

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



Definições

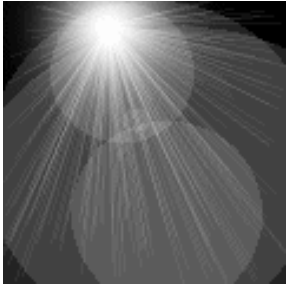
- Ciência dos Materiais
 - Investigação das relações entre composição/estrutura e propriedades dos materiais

- Engenharia dos Materiais
 - Projeto, desenvolvimento ou aperfeiçoamento de técnicas de processamento de materiais (= técnicas de fabricação) com base nas relações composição/estrutura e propriedades.
 - E também:
 - Desenvolvimento de formas de produção de materiais socialmente desejáveis a custo socialmente aceitável.

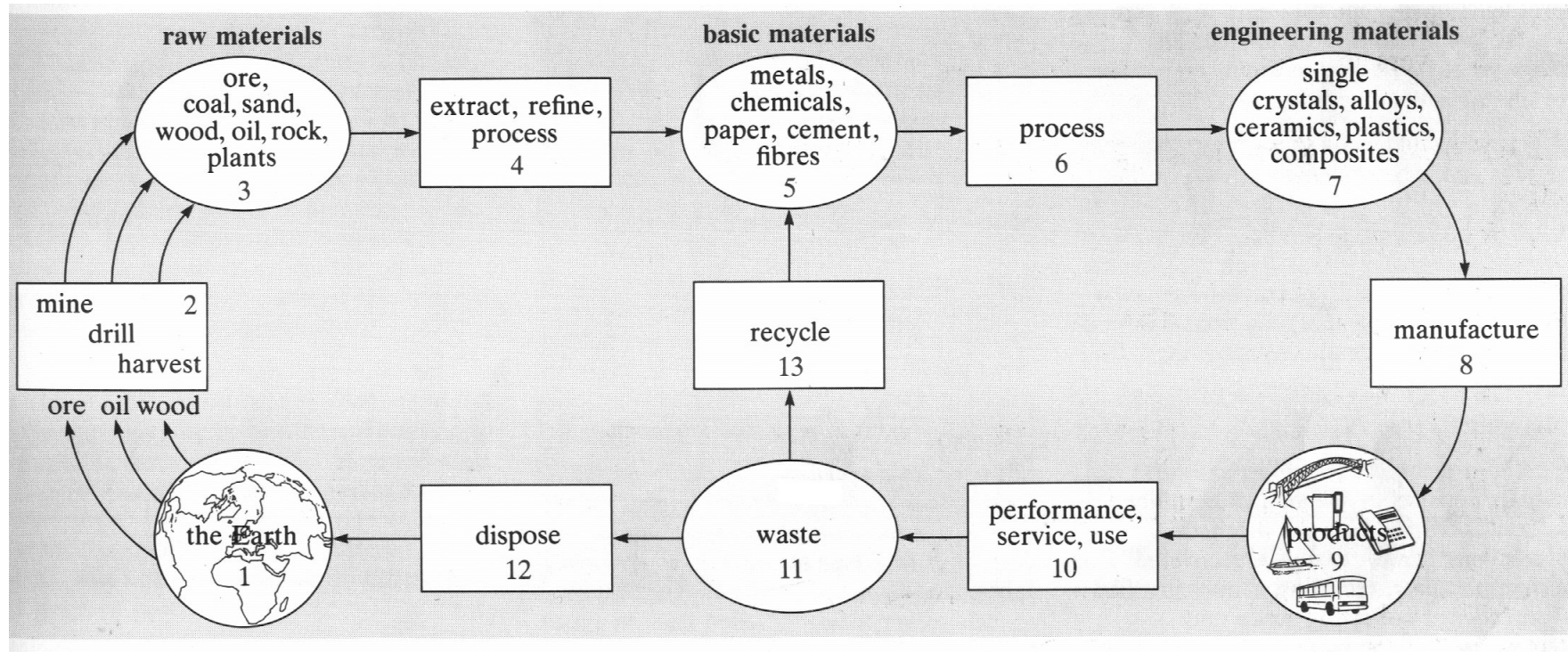


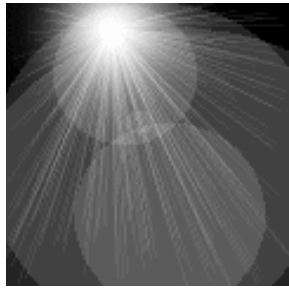
Definições

- Ciência e Engenharia dos Materiais são campos intimamente interligados e interdisciplinares.
- “Ciência e Engenharia dos Materiais é a área da atividade humana associada com a geração e a aplicação de conhecimentos que relacionem composição, estrutura e processamento de materiais às suas propriedades e usos.”
Morris Cohen, MIT (in Padilha, A.F. – Materiais de Engenharia, Hemus, 1997, cap. 1)
- Objetivos:
 - Desenvolvimento de materiais já conhecidos visando novas aplicações ou visando melhorias no desempenho.
 - Desenvolvimento de novos materiais para aplicações conhecidas.
 - Desenvolvimento de novos materiais para novas aplicações.

