face centrada

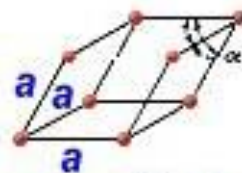


de corpo centrado

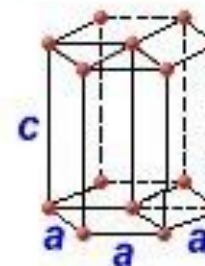
cúbico



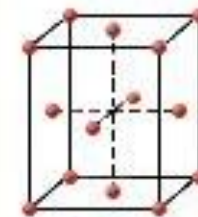
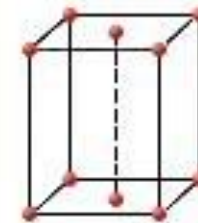
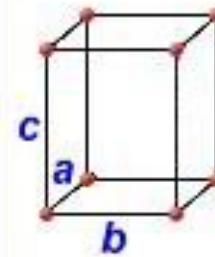
de corpo centrado tetragonal



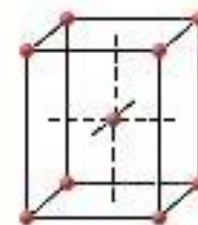
romboédrico



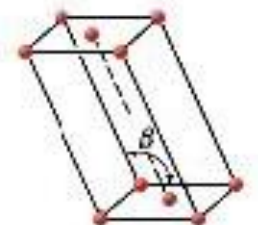
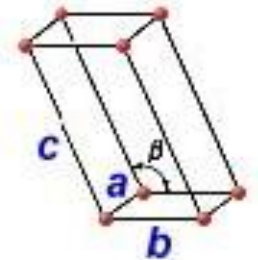
hexagonal



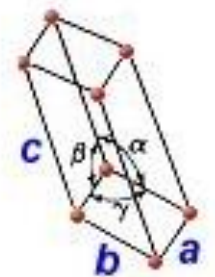
de face centrada



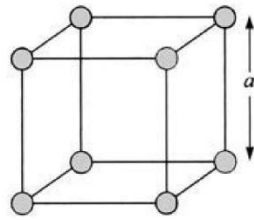
ortor-
rômbico



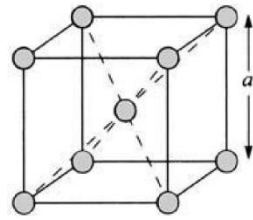
monoclinico



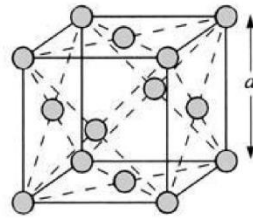
triclinico



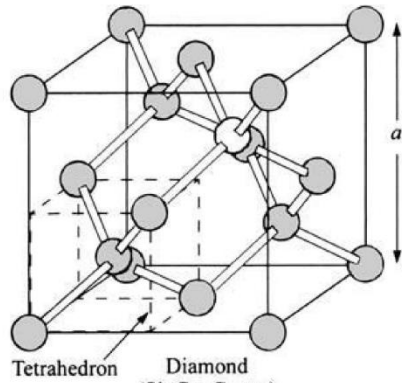
Simple cubic
(Po)
(a)



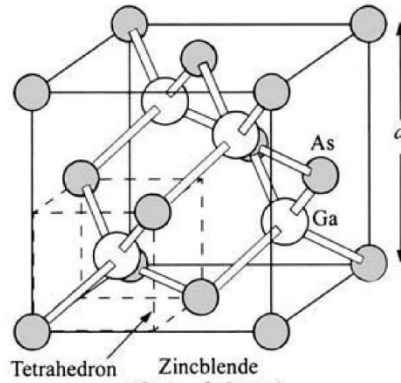
Body-centered cubic
(Na, W, etc.)
(b)



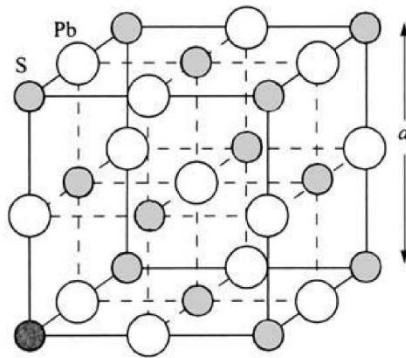
Face-centered cubic
(Al, Au, etc.)
(c)



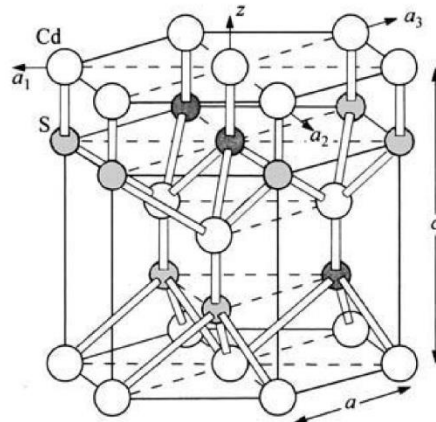
Tetrahedron
Diamond
(Si, Ge, C, etc.)
(d)



Tetrahedron
Zincblende
(GaAs, GaP, etc.)
(e)



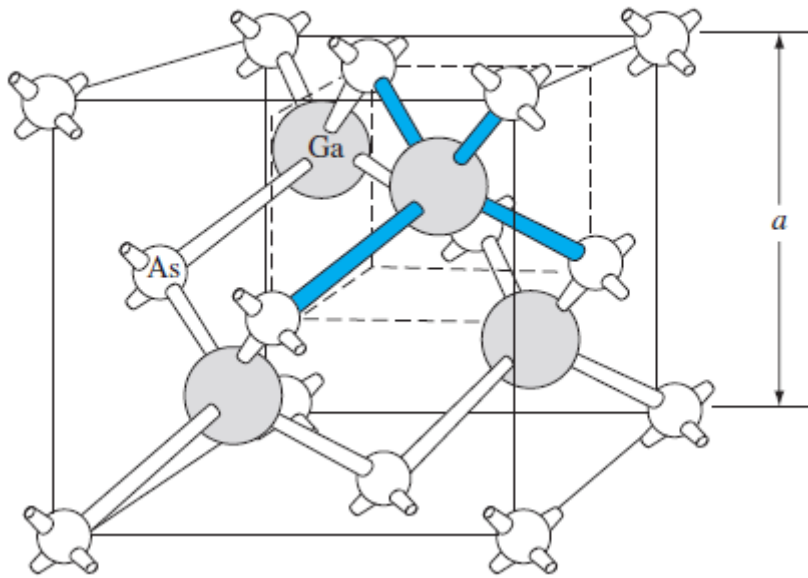
Rock-salt
(PbS, PbTe, etc.)
(f)



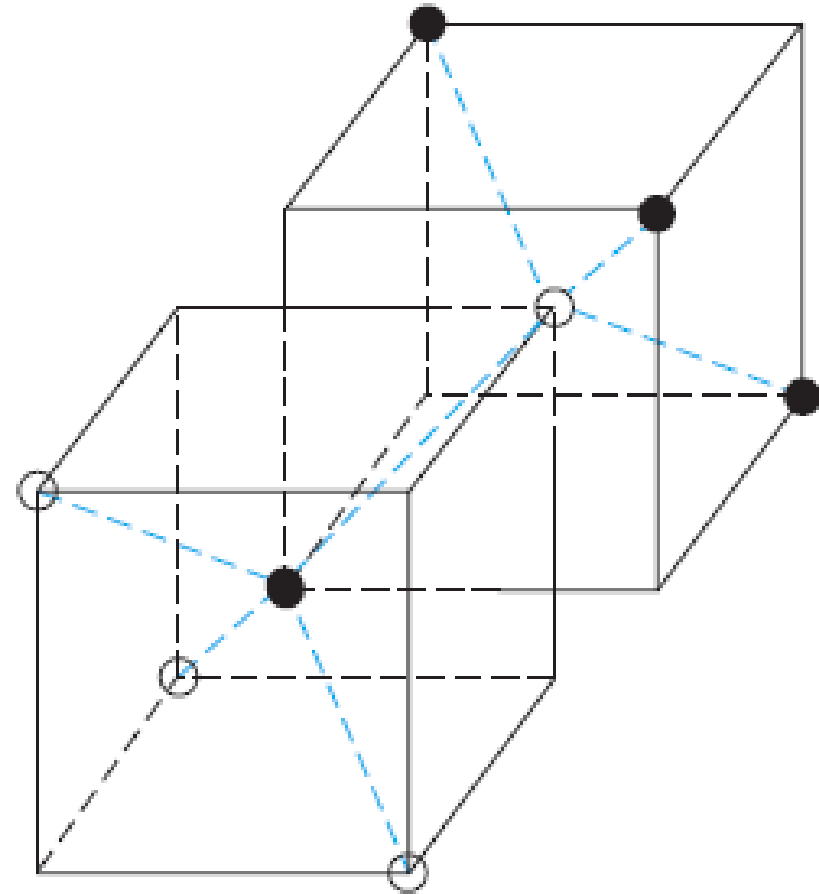
Wurtzite
(CdS, ZnS, etc.)
(g)

Semicondutores típicos

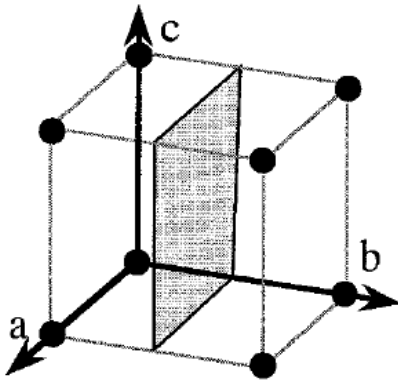
Rede Zinblend (2 átomos) ou diamante (1 átomo)



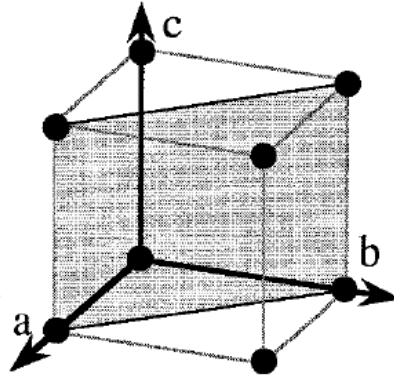
Ligações tetraédricas



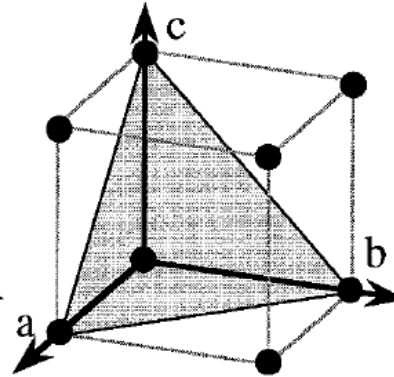
Planos e índices de Miller



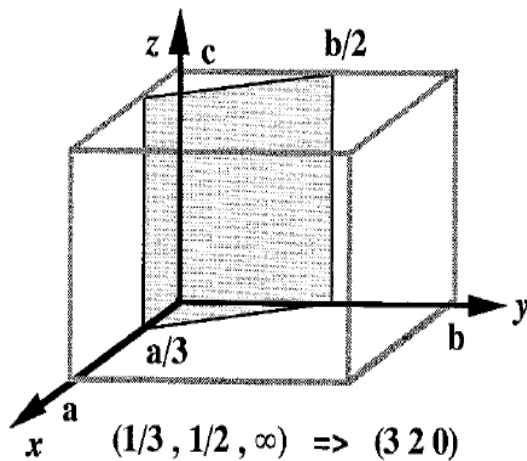
intercepts: $(-, 1/2, -)$
index: $(0\ 2\ 0)$



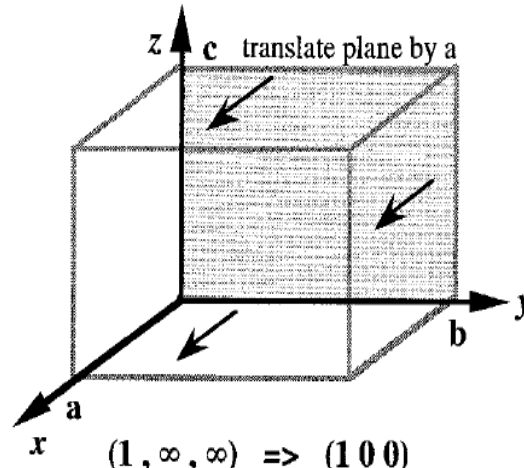
intercepts: $(1, 1, -)$
index: $(1\ 1\ 0)$



intercepts: $(1, 1, 1)$
index: $(1\ 1\ 1)$



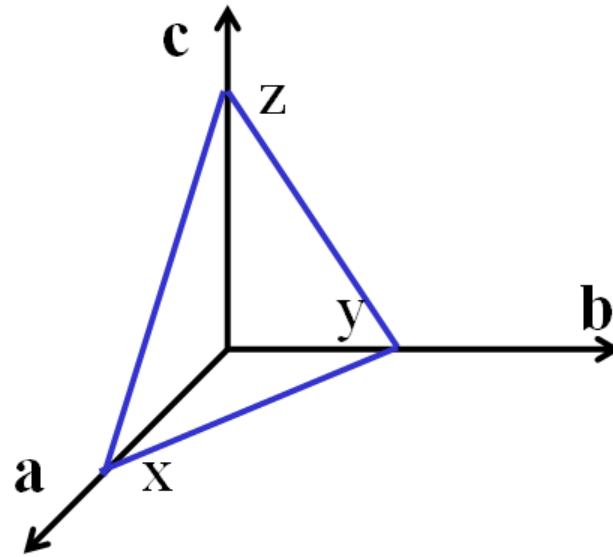
$(1/3, 1/2, \infty) \Rightarrow (3\ 2\ 0)$



$(1, \infty, \infty) \Rightarrow (1\ 0\ 0)$

- determine as intersecções com os eixos;
- determine o inverso de cada intersecção;
- determine um fator comum entre eles

Forma mais elegante (prova para os passos anteriores)



$$\vec{r}_1 = y\vec{b} - x\vec{a}; \quad \vec{r}_2 = z\vec{c} - x\vec{a}$$

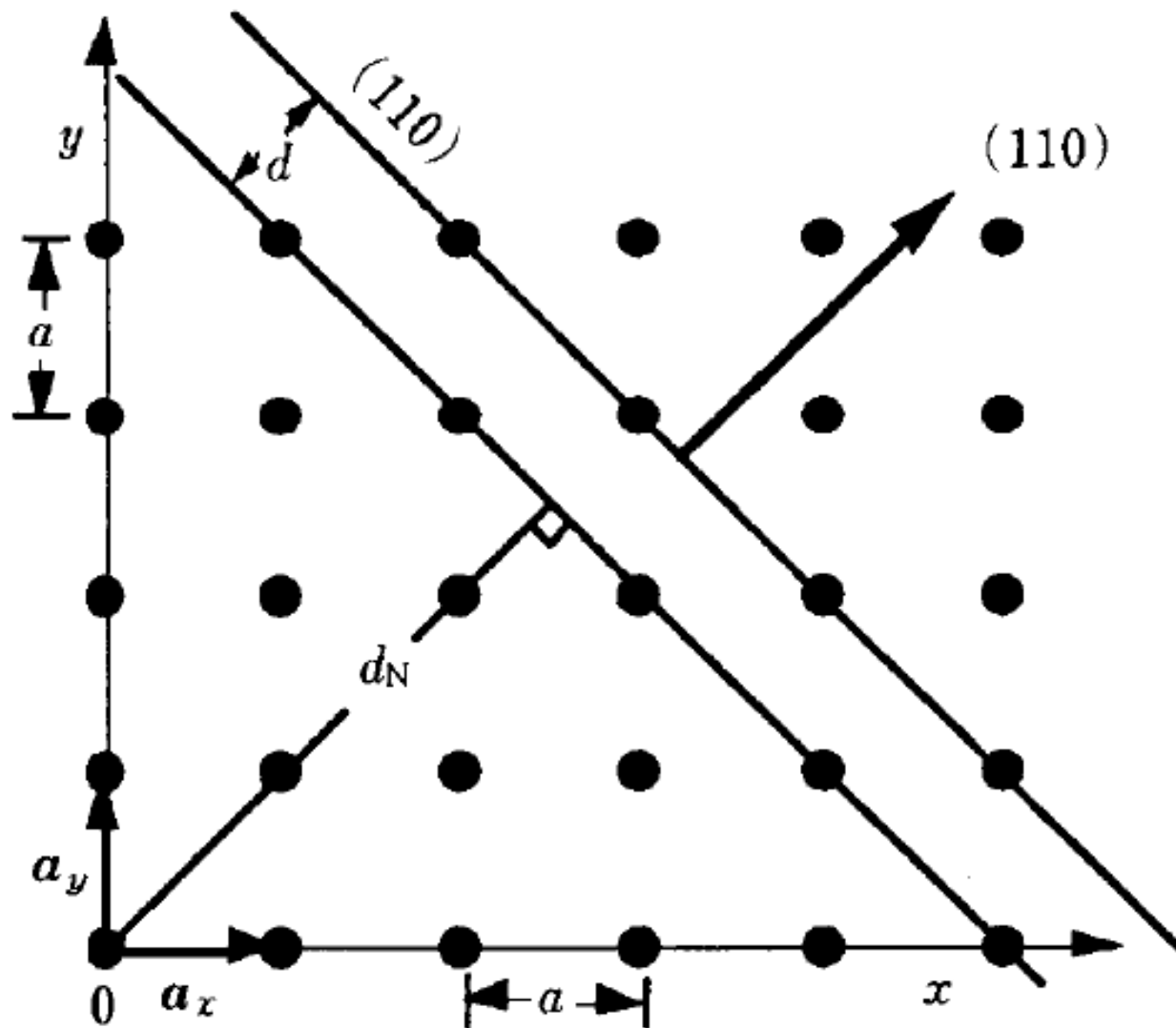
$$\vec{r}_1 \times \vec{r}_2 = \vec{a}(yz) + \vec{b}(xz) + \vec{c}(xy) \quad (\text{normal ao plano})$$

$$= xyz \left[\frac{\vec{b} \times \vec{c}}{x} + \frac{\vec{c} \times \vec{a}}{y} + \frac{\vec{a} \times \vec{b}}{z} \right] = \frac{xyz}{x} \vec{a} + \frac{xyz}{y} \vec{b} + \frac{xyz}{z} \vec{c}$$

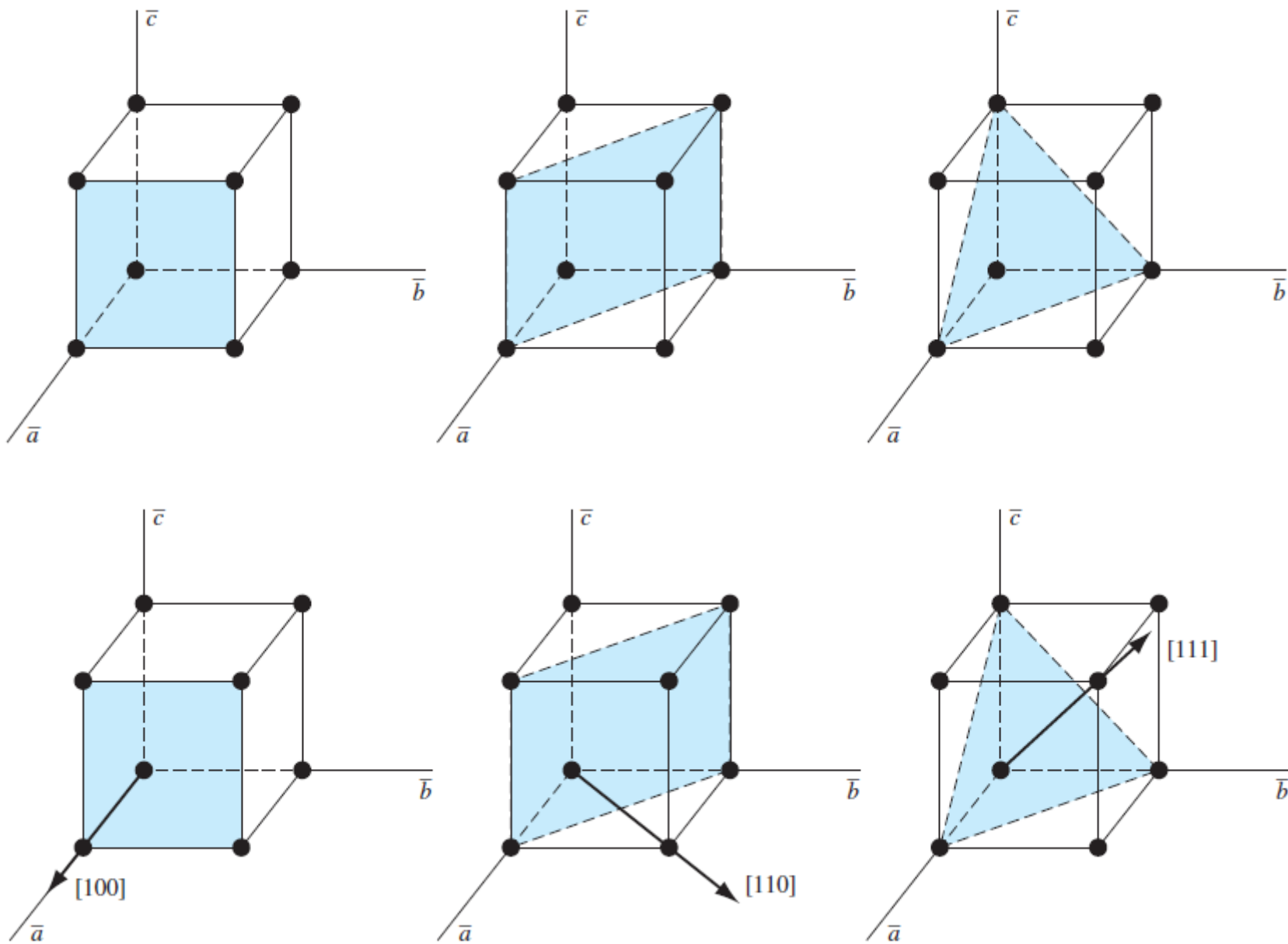
$$= A \left[\frac{1}{x} \vec{a} + \frac{1}{y} \vec{b} + \frac{1}{z} \vec{c} \right]$$

**Direção normal ao plano:
índices de Miller**

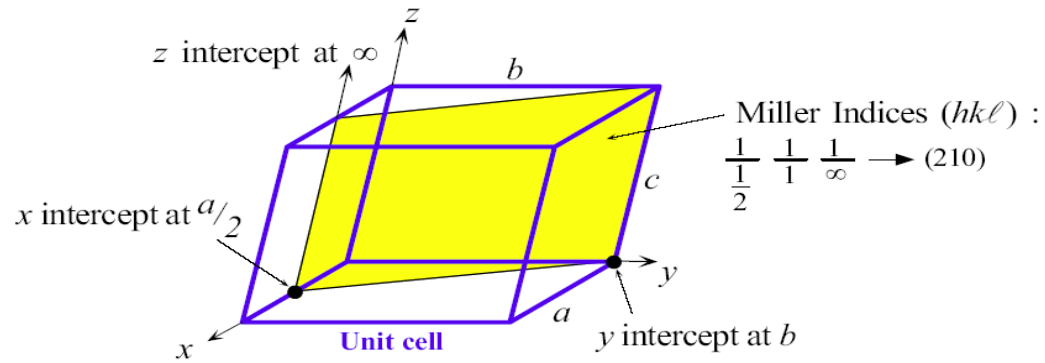
Direção normal ao plano: índices de Miller