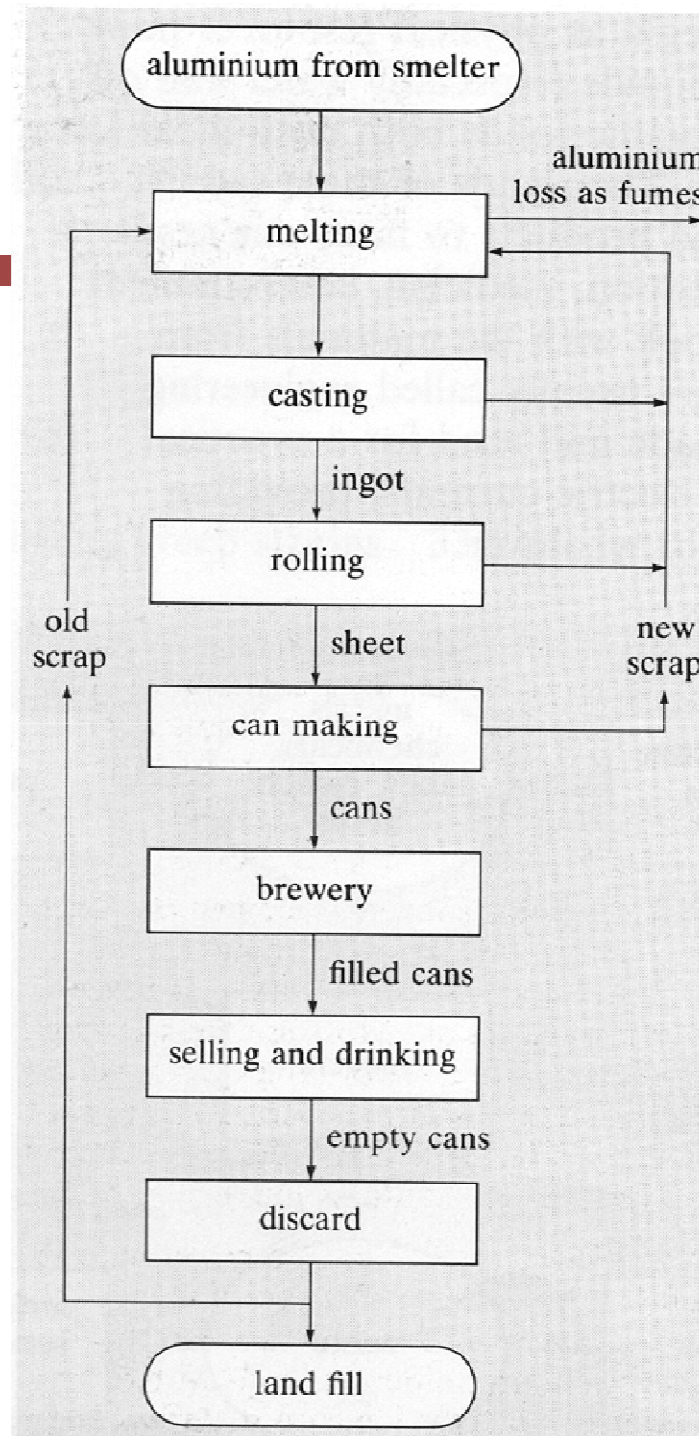


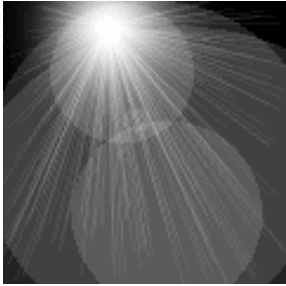
CICLO DE VIDA DOS MATERIAIS DE ENGENHARIA





RECYCLAGEM



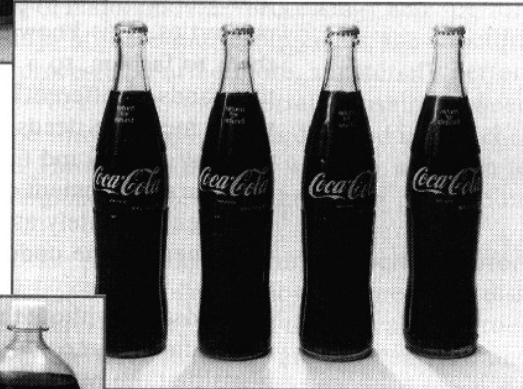


CLASSIFICAÇÃO DOS MATERIAIS

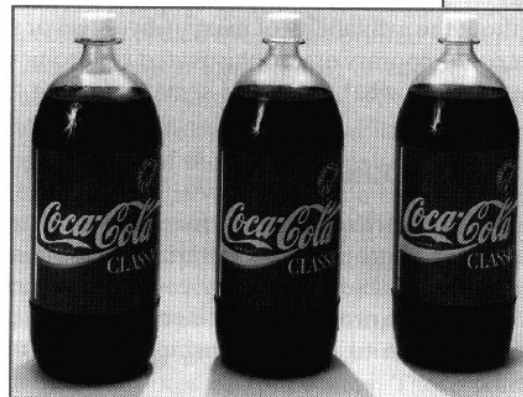
Metálico

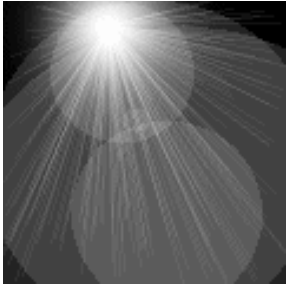


Cerâmico



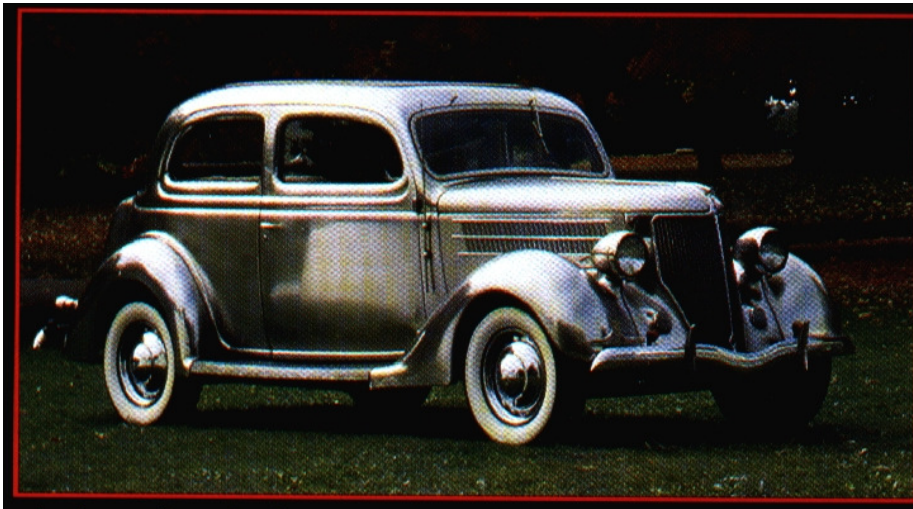
Polimérico

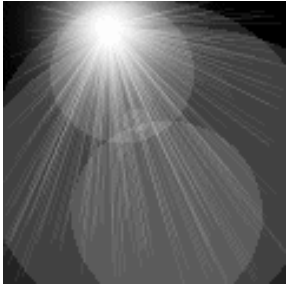




UTILIZAÇÃO DOS MATERIAIS

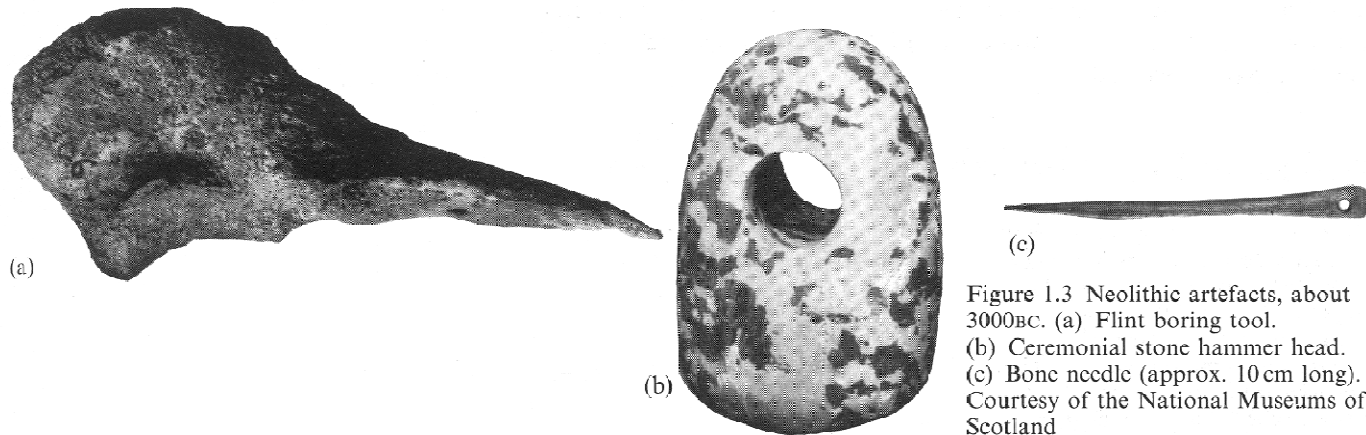
- transportes (carro, avião, ônibus espacial, trens, navios, bicicletas, carros de F-1)
- construção (casas, prédios, viadutos, túneis)
- vestuário (tecidos impermeáveis, tecidos de alta performance para práticas esportivas, calçados)
- comunicação (TV, telefone, telefone celular, microcomputador, fibras óticas, fios de cobre, CD, walkman)
- alimentação (embalagens, tanques armazenamento de alimentos, sistemas de processamento de alimentos)