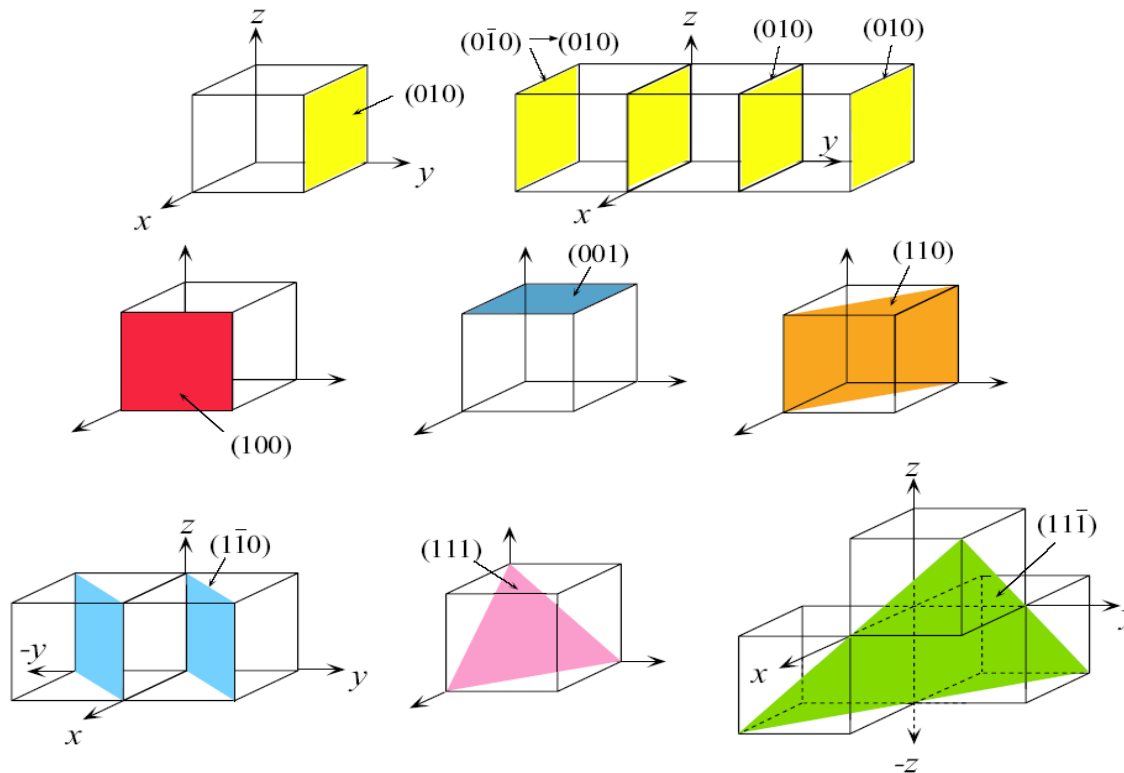
Planos e direções



Exemplos



(a) Identification of a plane in a crystal



(b) Various planes in the cubic lattice

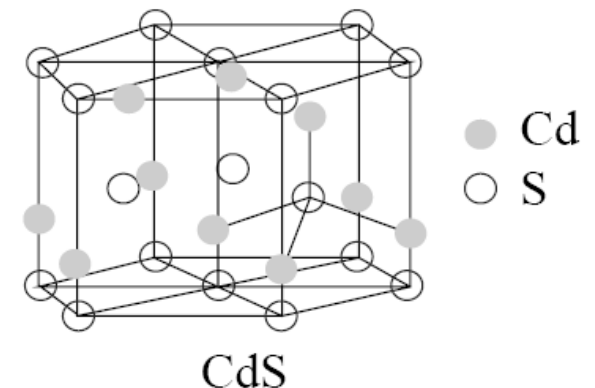
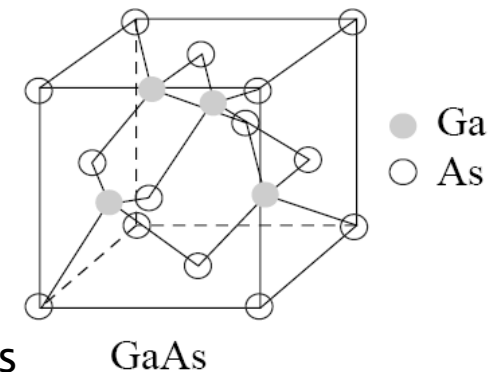
Semicondutores – Idéias gerais

Semicondutor é um isolante que possui algumas cargas livres mesmo em equilíbrio térmico. No zero absoluto um cristal semicondutor perfeito será isolante

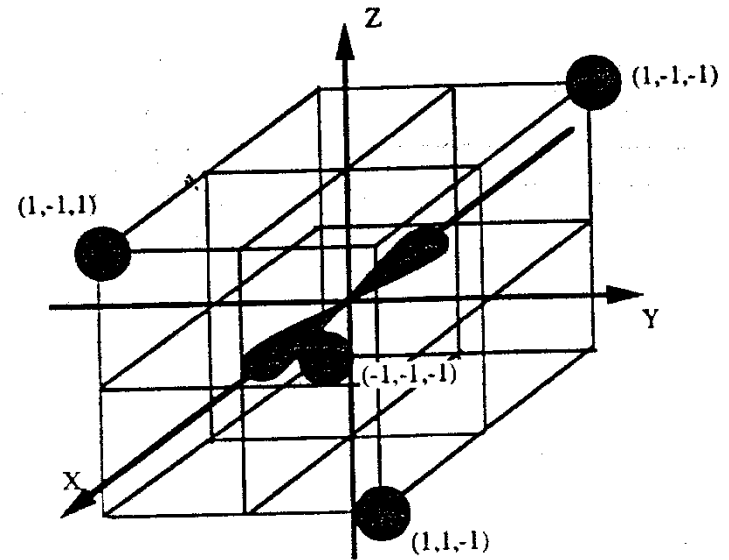
Semicondutores: Estrutura e ligações químicas

Semicondutores incluem um grande número de substâncias com diferentes propriedades químicas e físicas

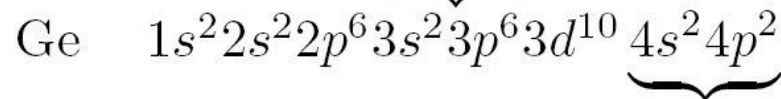
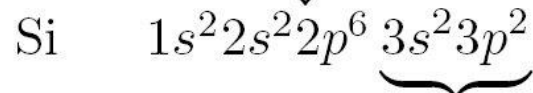
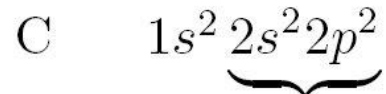
- Grupo IV – semicondutores (Si, Ge)
 - estrutura diamante (duas FCC deslocadas com átomos idênticos)
 - cristais covalentes
 - é comum a hibridização sp^3
- Grupos III–V (GaAs, InP) e II–VI (ZnSe, ZnS) – semicondutores e ligas
 - estrutura zincblend ou wurtzita hexagonal
 - covalente e polares (distribuição de elétrons não é simétrica)
- Outros compostos
 - compostos orgânicos, halogênios, calcogênios, óxidos...



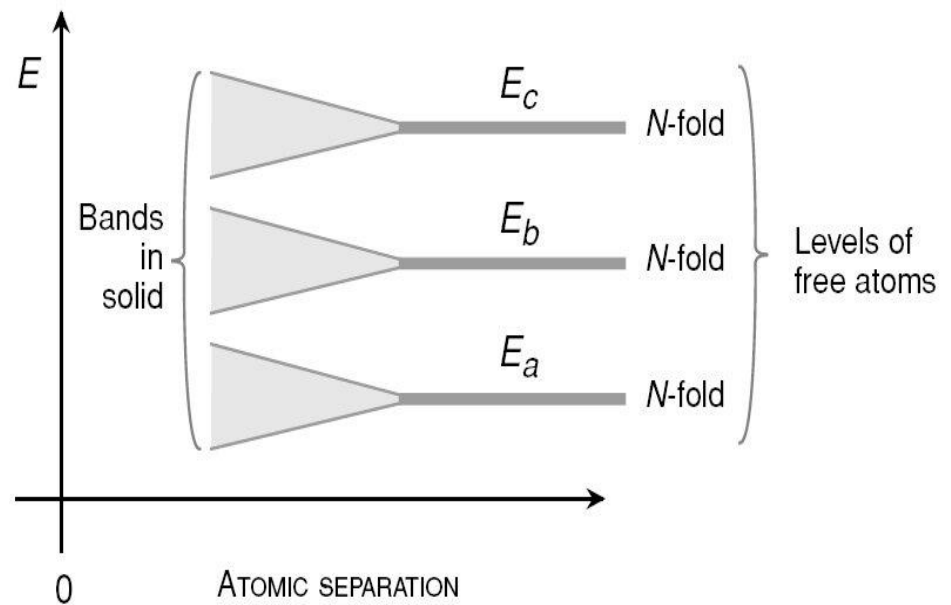
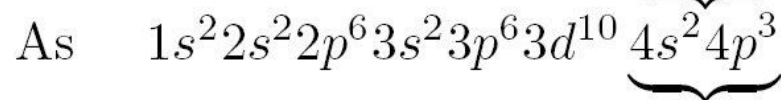
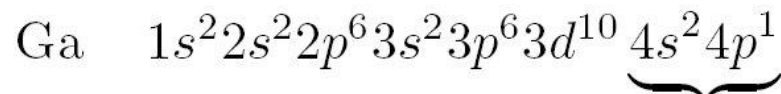
A maioria dos cristais que dão origem a semicondutores tem elétrons de valência nos orbitais s e p, que darão origem a estados estendidos com características s ou p (*como sabemos da teoria de bandas*)



IV Semiconductors



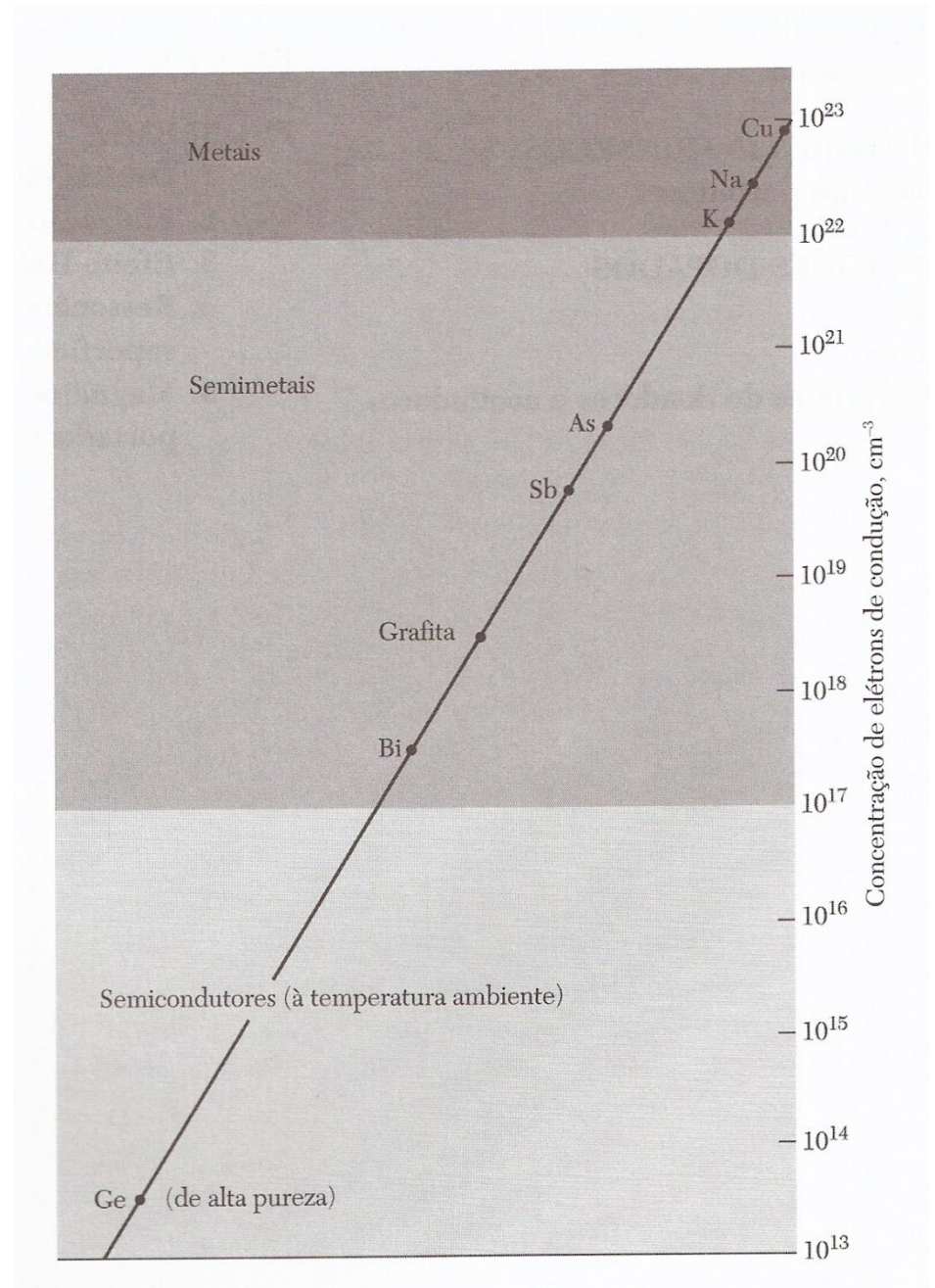
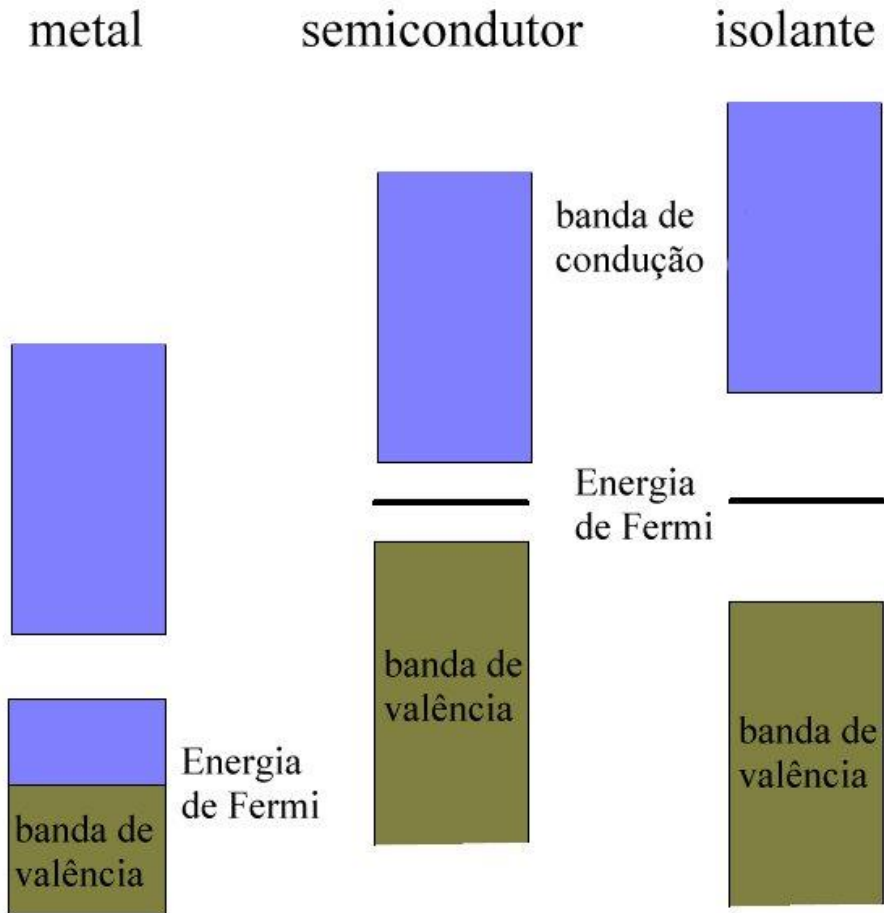
III–V Semiconductors



Configurações eletrônicas para alguns elementos

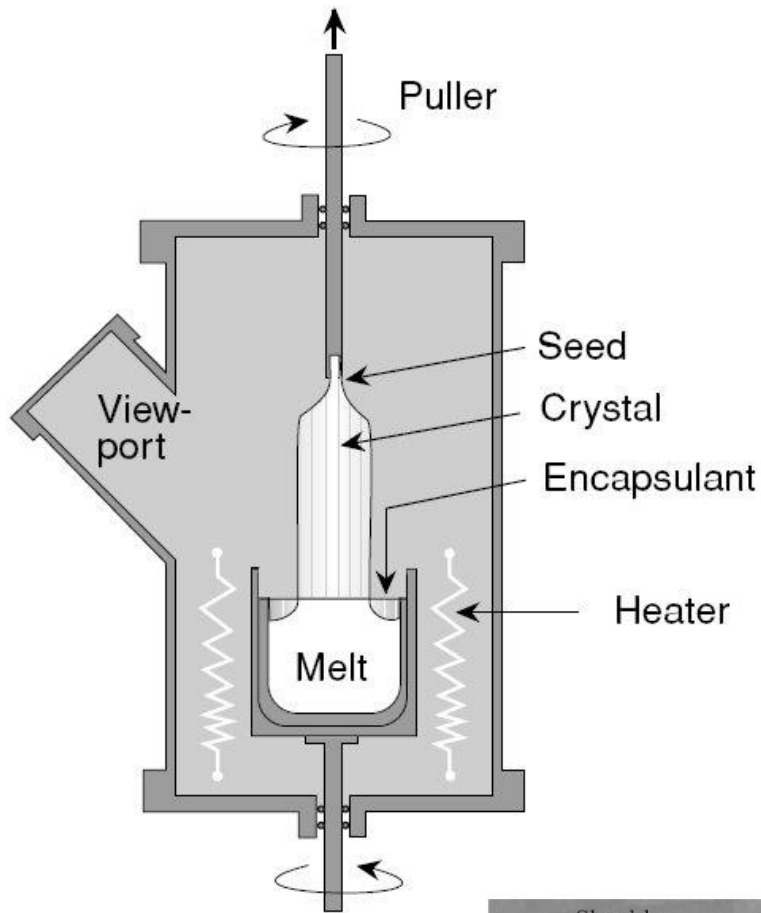
<i>Element</i>	<i>Symbol</i>	<i>Atomic Number</i>	<i>Electron Configuration</i>
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 2s^2 2p^6$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
Potassium	K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium	Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium	Sc	21	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
Titanium	Ti	22	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Vanadium	V	23	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
Chromium	Cr	24	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Manganese	Mn	25	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$

Condutores versus semicondutores



Processos de crescimento de cristais semicondutores

Método Czochraslki



$$\left(-k_l A \frac{dT}{dx} \Big|_l \right) - \left(-k_s A \frac{dT}{dx} \Big|_s \right) = L \frac{dm}{dt}$$

k_l, k_s = thermal conductivity, at the melting point, of the liquid and solid, respectively

A = boule cross-sectional area

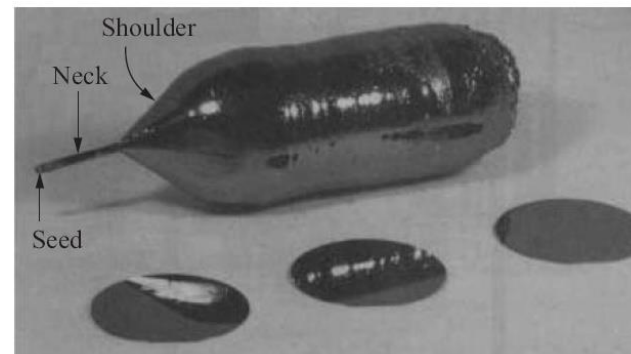
T = temperature

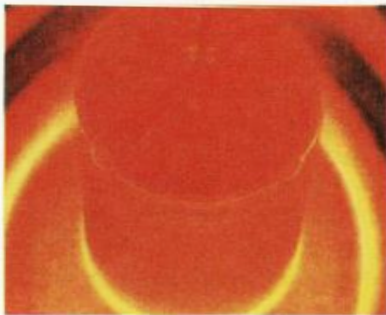
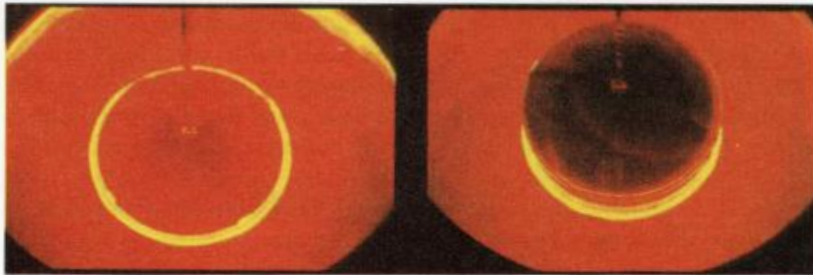
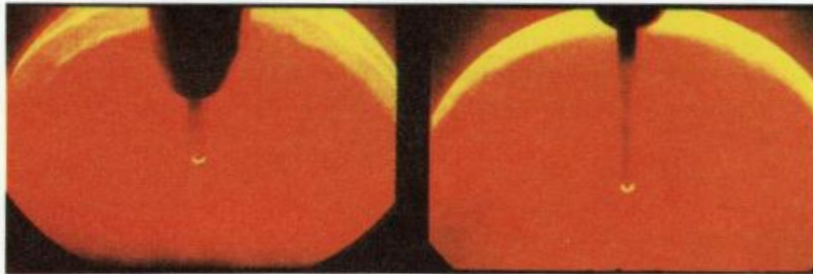
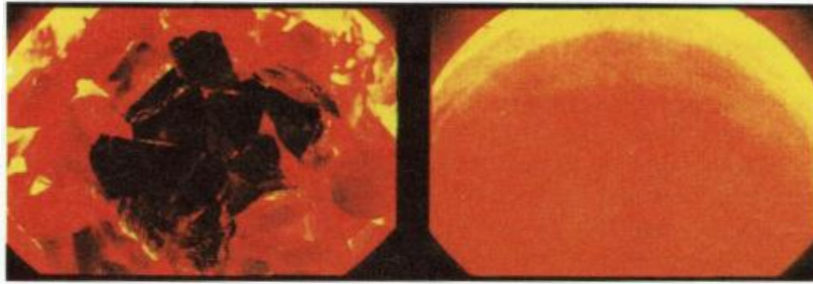
L = latent heat of fusion

m = mass of growing solid

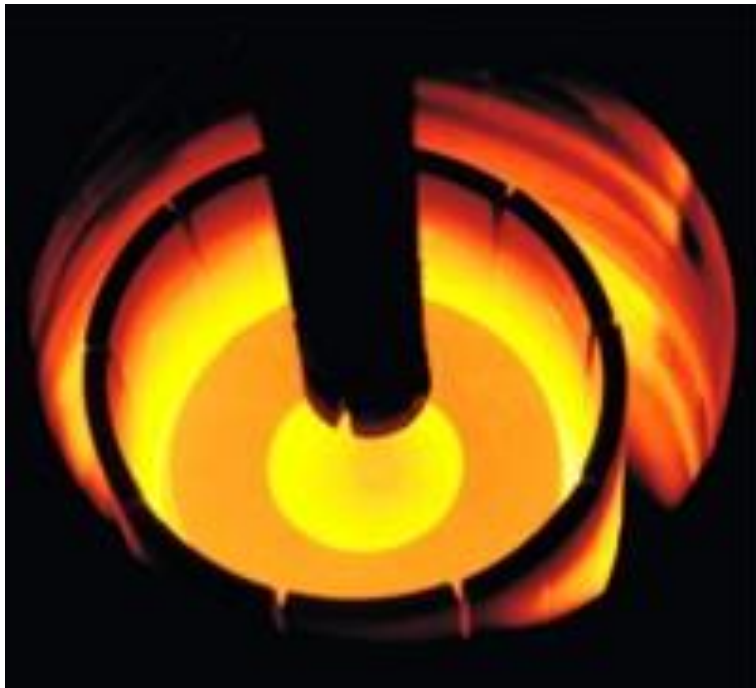
t = time

$$v_{\max} \approx \frac{k_s A dT}{L dm} = \frac{k_s}{M_v L} \frac{dT}{dx} \Big|_s$$