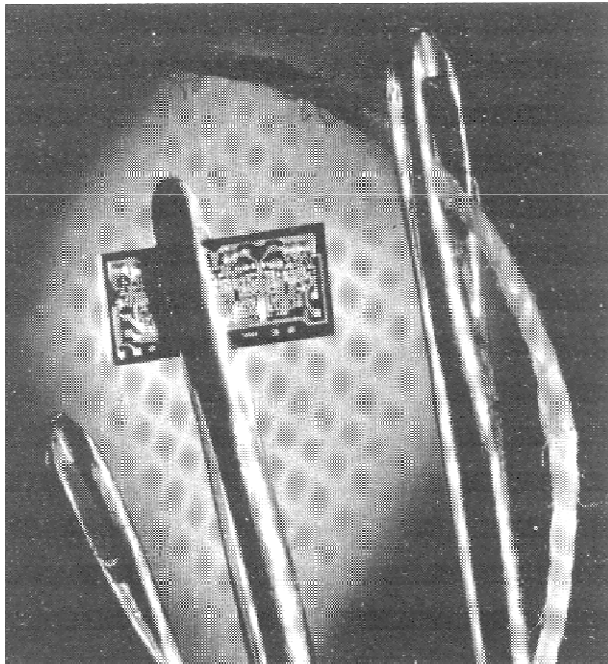
PERSPECTIVA HISTÓRICA

- Inicialmente se utilizavam somente materiais naturais: pedra, madeira, argila, peles.

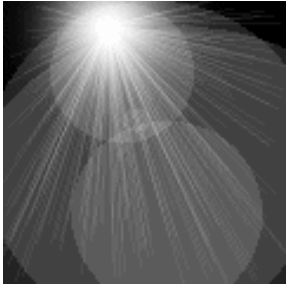




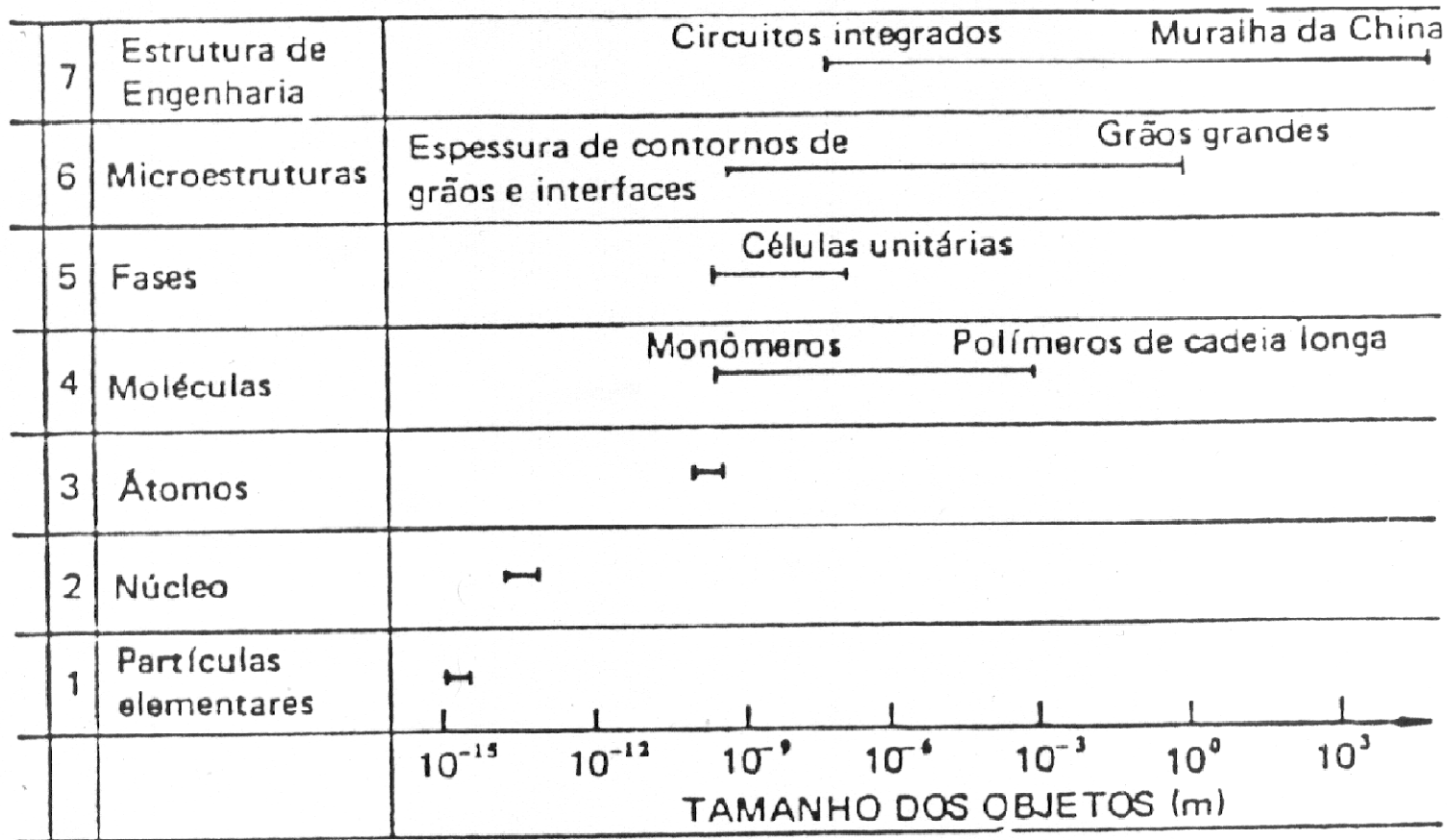
PERSPECTIVA HISTÓRICA



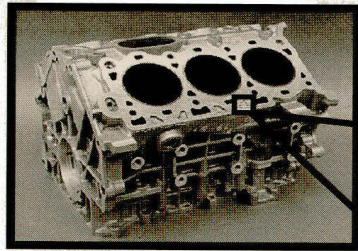
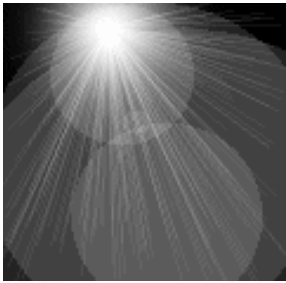
- Descobrimiento de técnicas para a produção de materiais: porcelana, alguns metais.
- Descobrimiento de processos que permitiram modificar as propriedades dos materiais: mistura de diferentes materiais, tratamento térmico e termomecânico.
- Há aproximadamente 60 anos se iniciou o estudo sistemático da relação estrutura-propriedades.



ESTRUTURAS DE ENGENHARIA



ESTRUTURAS