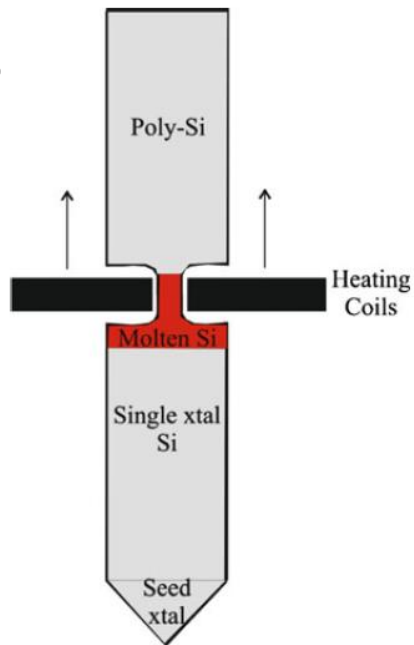


Sequencia de
produção - método
Czochralski



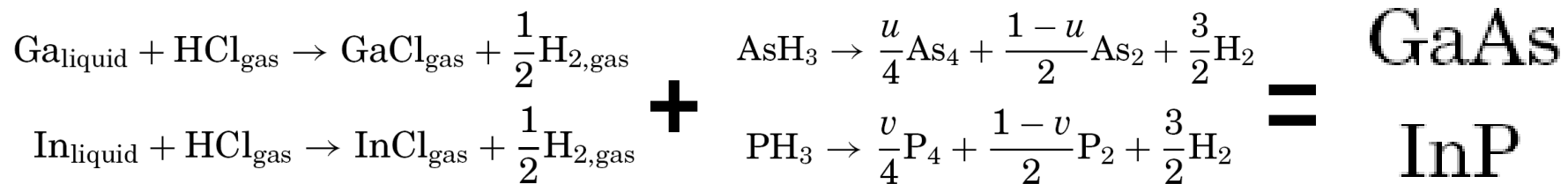
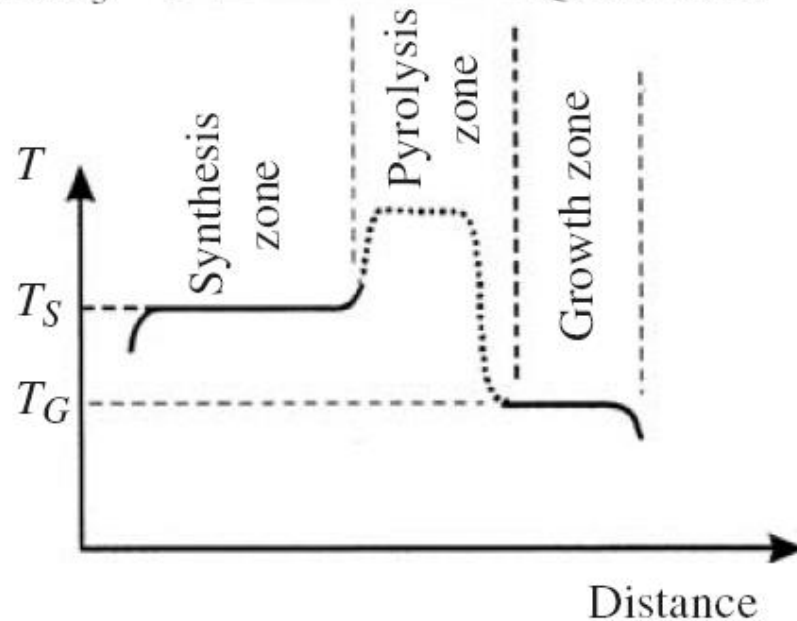
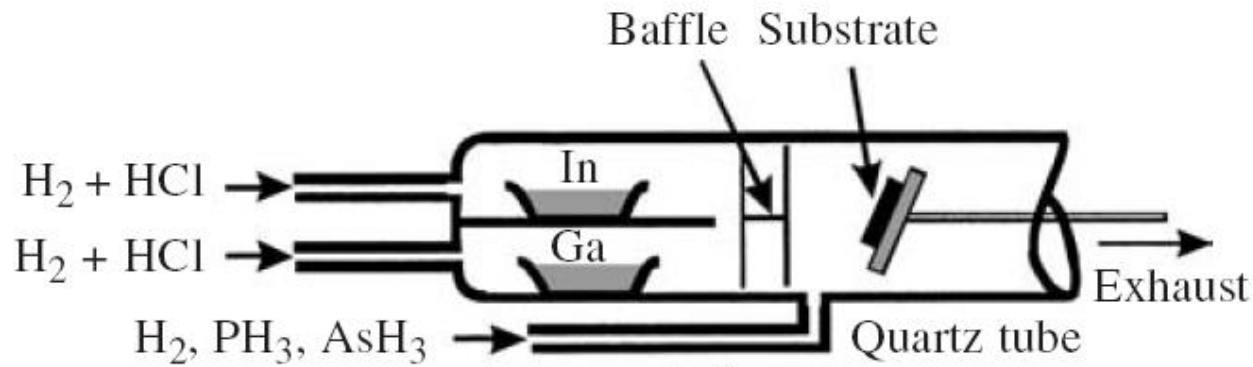
Silício em fusão

Purificação



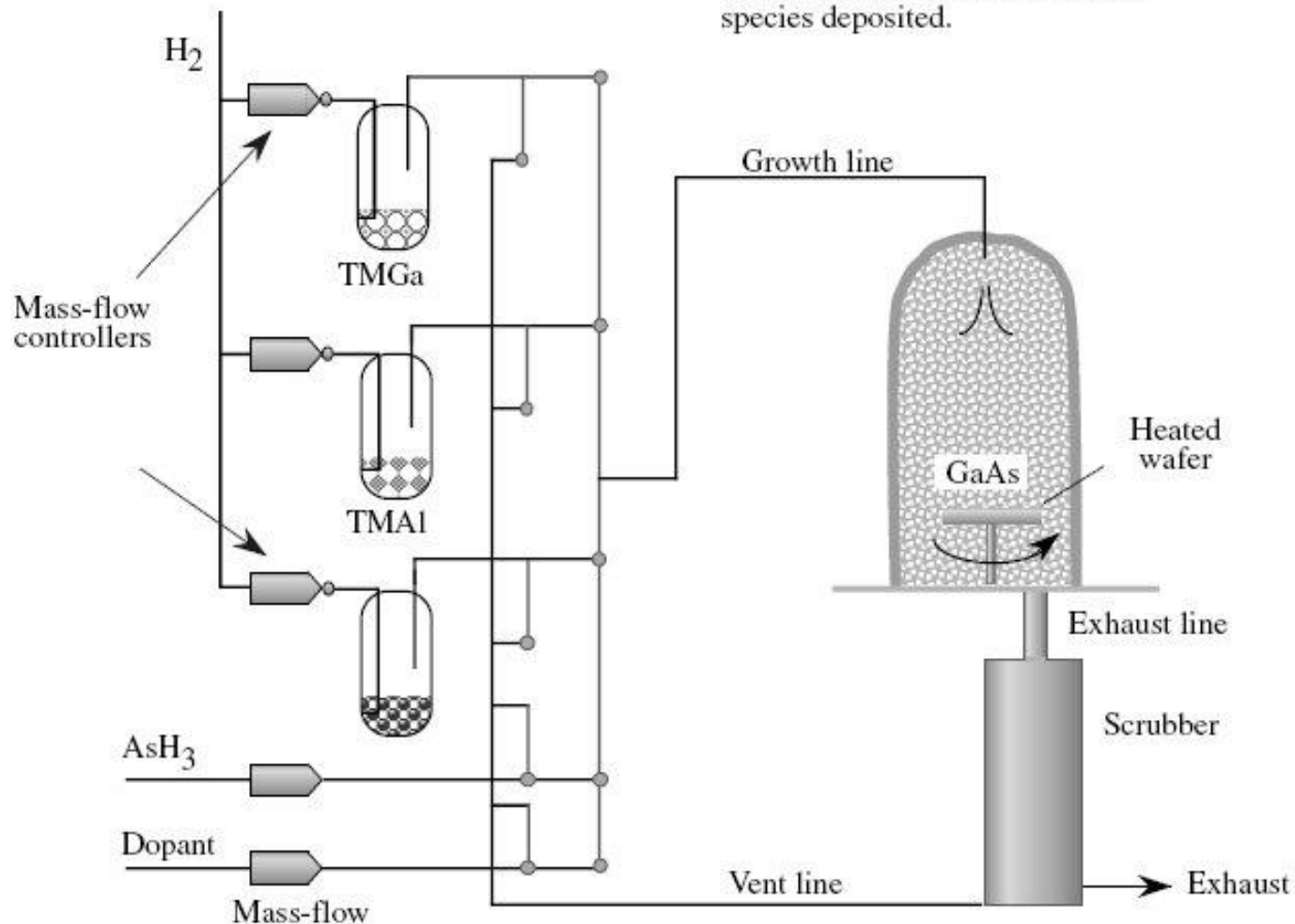
Planta industrial

VPE - Vapour phase epitaxy (*epi* = sobre ; *taxis* = arranjo)



MOCVD - Metal Organic Chemical Vapour Deposition

Chemical reaction at the heated substrate deposits GaAs or AlAs. Mass flow controllers control the species deposited.

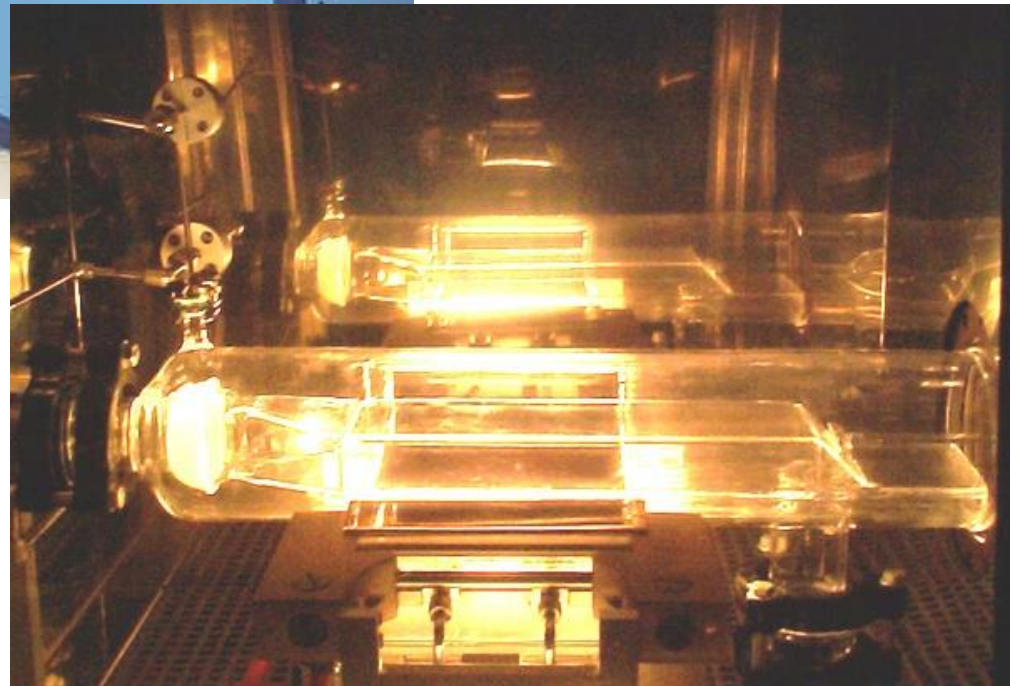


TMGa : Gallium containing organic compound
TMAI : Aluminum containing organic compound
 AsH_3 : Arsenic containing compound



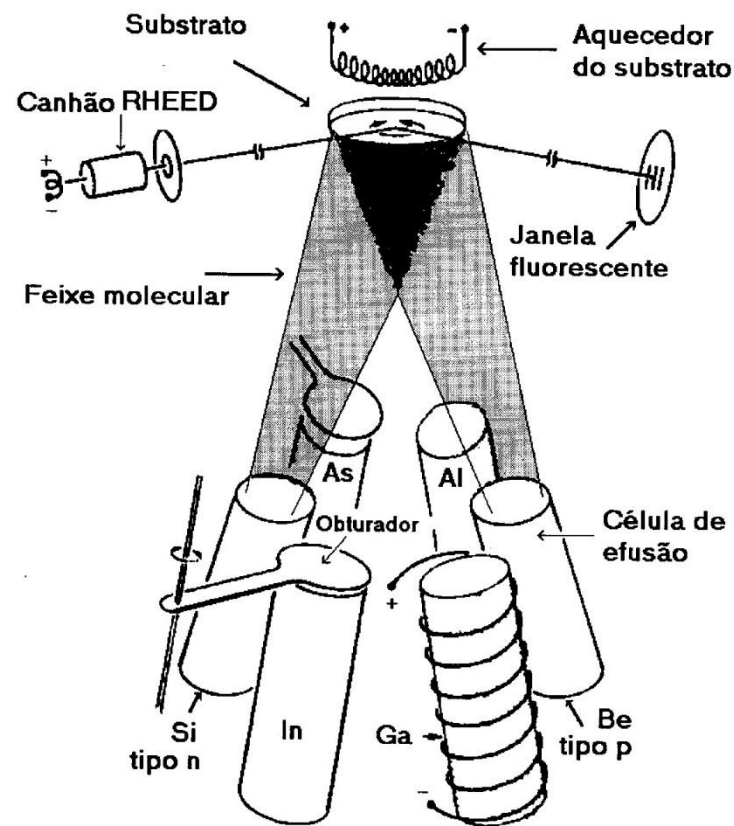
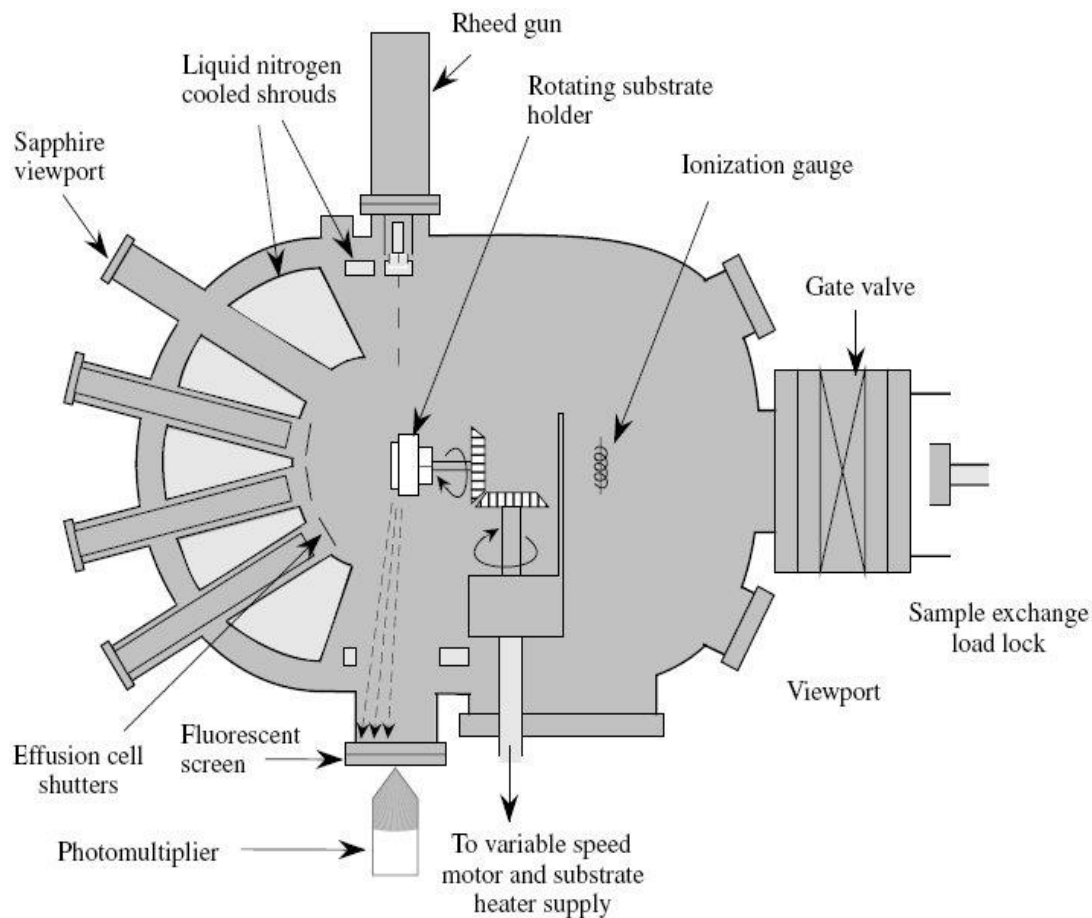
Reator MOCVD

Reator MOCVD:
câmara de síntese

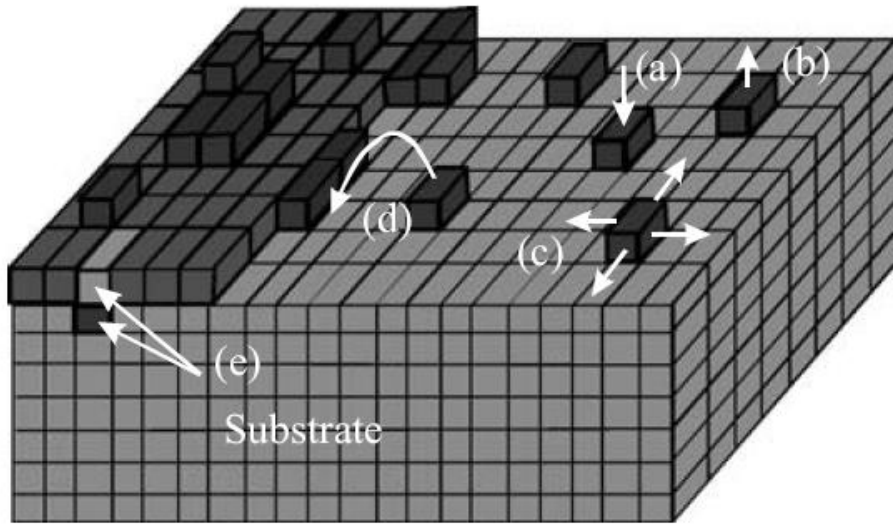


MBE- Molecular Beam Epitaxy - epitaxia por feixes moleculares

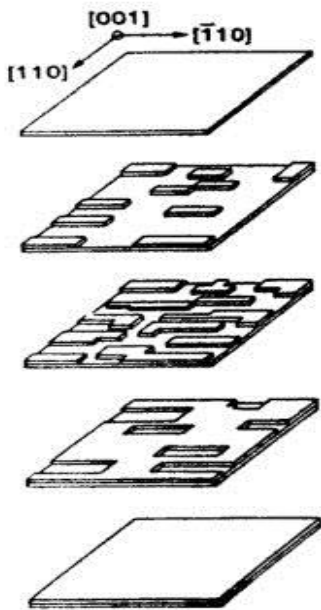
Epi = sobre; taxis = arranjo



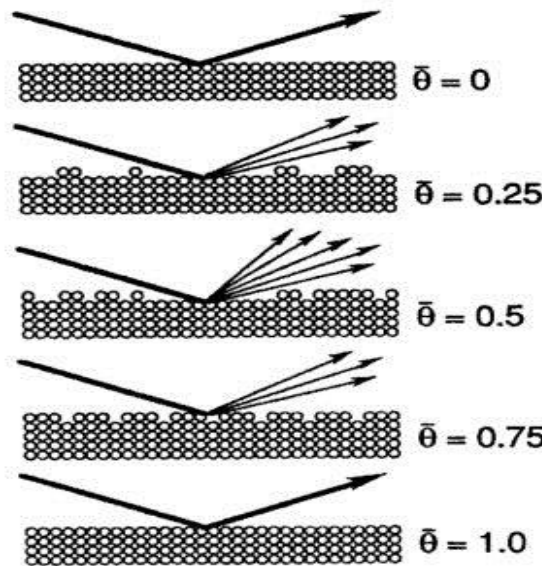
Construção controlada, camada por camada atômica !!!



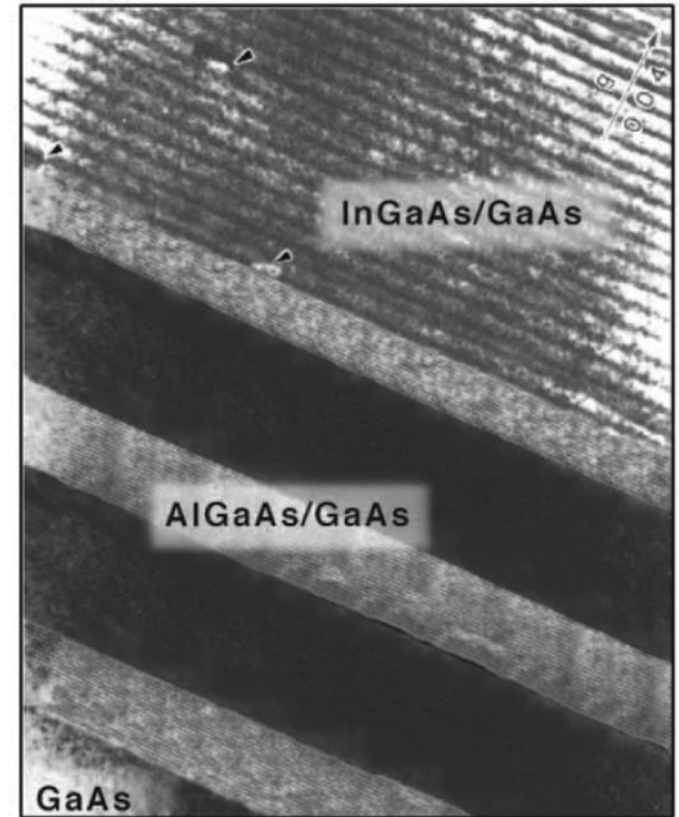
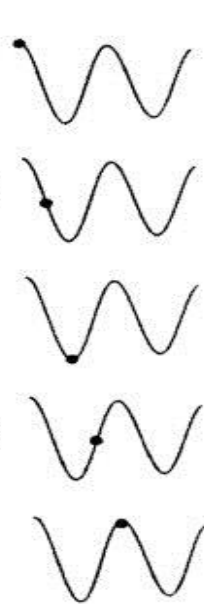
MONOLAYER GROWTH



ELECTRON BEAM



RHEED SIGNAL

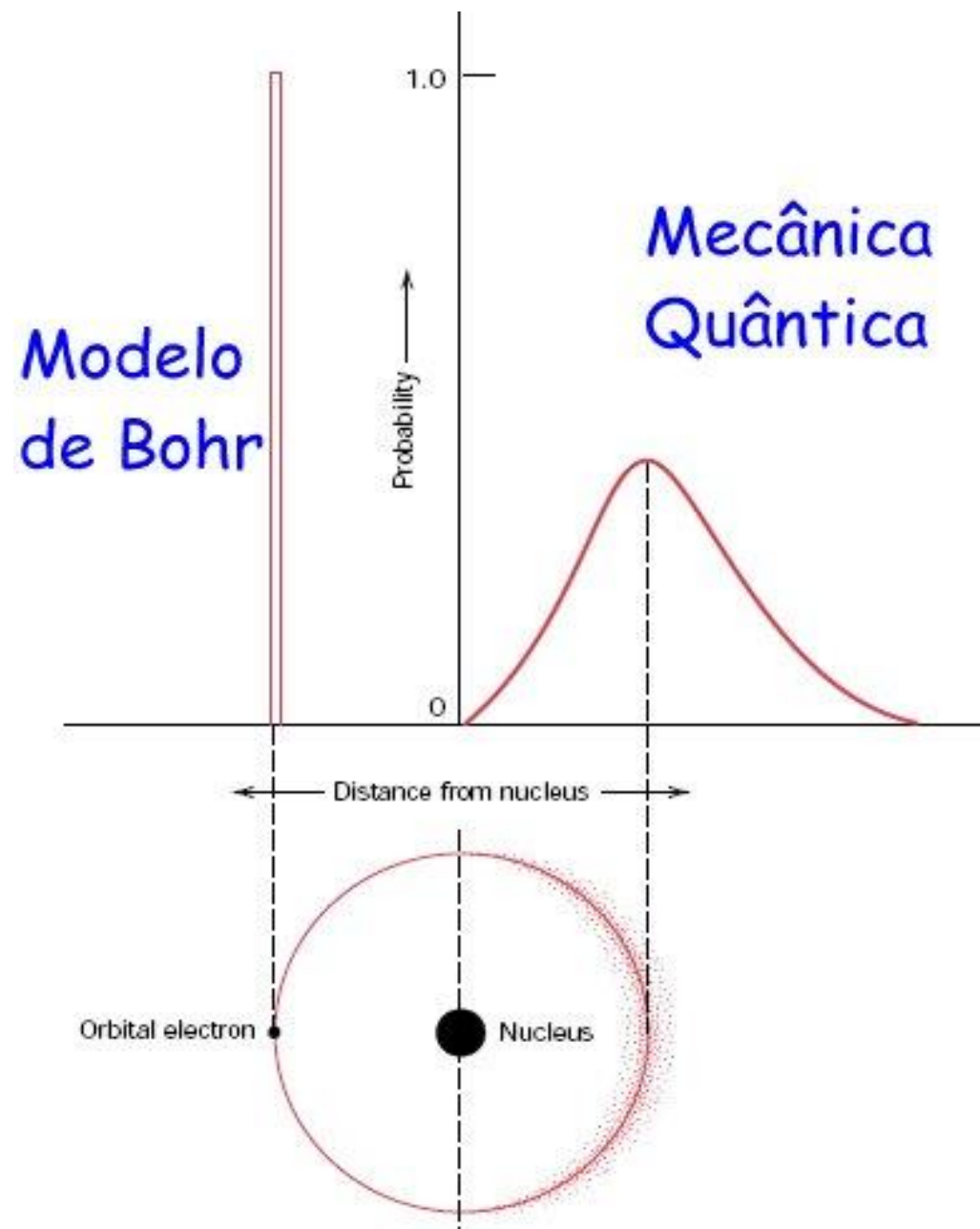


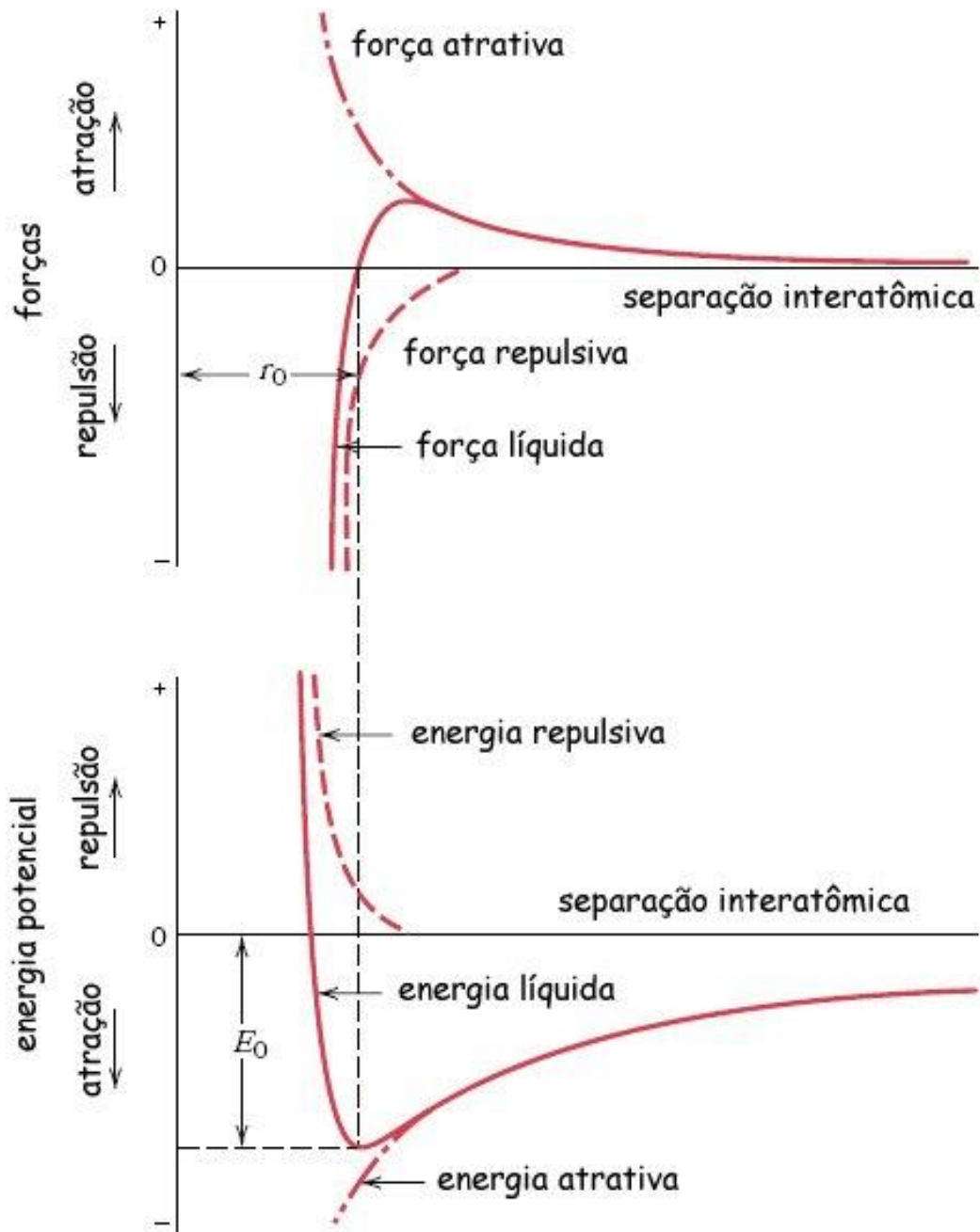
... camada por camada atômica !!!



Ligações químicas

Ligações Químicas: a base para a formação de sólidos



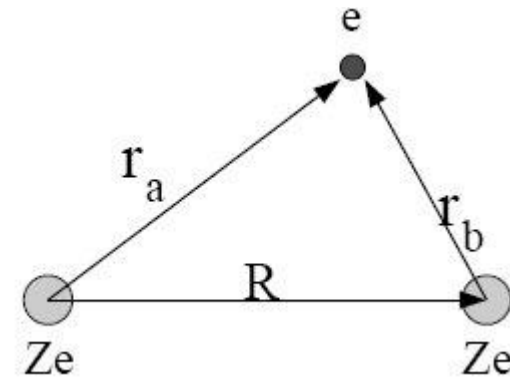


Esquema de interação entre forças em uma molécula e sua relação com a energia potencial

Ligações covalentes

Considere uma molécula de O_2 : o hamiltoniano correspondente às interações será

$$H = -\frac{\nabla^2}{2m} - \frac{Ze^2}{r_a} - \frac{Ze^2}{r_b} + \frac{Z^2e^2}{R}$$



Solução variacional para o problema de auto-valores $H\Psi_{mol} = E\Psi_{mol}$ construindo uma autofunção variacional (*tentativa*) para os orbitais atômicos dos dois átomos

Função variacional e energia correspondente (a melhor escolha de Ψ' minimiza E')

$$\Psi' = c_a\psi_a + c_b\psi_b$$

$$E' = \frac{\int \Psi'^* H \Psi'}{\int \Psi'^* \Psi'} \geq E$$

Definindo

$$S = \int \psi_a^* \psi_b \quad H_{aa} = H_{bb} = \int \psi_a^* H \psi_a \quad H_{ab} = \int \psi_a^* H \psi_b$$

S: integral de “superposição” (0 até 1)

Encontramos

$$E' = \frac{(c_a^2 + c_b^2)H_{aa} + 2c_a c_b H_{ab}}{c_a^2 + c_b^2 + 2c_a c_b S}$$

que deve ser minimizada, ou seja, $\frac{\partial E'}{\partial c_a} = \frac{\partial E'}{\partial c_b} = 0$

e considerando as duas derivadas anteriores,

$$\begin{cases} c_a(H_{ab} - E'S) + c_b(H_{aa} - E') = 0 \\ c_a(H_{aa} - E') + c_b(H_{ab} - E'S) = 0 \end{cases}$$

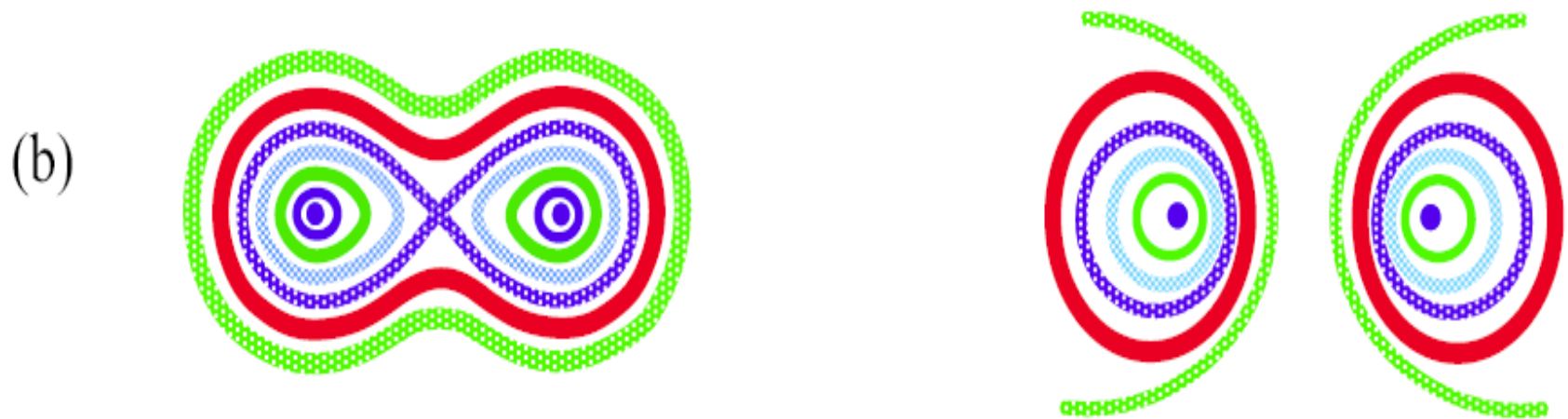
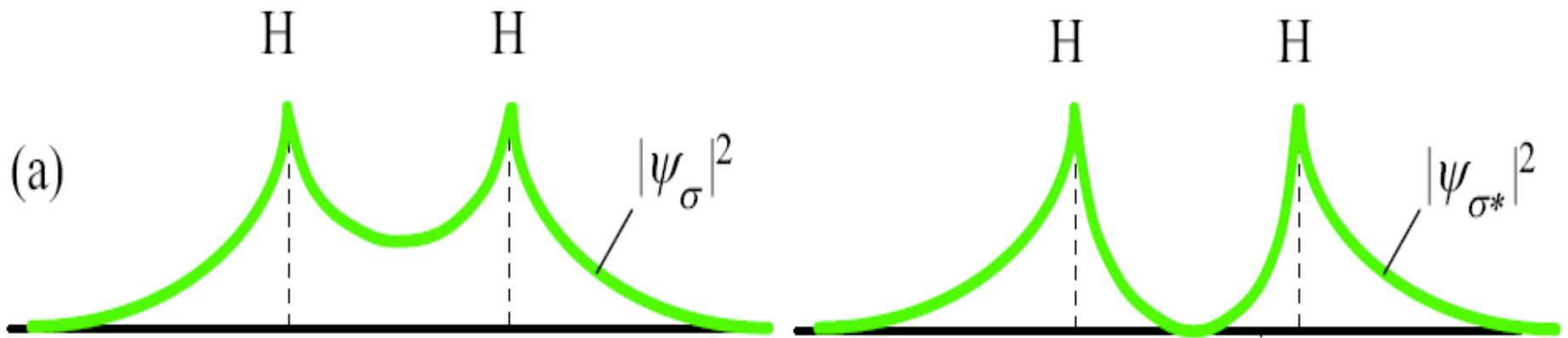
Finalmente, $E' = \frac{H_{aa} \pm H_{ab}}{1 \pm S}$, e tomando uma das soluções,

$$c_a = c_b = 1/\sqrt{2}$$



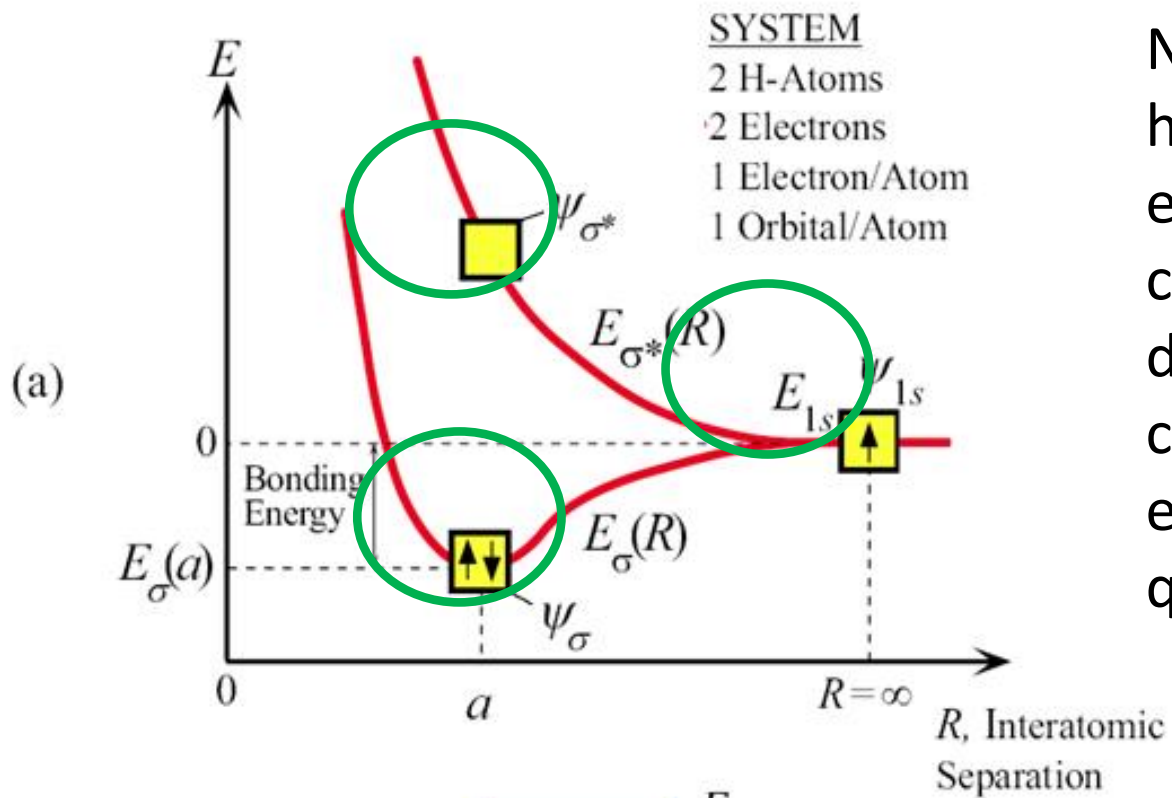
$$\Psi'_{bonding} = \frac{1}{\sqrt{2}} (\psi_a + \psi_b)$$

$$E'_{bonding} = \frac{H_{aa} + H_{ab}}{1 + S}$$

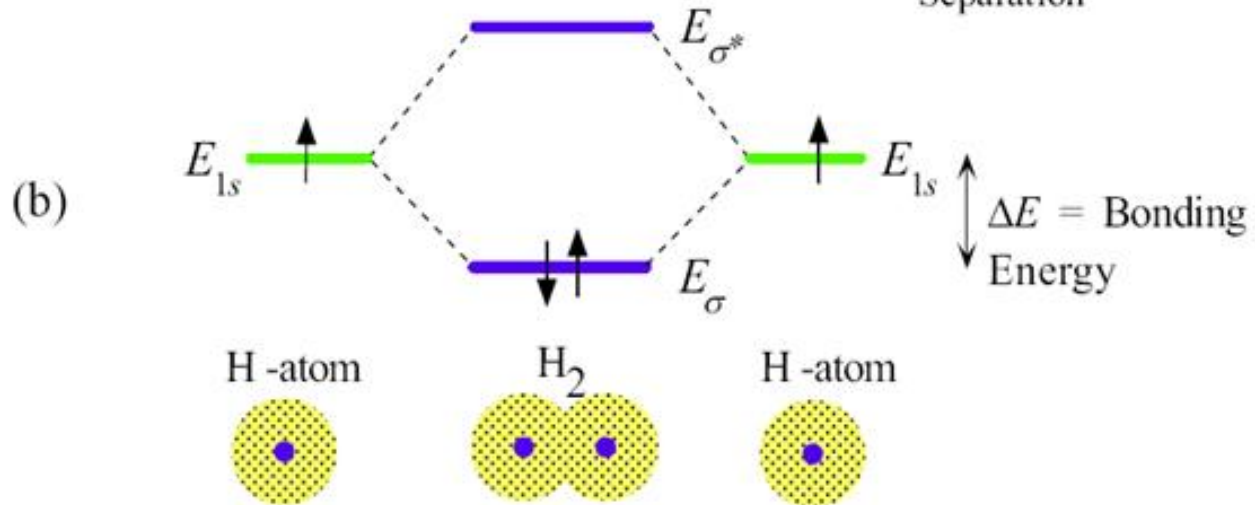


(a) Probabilidade dos estados ligados e não ligados em uma molécula de H_2

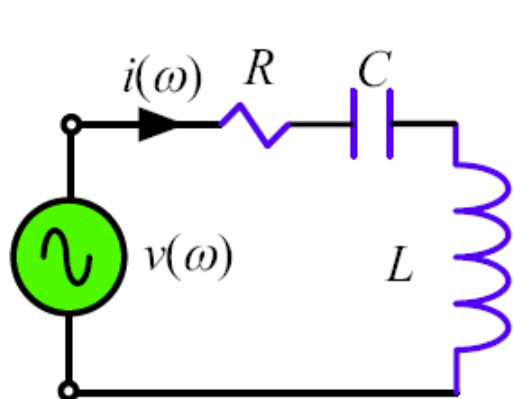
(b) Contornos de probabilidade constante



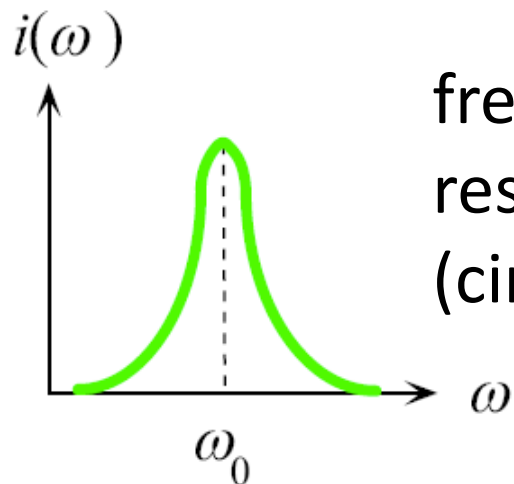
Na distância de equilíbrio há a formação da molécula e como o orbital ligado comporta os dois elétrons do sistema, esta configuração é a mais estável (menor energia que quando separados)



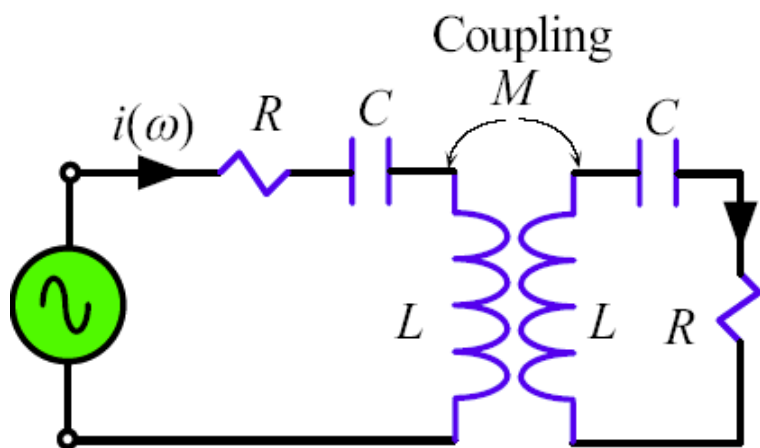
Analogia entre a molécula de H₂ e um circuito ressonante RLC



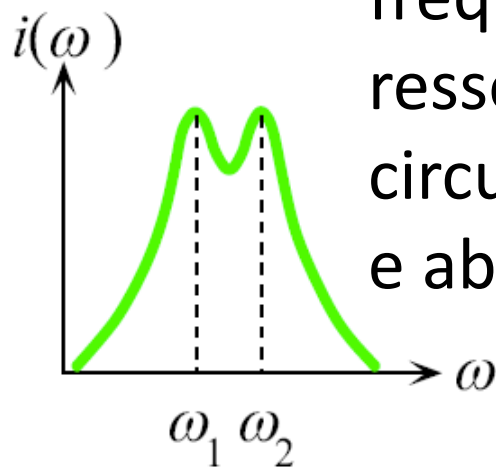
(a)



freqüência de ressonância, ω_0
(circuito RLC isolado).