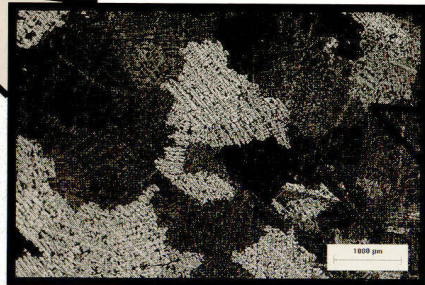


*Escala
"Macro"*

Macro-Scale Structure
Engine Block
≅ upto 1 meter

Performance Criteria

- Power generated
- Efficiency
- Durability
- Cost

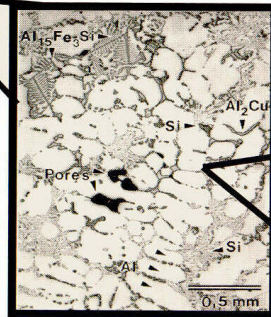


Microstructure
- Grains
≅ 1 – 10 millimeters

Properties affected

- High cycle fatigue
- Ductility

*Escala
"Micro"*

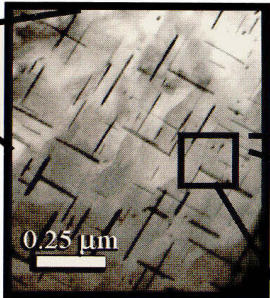


Microstructure
- Dendrites & Phases
≅ 50 – 500 micrometers

Properties affected

- Yield strength
- Ultimate tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility

*Escala
"Nano"*

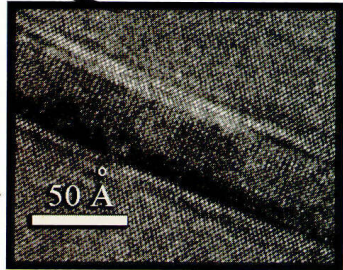


Nano-structure
- Precipitates
≅ 3-100 nanometers

Properties affected

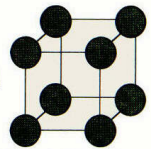
- Yield strength
- Ultimate tensile strength
- Low cycle fatigue
- Ductility

*Escala
Atômica*



Atomic-scale structure
≅ 1-100 Angstroms
Property affected

- Young's modulus
- Thermal Growth



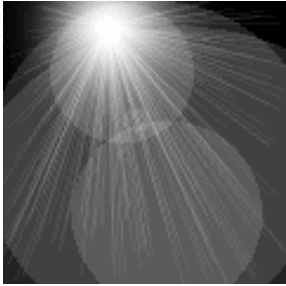
*Bloco de motor em liga
de alumínio fundido
(material em
desenvolvimento)
Ford Motor Company*



ESTRUTURA DOS MATERIAIS

Associada ao arranjo dos componentes do material em escala:

- subatômica
- atômica (átomos ou moléculas)
- microscópica (microestrutura)
- macroscópica (macroestrutura)



MACROESTRUTURAS

▼ Reinforced concrete ▲

Reinforced concrete at different levels of scale. The techniques for revealing structure are considered later.

Concrete is a mixture of cement and an aggregate of sand and stone:

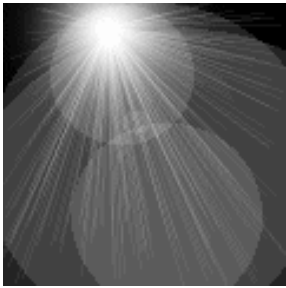


Figure 2.4

Reinforced concrete (left) in action. It is a composite material on the grand scale. Concrete is weak in tension; steel is strong in tension. The reinforcing steel rods allow the use of concrete in components which carry tensile loads — beams, tall columns etc.

The reinforcing rods are a plain carbon steel (an alloy of iron with about 0.15% carbon).





MICROESTRUTURAS

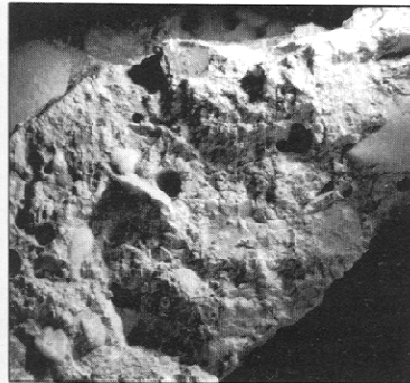


Figure 2.5

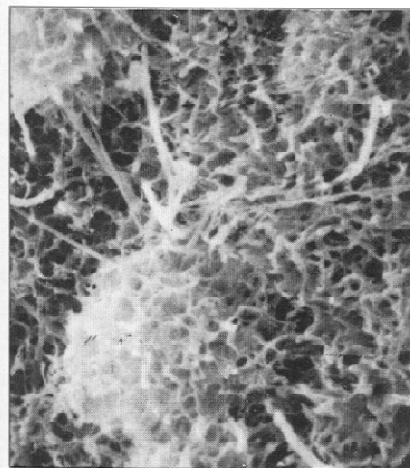


Figure 2.7

0 1 mm

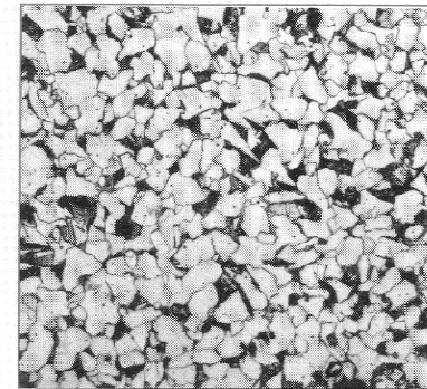


Figure 2.6

0 50 μm

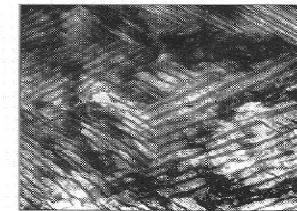


Figure 2.8 (a)