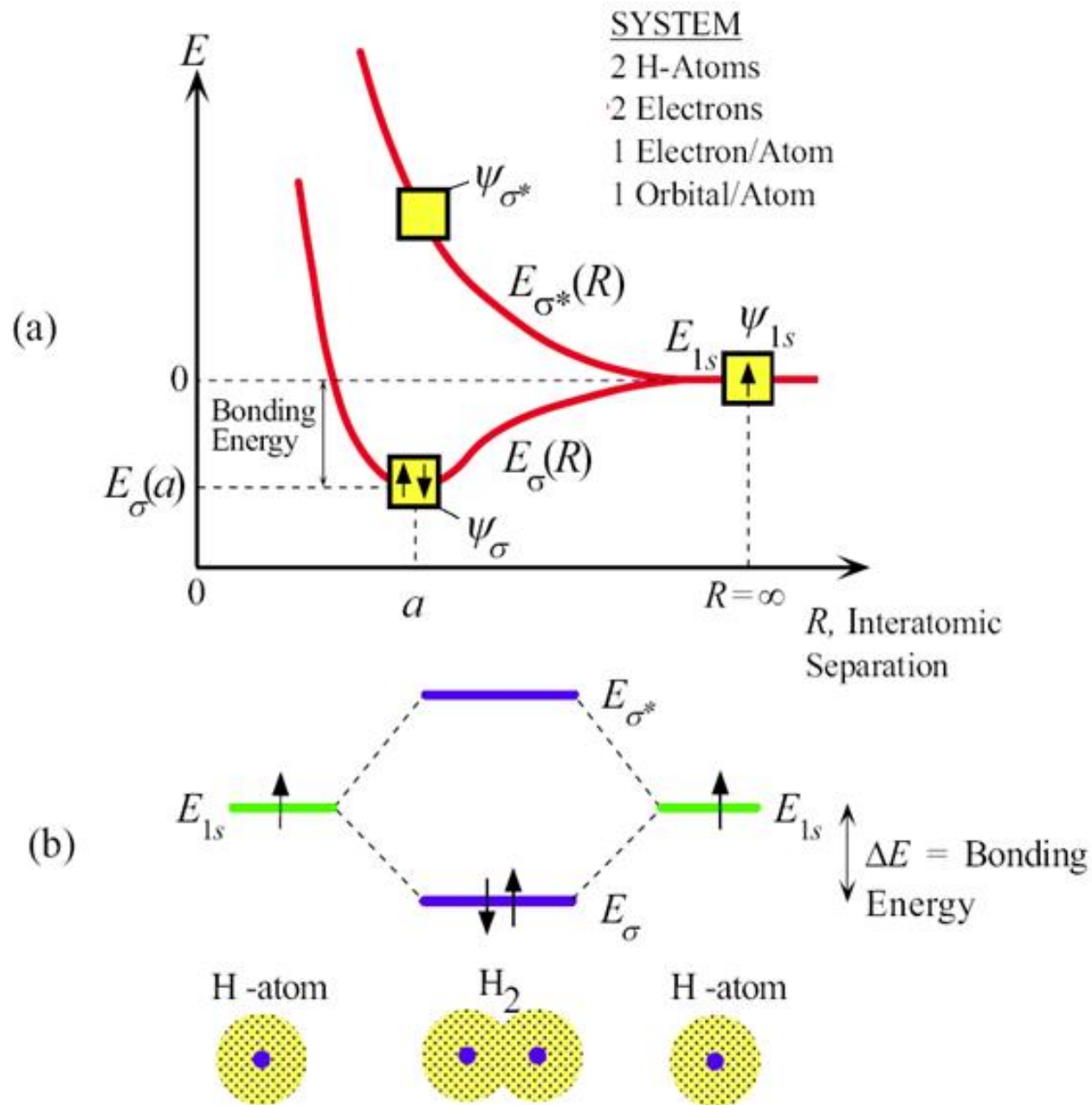


(b)

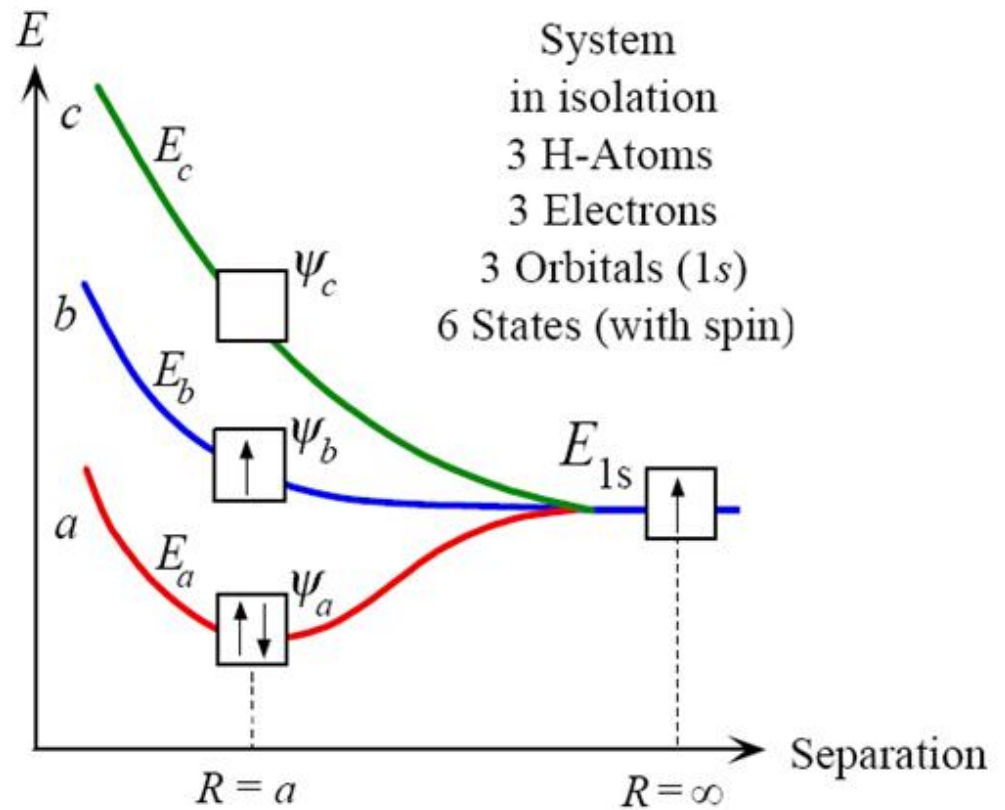
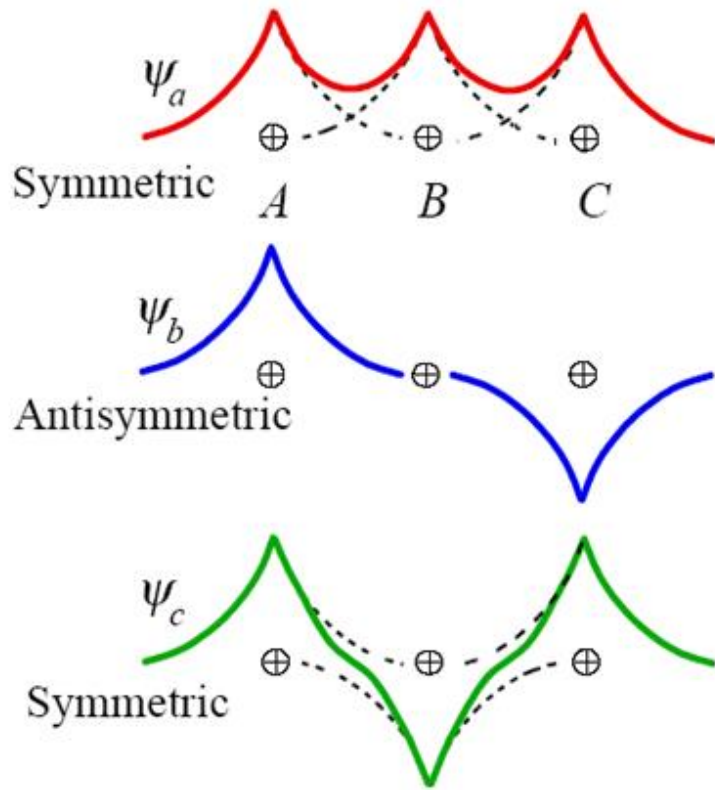


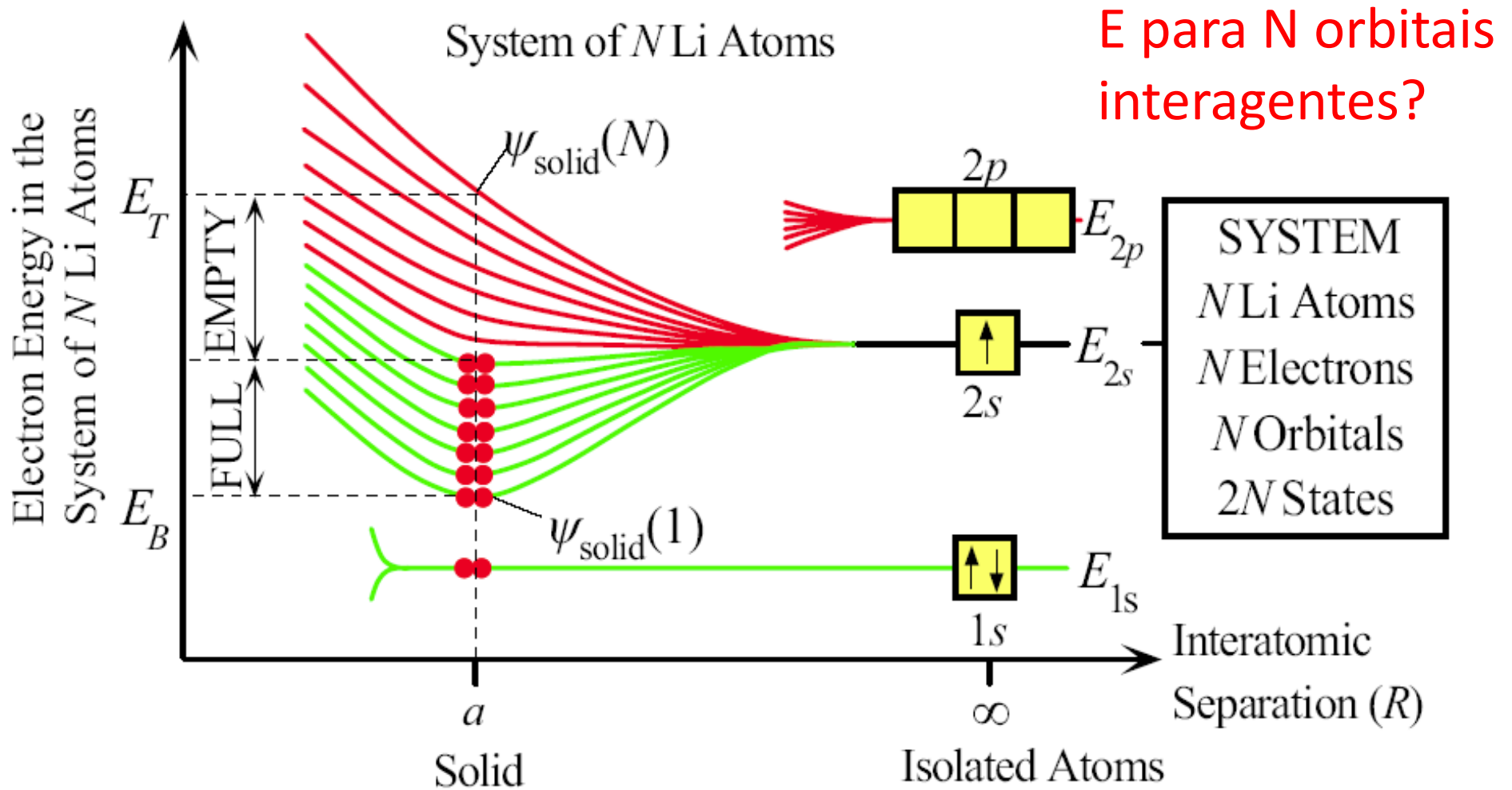
freqüências de ressonância, para dos circuito acoplados (acima e abaixo de ω_0)

Ligações covalentes



E para três orbitais interagentes?

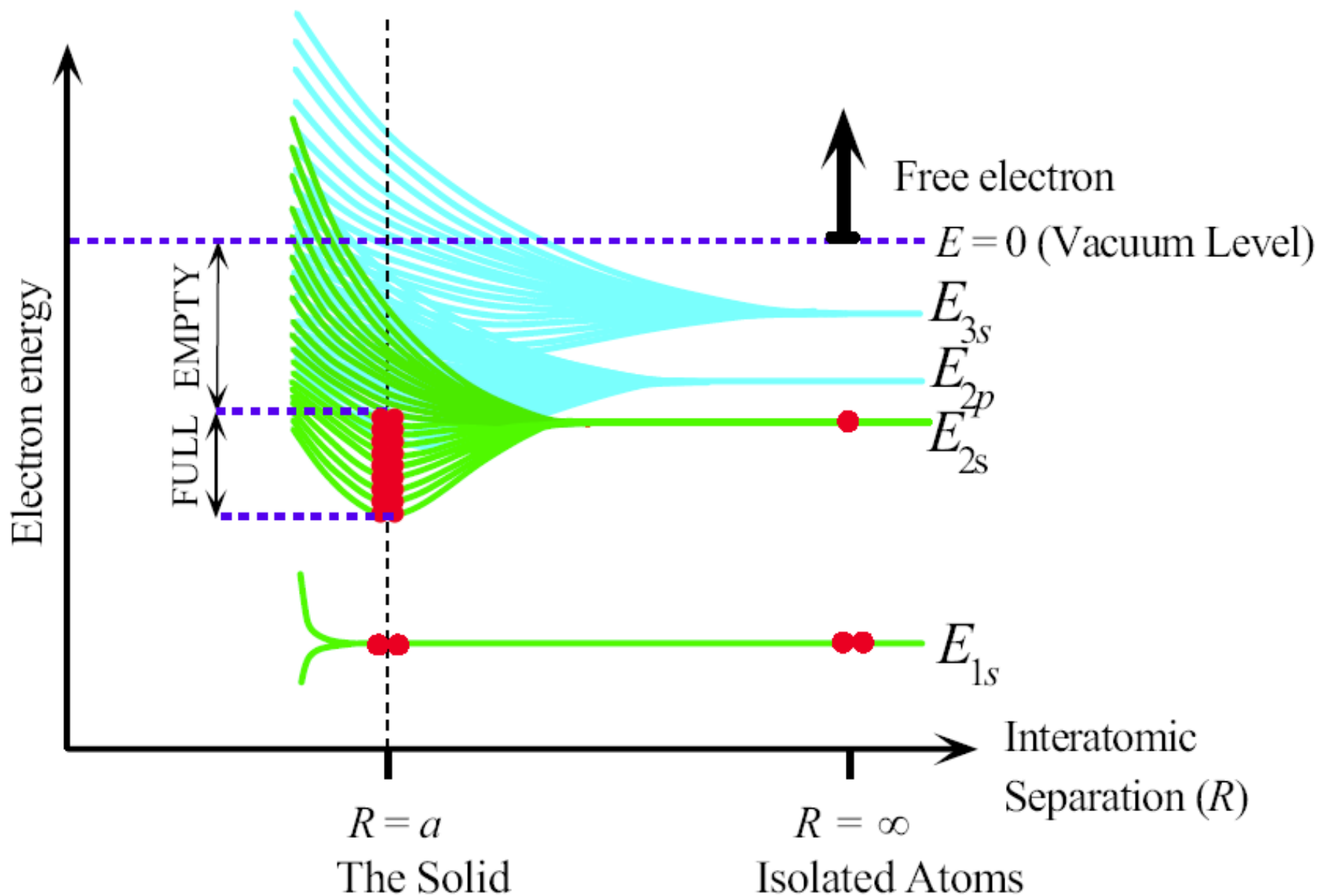


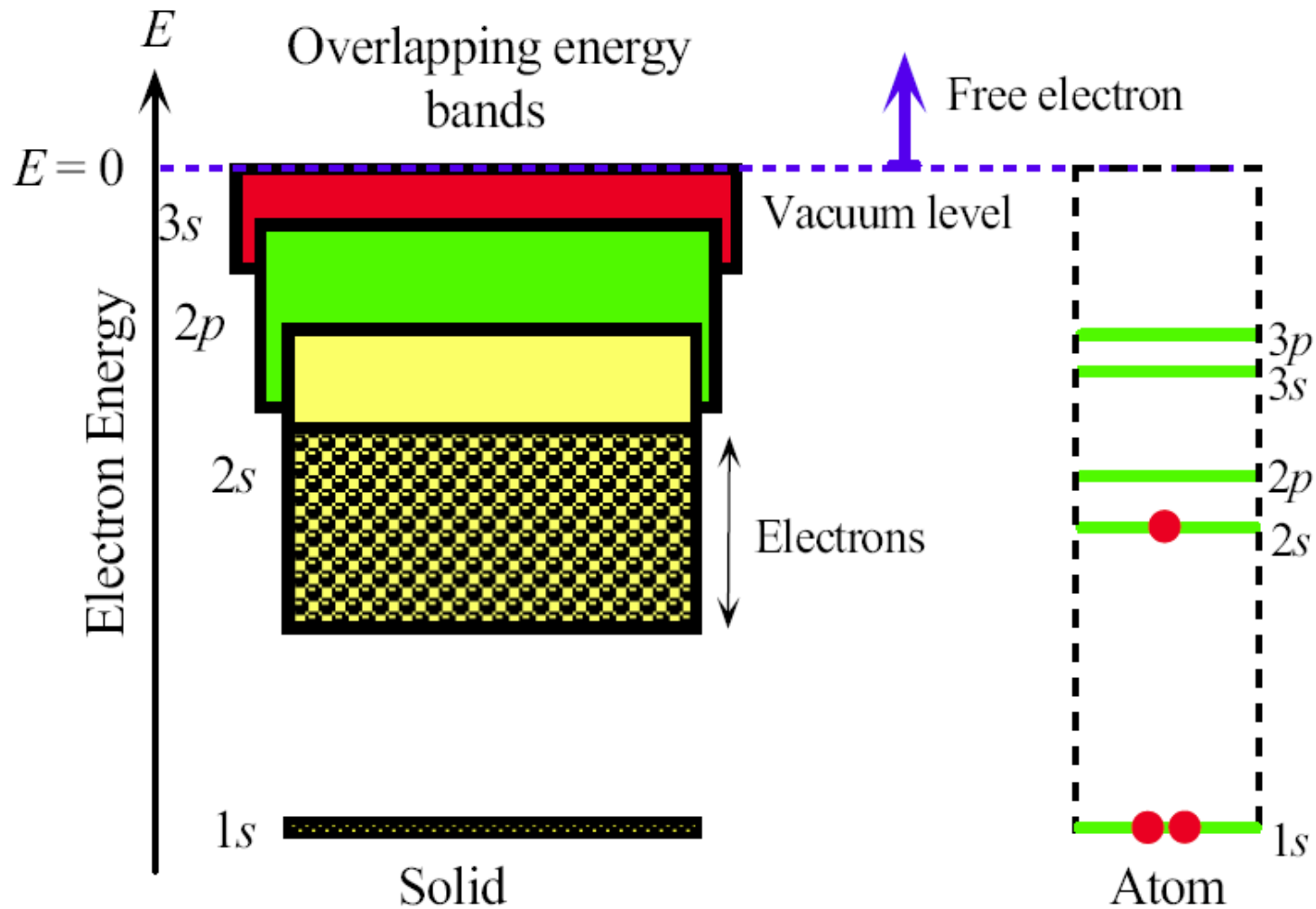


Formação da banda 2s devido aos orbitais 2s quando N átomos de Li se aproximam formando o Li sólido. Existem N 2s elétrons e N estados na banda (ocupação parcial). Observem que a camada 1s não é perturbada.

Obs: $\text{Li} \rightarrow 1s^2 2s^1$

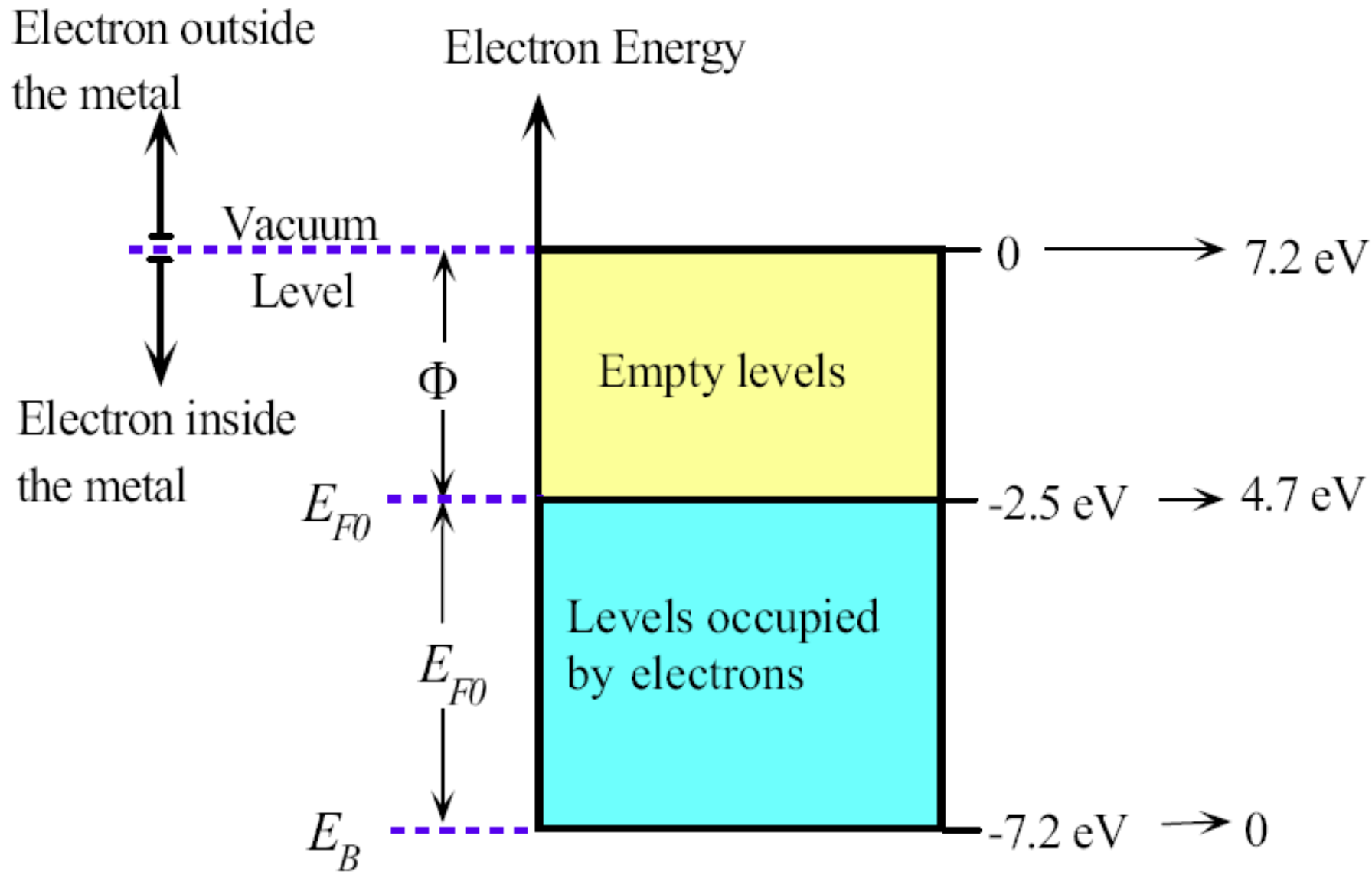
Ainda Lítio...





Em metais há superposição das várias bandas e a ocupação dos estados, como sempre, vai depender da quantidade de elétrons no sistema

Diagrama de bandas típico para um metal



Formação das bandas pela hibridização dos orbitais 3s e 3p que fazem 109.5° entre si

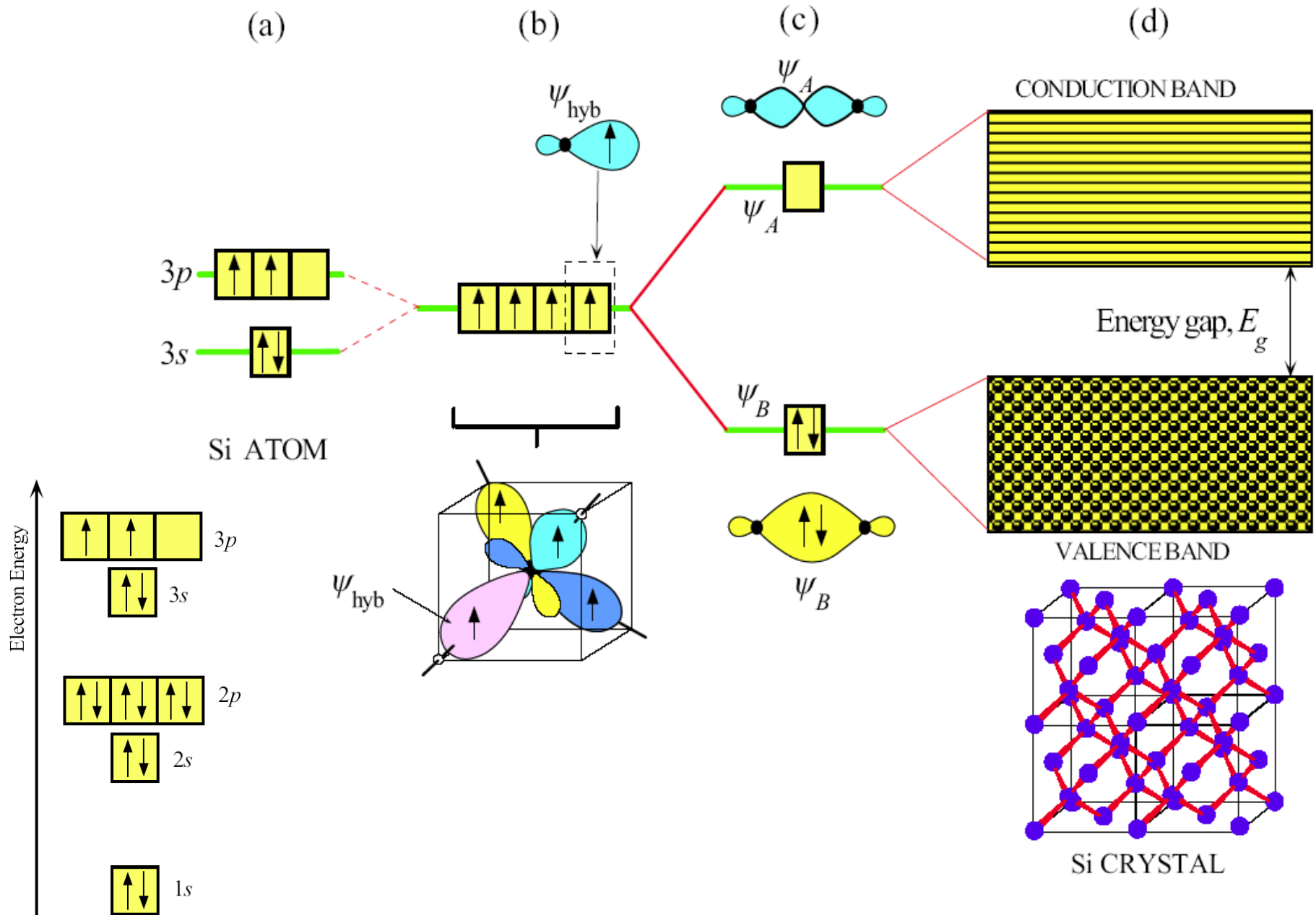
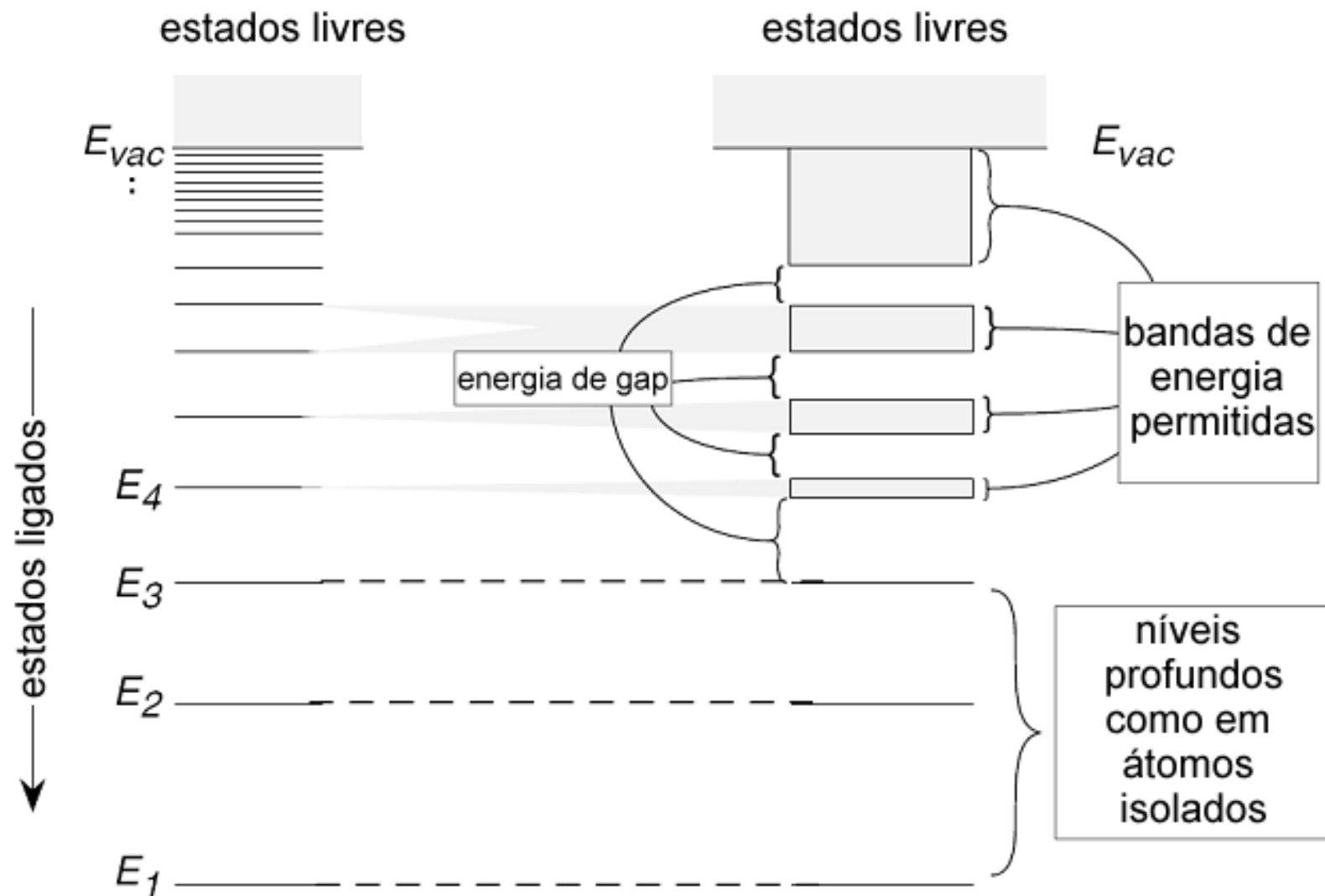


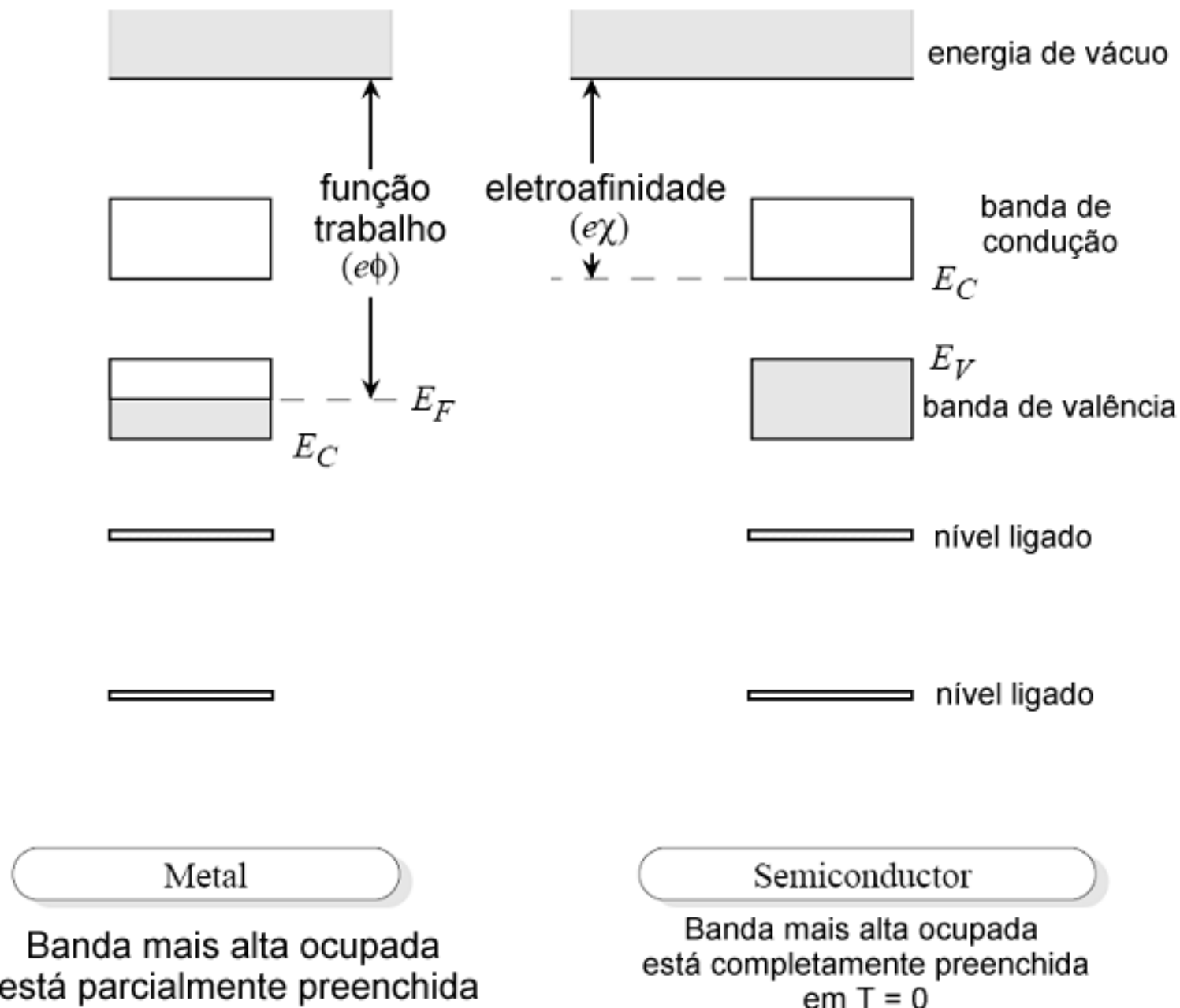
Diagrama de bandas típicos e ocupação – descrição qualitativa

átomos isolados

cristal: separação atômica ~1-2 Å

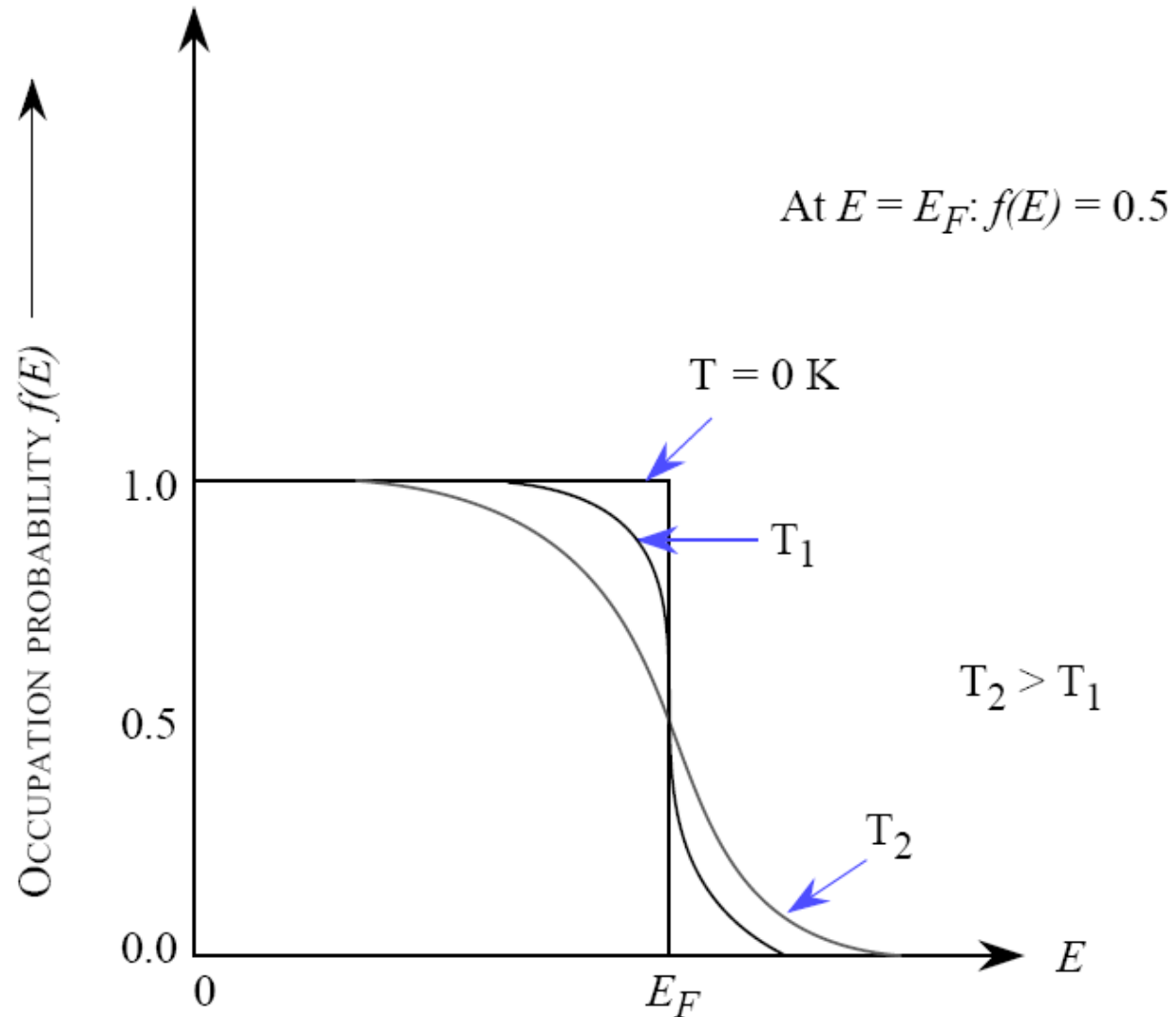


Comparação entre um METAL e um SEMICONDUTOR

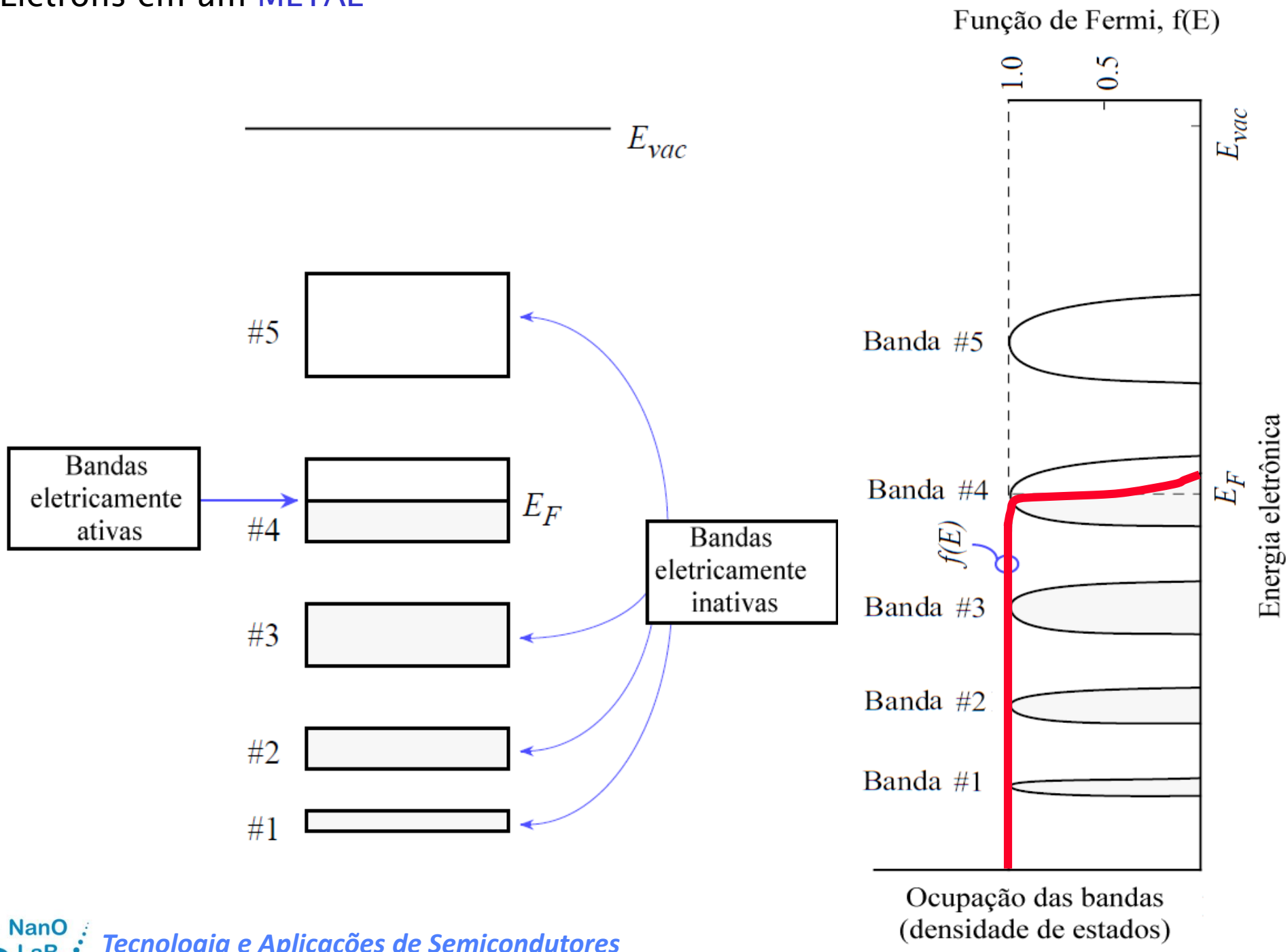


Preenchimentos dos níveis com elétrons – Distribuição de Fermi-Dirac

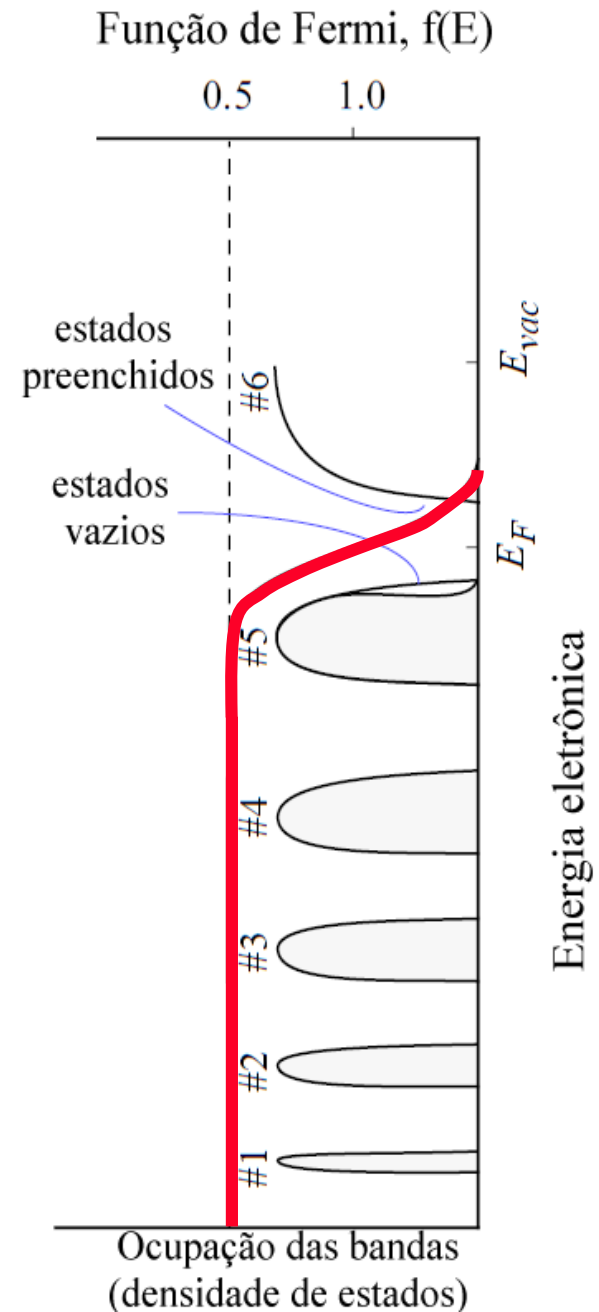
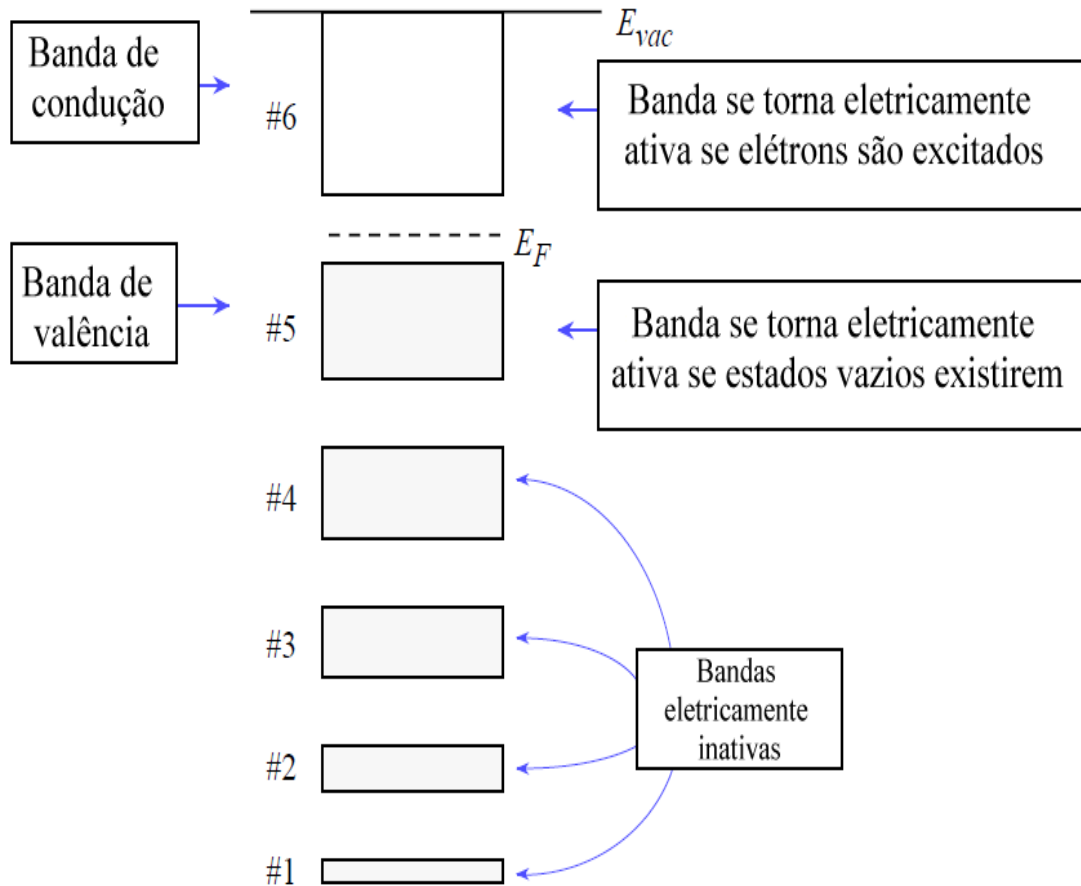
“A distribuição específica, em condições de equilíbrio, a probabilidade de um determinado nível de energia estar ocupado por elétrons”



Elétrons em um METAL

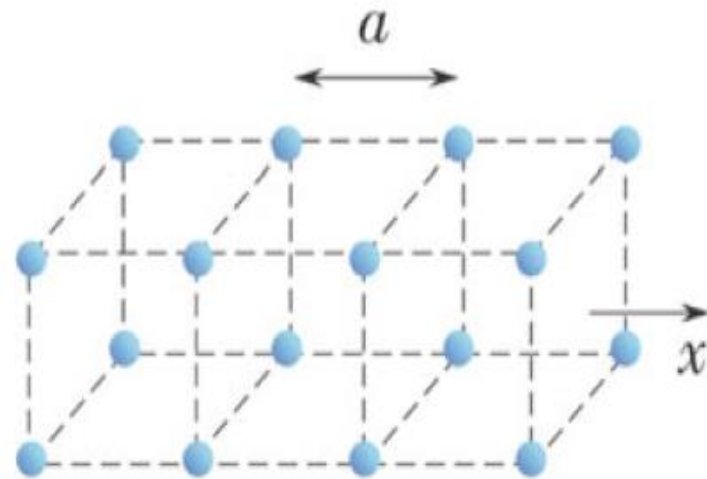
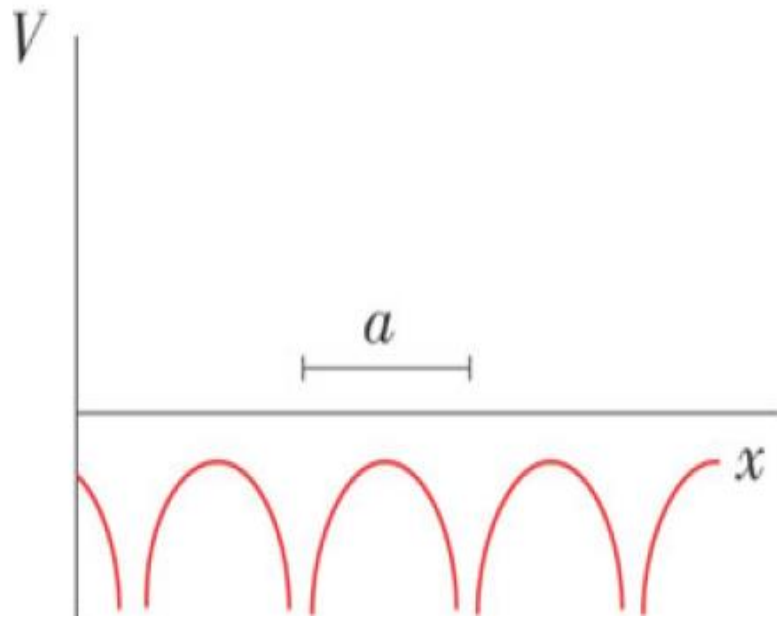


Elétrons em um SEMICONDUTOR



Cristal: periodicidade

Potencial atômico periódico



Periodicidade no cristal: potencial, energia, funções de onda, densidade de cargas, etc. Assim,

$$V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r})$$

Levando em conta a forma geral de uma transformada de Fourier para um potencial periódico,

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \quad \text{com}$$

$$V_{\mathbf{G}} = \frac{1}{v_D} \int_{v_D} V(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r}$$

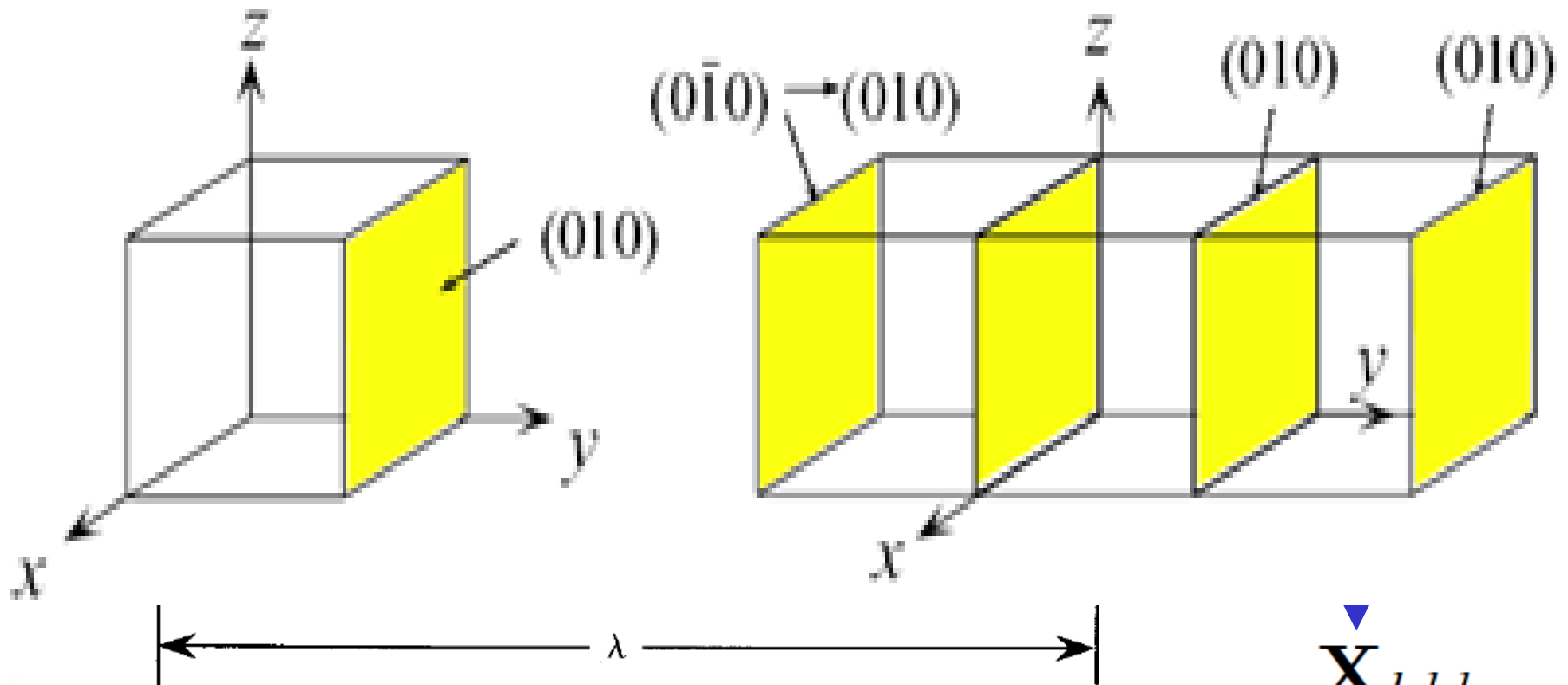
e sendo v_D o volume da célula do cristal

O vetor \mathbf{G} é um índice de soma na série de Fourier e deve ter dimensão inversa da distância; sendo um índice, assume valores inteiros.

$$\mathbf{G} \propto \frac{2\pi}{a} (\ell, m, p)$$

Considere uma onda plana viajando através de um cristal

$$\psi(\mathbf{r}) = A e^{i\mathbf{k} \cdot \mathbf{r}}$$



$$\mathbf{X}_{hkl}$$

Ou

$$\mathbf{X}_{hkl} \rightarrow \mathbf{G}_{hkl}$$

Nesse caso,

$$e^{i\mathbf{G}_{hkl}(\mathbf{r}+\mathbf{R})} = e^{i\mathbf{G}_{hkl}\mathbf{r}} e^{i\mathbf{G}_{hkl}\mathbf{R}} = e^{i\mathbf{G}_{hkl}\mathbf{r}}$$

$$\Leftrightarrow e^{i\mathbf{G}_{hkl}\mathbf{R}} = 1 \Rightarrow \mathbf{G}_{hkl}\mathbf{R} = 2\pi\mathbf{N}$$

Definindo um vetor da REDE RECÍPROCA

$$\mathbf{G}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

Temos $\mathbf{G}_{hkl}\mathbf{R} = 2\pi\mathbf{N} \implies$

$$\begin{aligned}\mathbf{G}_{hkl}\mathbf{R} &= (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \cdot (m\mathbf{a}_1 + n\mathbf{a}_2 + p\mathbf{a}_3) \\ &= 2\pi\mathbf{N} = \text{inteiro}\end{aligned}$$

Ou seja,

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{i,j}$$

Exemplo:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot |\mathbf{a}_2 \times \mathbf{a}_3|}$$

$$\mathbf{R} = m\mathbf{a}_1 + n\mathbf{a}_2 + p\mathbf{a}_3 \equiv m\mathbf{a} + n\mathbf{b} + p\mathbf{c}$$

Construção das redes recíprocas para algumas geometrias

Cúbica simples (rede direta e recíprocas são cúbicas simples)

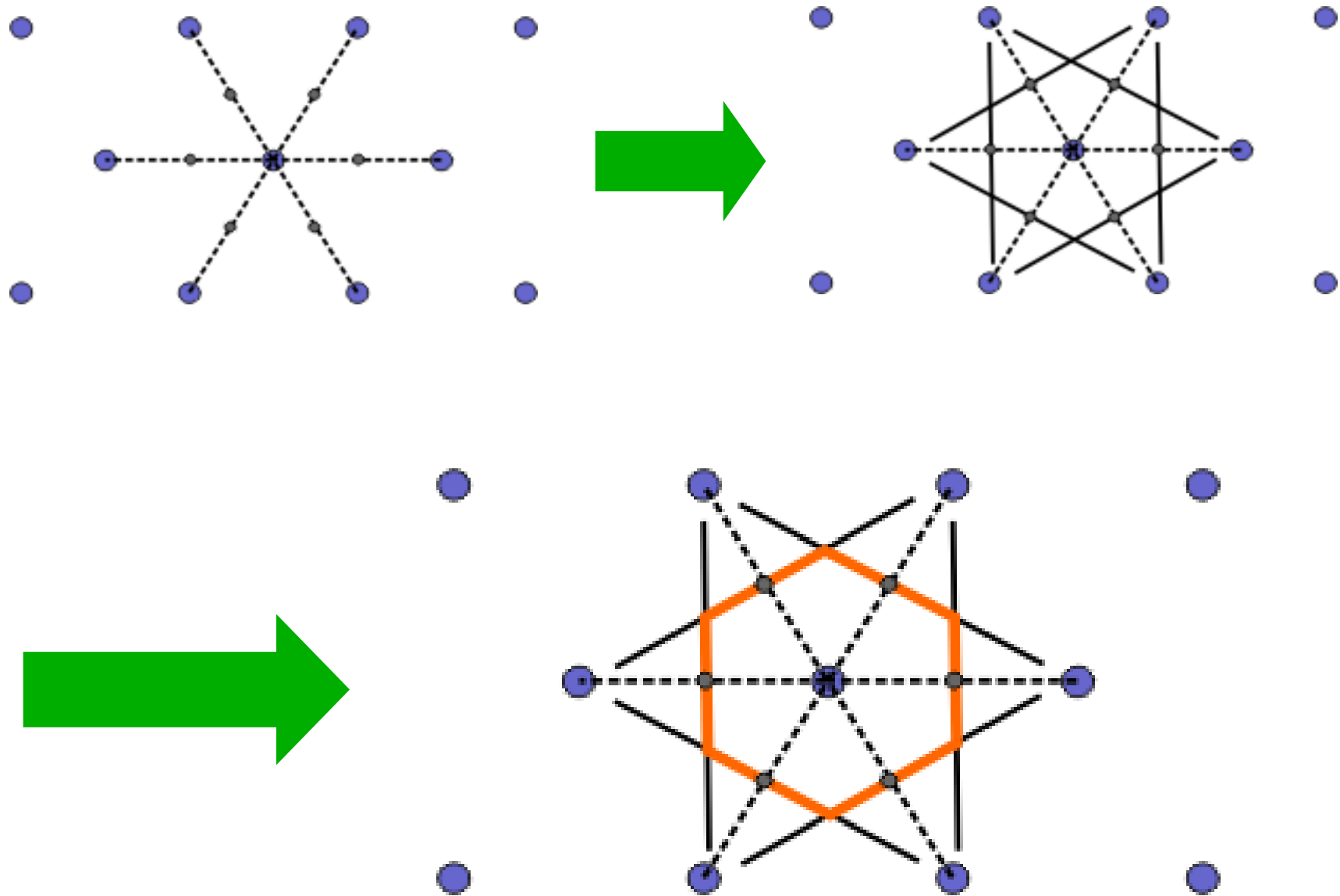
$$\begin{array}{l} \mathbf{a} = a\mathbf{x} \\ \mathbf{b} = by \\ \mathbf{c} = cz \end{array} \quad \longrightarrow \quad \begin{array}{l} \mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\ \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\ \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \end{array} \quad \longrightarrow \quad \begin{array}{l} \mathbf{A} = \frac{2\pi}{a} \mathbf{x} \\ \mathbf{B} = \frac{2\pi}{b} \mathbf{y} \\ \mathbf{C} = \frac{2\pi}{c} \mathbf{z} \end{array}$$

Obs: $|\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}|$

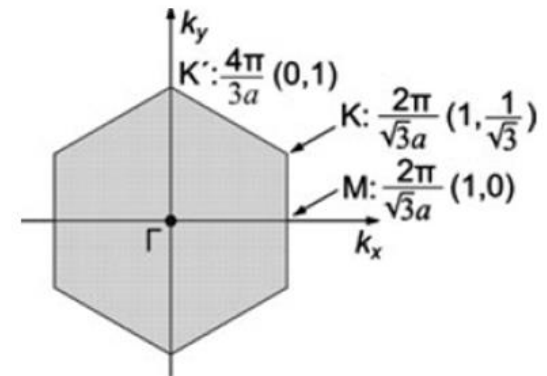
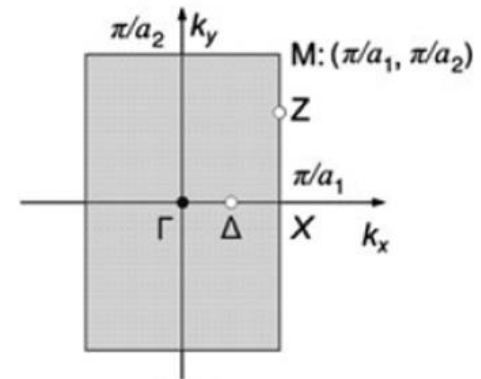
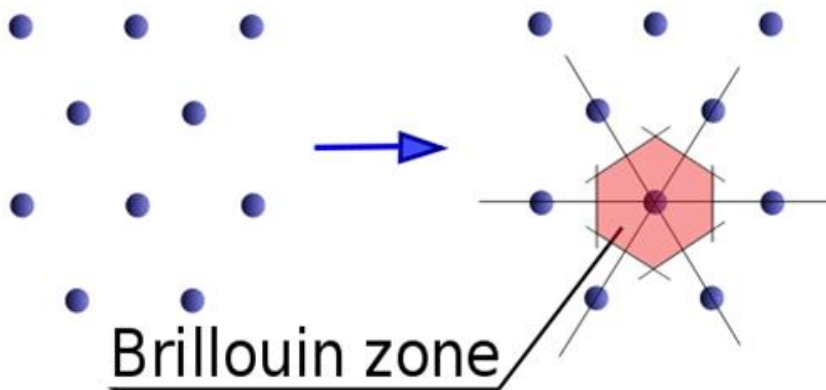
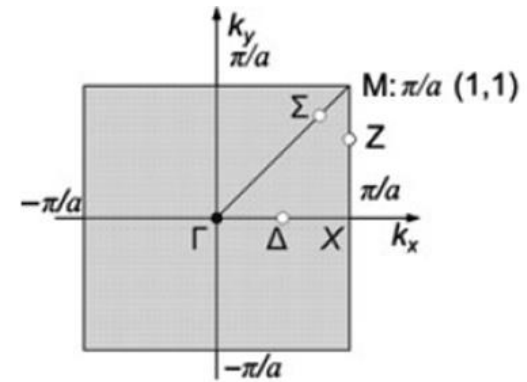
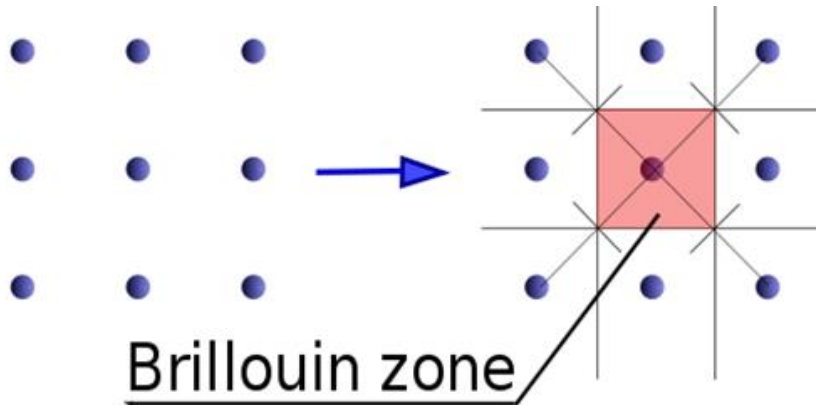
FCC (recíproca é uma BCC)

$$\begin{array}{l} \mathbf{a} = \frac{a}{2} (\mathbf{y} + \mathbf{z}) \\ \mathbf{b} = \frac{a}{2} (\mathbf{z} + \mathbf{x}) \\ \mathbf{c} = \frac{a}{2} (\mathbf{x} + \mathbf{y}) \end{array} \quad \longrightarrow \quad \begin{array}{l} \mathbf{A} = \frac{4\pi}{a} \left[\frac{1}{2} (-\mathbf{x} + \mathbf{y} + \mathbf{z}) \right] \\ \mathbf{B} = \frac{4\pi}{a} \left[\frac{1}{2} (\mathbf{x} - \mathbf{y} + \mathbf{z}) \right] \\ \mathbf{C} = \frac{4\pi}{a} \left[\frac{1}{2} (\mathbf{x} + \mathbf{y} - \mathbf{z}) \right] \end{array}$$

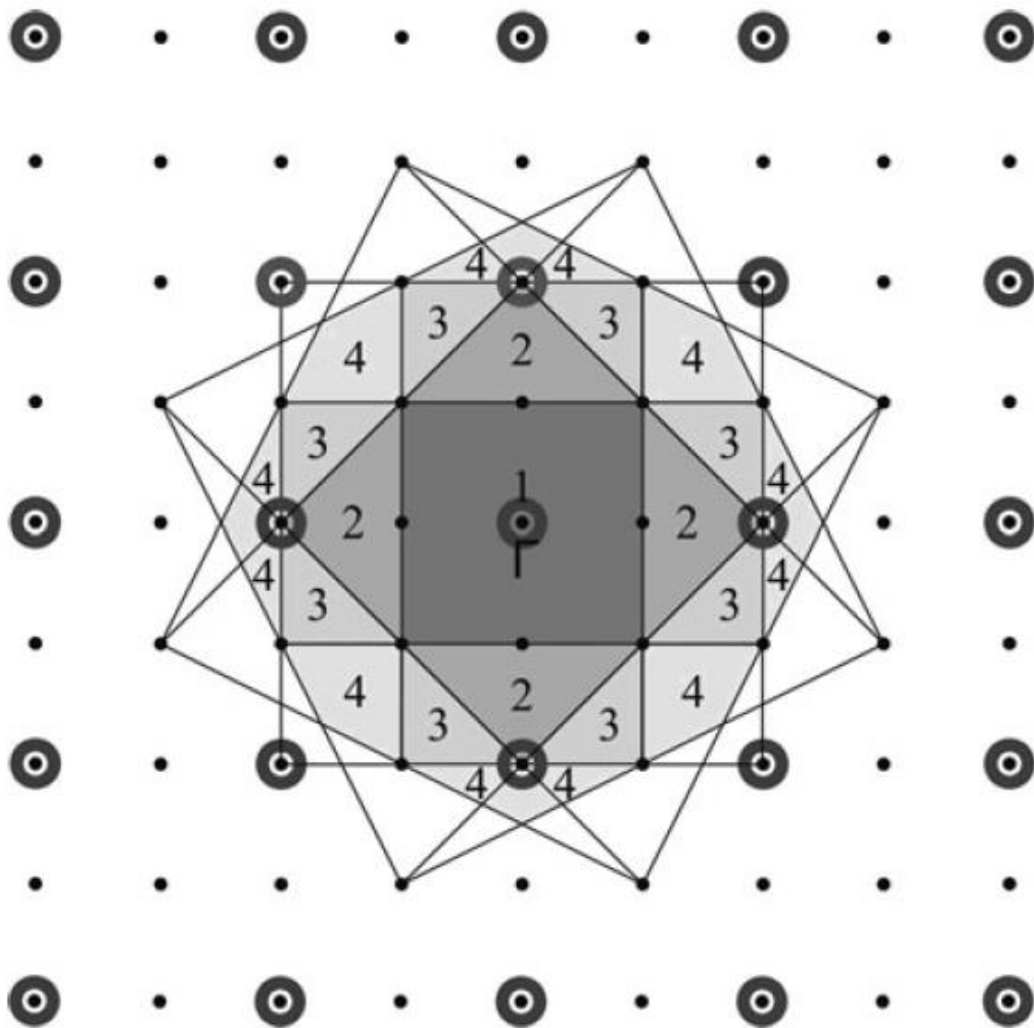
Células unitárias na RR: Zonas de Brillouin 2D



A primeira Zona de Brillouin é a célula de Wigner-Seitz na rede recíproca

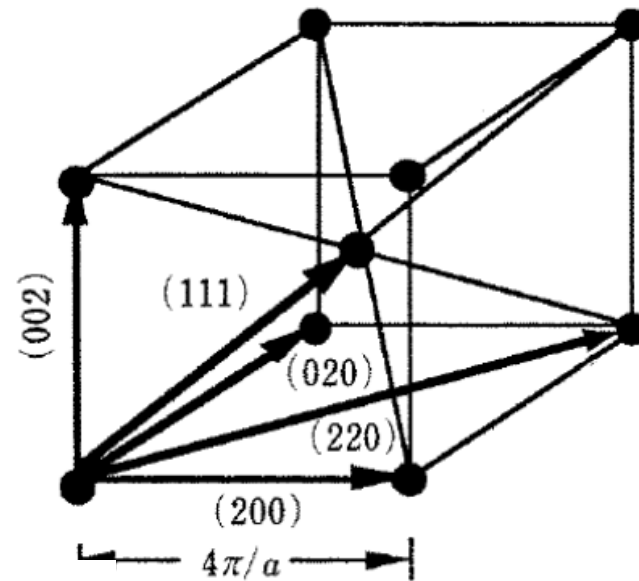
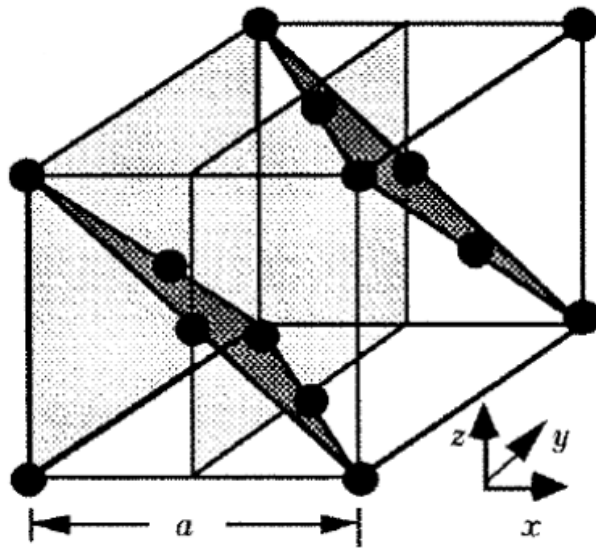


Uma Zona de Brillouin é uma célula primitiva tal que a distância de todos os seus pontos (k) em relação a um ponto central é menor ou igual à distância em relação a qualquer outro ponto da rede recíproca.



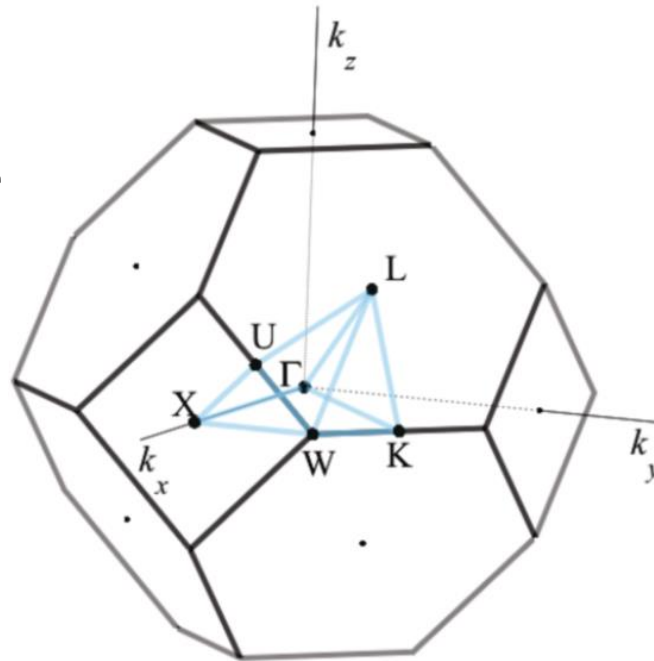
As 4 primeiras ZB para uma rede 2D quadrada

FCC (recíproca é uma BCC)



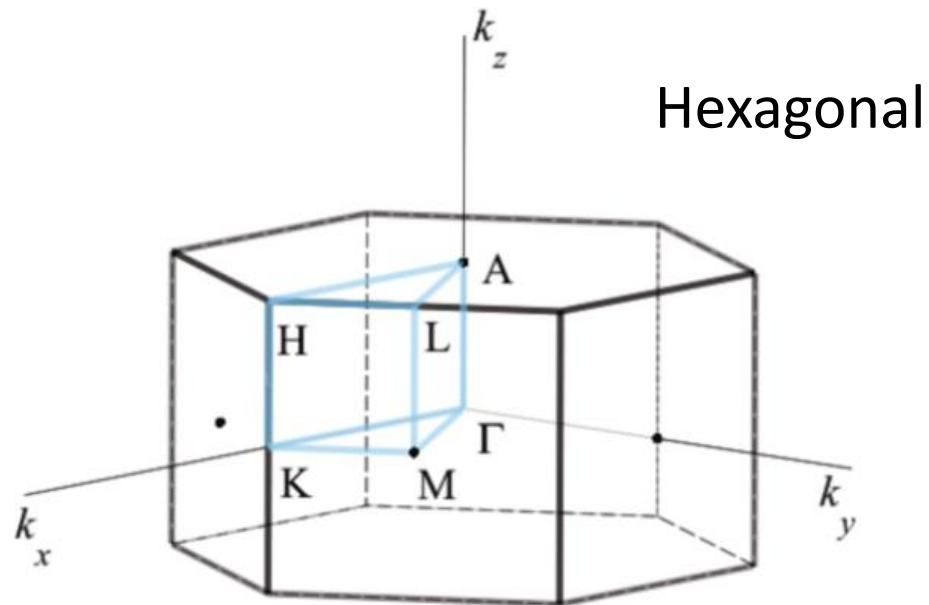
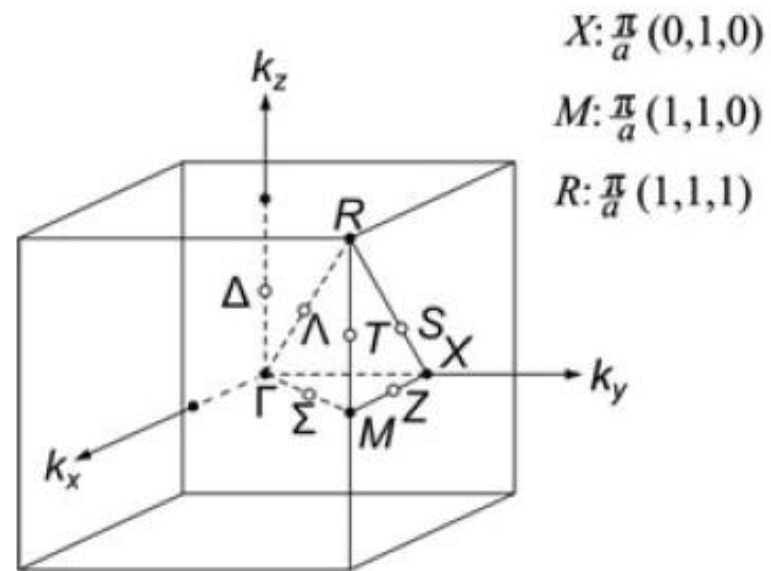
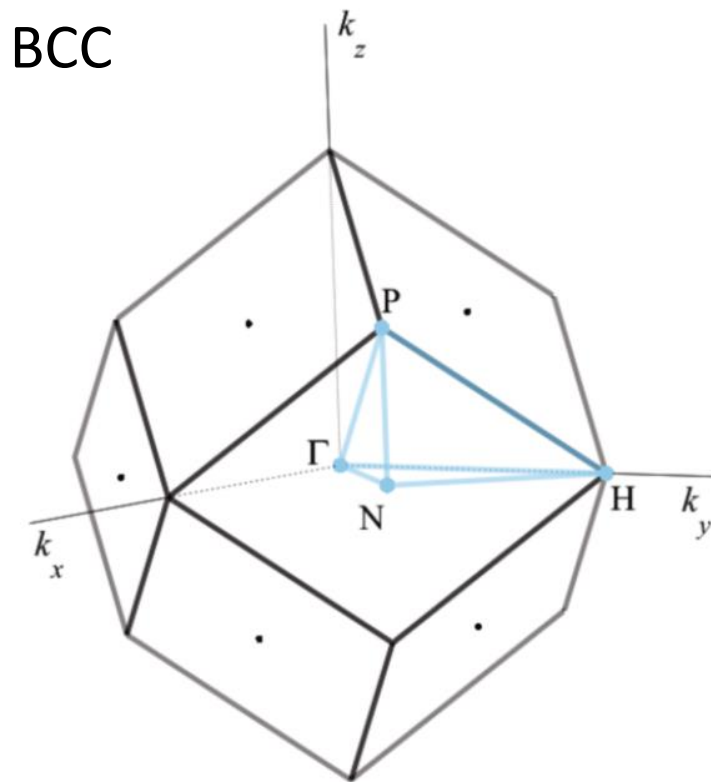
Pontos e planos
(RR x RD)

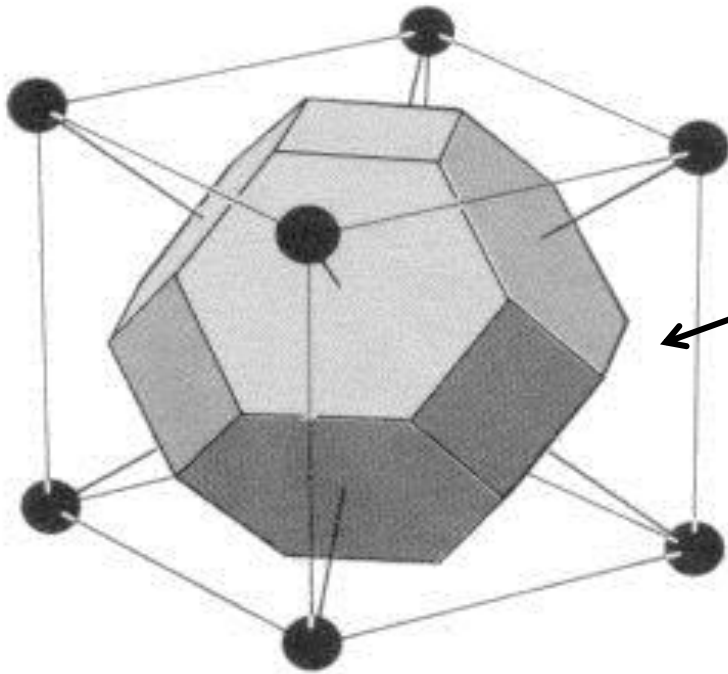
1ª Zona de Brillouin para uma FCC



Γ – identifica o centro da ZB
X – identifica o limite de zona na direção [100]
L – identifica o limite de zona na direção [111]

1ª Zona de Brilloiun para outras redes

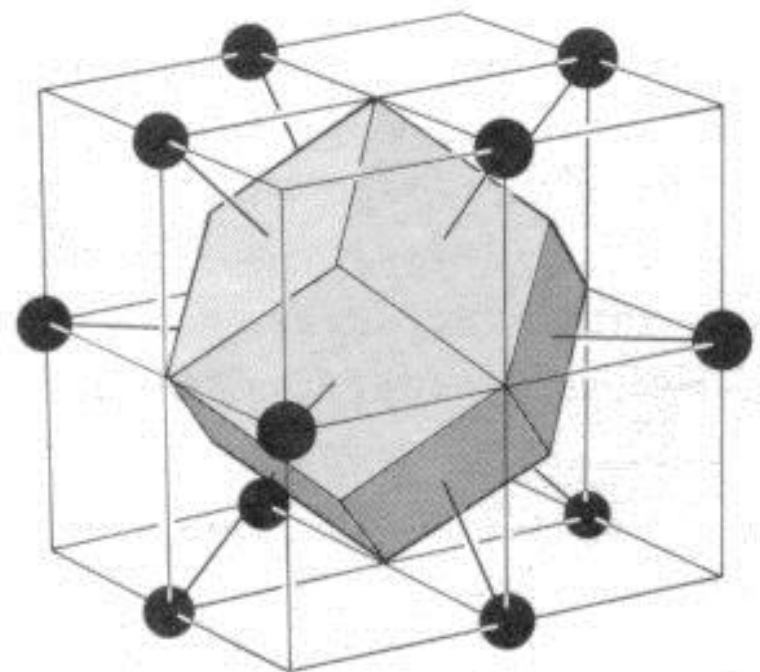




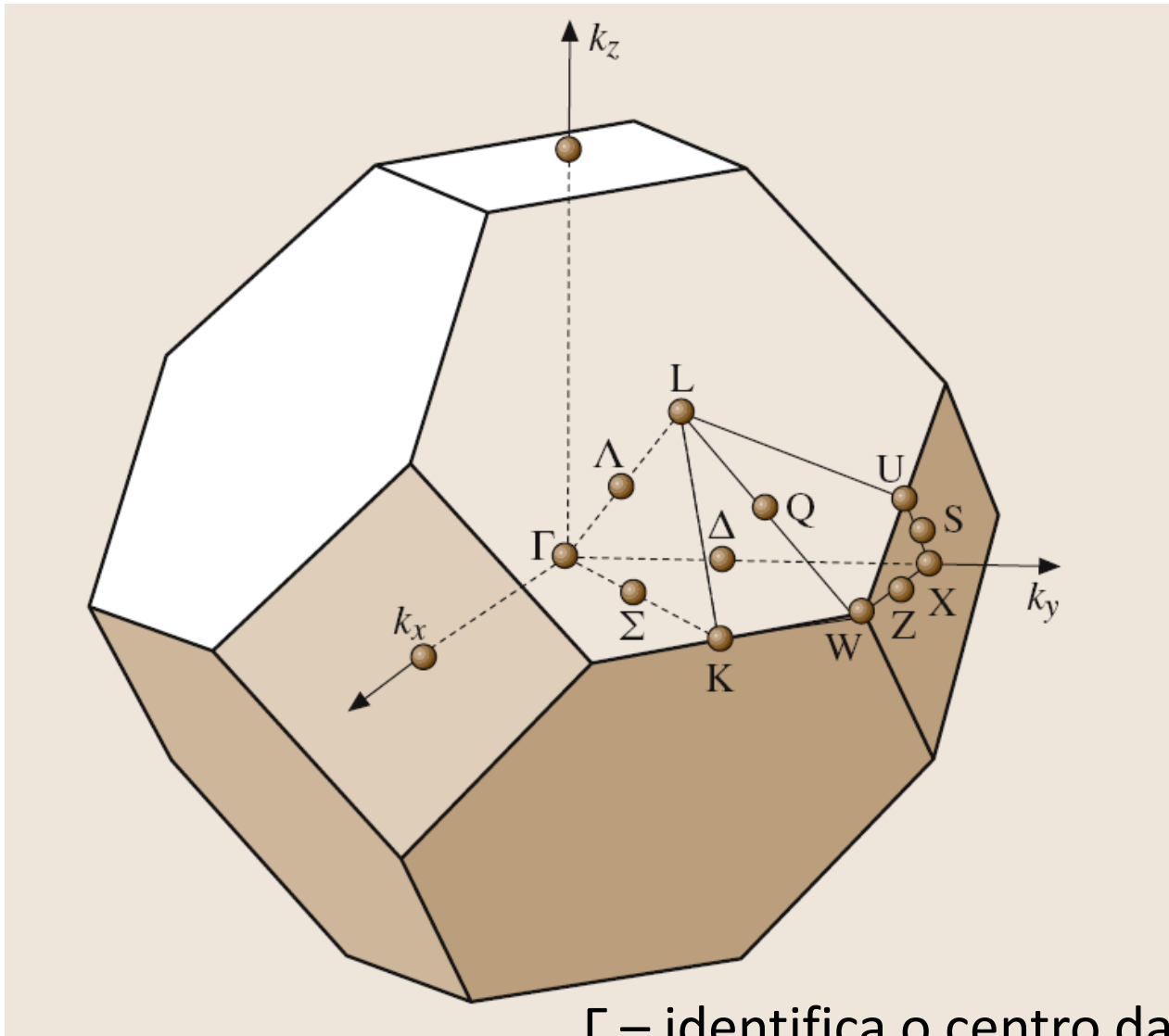
FCC no espaço
real torna-se
BCC no espaço
recíproco

BCC no espaço
real torna-se
FCC no espaço
recíproco

*1ª Zona de Brillouin:
célula de Wigner-Seitz no
espaço recíproco:*



Sistemas reais 3D: diagrama de bandas e zonas de Brillouin



Γ – identifica o centro da Zona de Brillouin

X – identifica o limite de zona na direção (100)

L – identifica o limite de zona da direção (111)

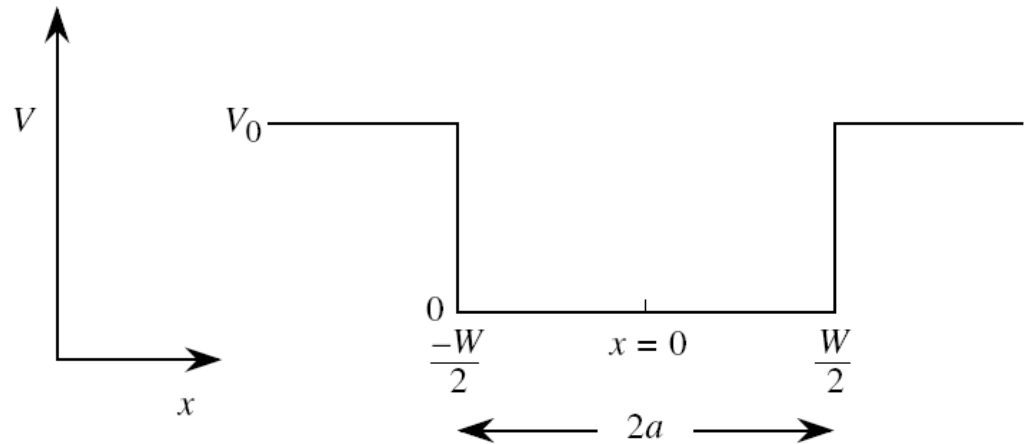
Estados eletrônicos em cristais

Os elétrons em um cristal se comportam segundo determina a Mec. Quântica, o que pode ser expresso pela **eq. de Schrödinger**:

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + V(r, t) \right] \Psi(r, t) = E \Psi(r, t)$$

Vamos supor que os elétrons estejam sujeitos a um potencial conhecido como o potencial quadrado 3D para representar “uma unidade de um cristal”

$$V(r) = V(x) + V(y) + V(z)$$



Para facilitar nossa discussão qualitativa, consideremos o potencial infinito fora do poço e nulo em seu interior! As eq. de Schrödinger e sua solução serão escritas como

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \text{e} \quad \psi(r) = \psi(x)\psi(y)\psi(z)$$

ou

$$\begin{aligned} \psi(x) &= B \cos \frac{n\pi x}{2a}, \quad n \text{ ímpar} \\ &= A \sin \frac{n\pi x}{2a}, \quad n \text{ par} \end{aligned} \quad \text{com} \quad E = \frac{\pi^2 \hbar^2 n^2}{8ma^2}$$

No caso de um potencial finito,

$$\begin{aligned} \alpha &= \sqrt{\frac{2mE}{\hbar^2}} \\ \beta &= \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \end{aligned} \quad \longrightarrow \quad \begin{aligned} \frac{\alpha W}{2} \tan \frac{\alpha W}{2} &= \frac{\beta W}{2} \\ \frac{\alpha W}{2} \cot \frac{\alpha W}{2} &= -\frac{\beta W}{2} \end{aligned}$$

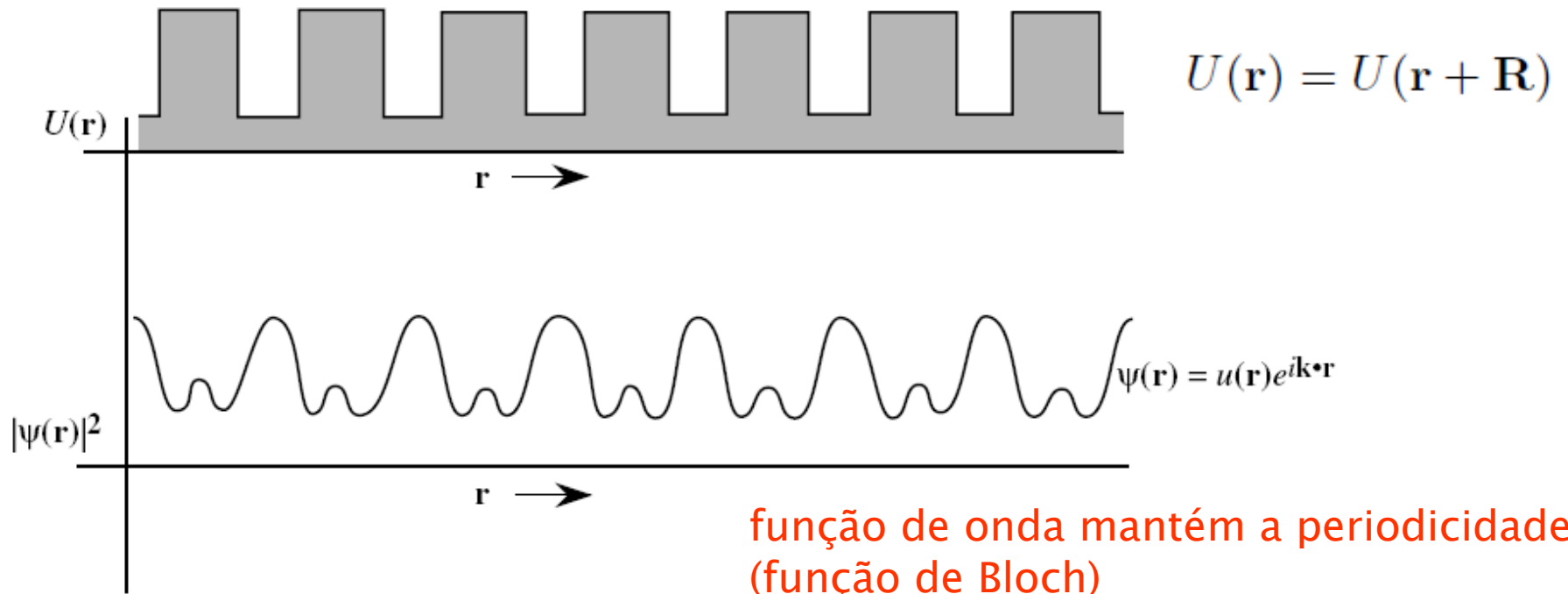
No caso de um potencial periódico,

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(\mathbf{r}) = (E - V_0)\psi(\mathbf{r})$$

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{\pm i\mathbf{k}\cdot\mathbf{r}}$$

$$E = \frac{\hbar^2 k^2}{2m} + V_0$$

potencial periódico



função de onda mantém a periodicidade
(função de Bloch)