0 400 nm

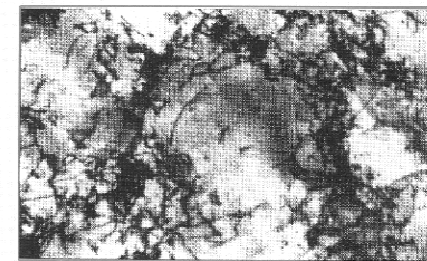
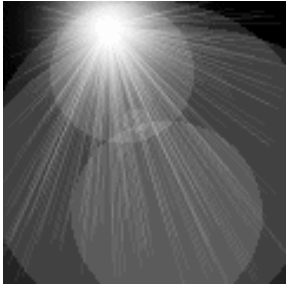


Figure 2.8 (b)

0 1 μm



ESTRUTURA DOS MATERIAIS



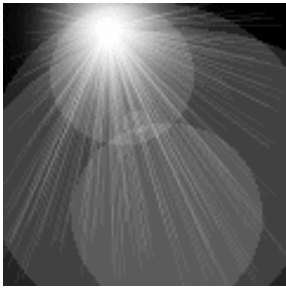
Macrografia de uma junta soldada.

Liga Nb-10%Hf-10%W. 15X



Micrografia óptica de uma camada cementada.

Aço AISI 9310. 320X



▼ A gallery of microstructures ▲

The techniques and terms are considered later in the chapter.

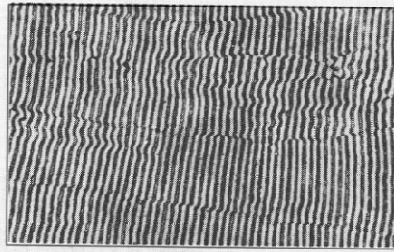


Figure 2.35 (a)

0 50 μm

(left) The intimate mixture of Pb-rich and Sn-rich regions found in electricians' solder.

(right) A powerful permanent magnet alloy. It is made of iron together with aluminium, nickel and cobalt (an alloy called Alnico). The two materials present (light and dark) form elongated regions because the alloy was cooled from the liquid in a magnetic field. Seen in an electron microscope.

Both of these microstructures are of a sample of tin bronze (copper + 4% tin).

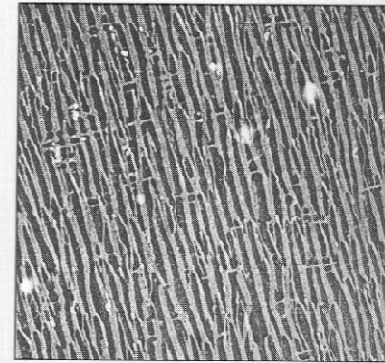


Figure 2.35 (b)

0 0.3 μm

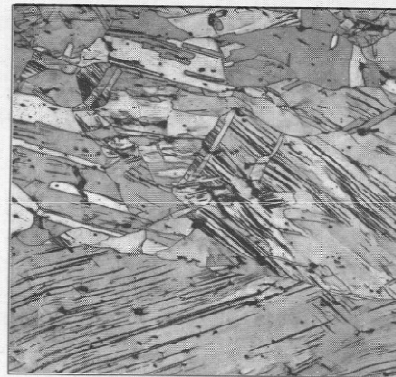


Figure 2.36 (a)

0 0.25 mm

(left) The surface after plastic deformation. The dark lines are slip lines — a manifestation of plastic flow in crystals. Notice the lines are at different angles in each grain.

(right) A polished and chemically etched section of the same material after heating to about $0.4 T_m$. The deformed material of Figure 2.36(a) recrystallizes to form a set of completely new grains.

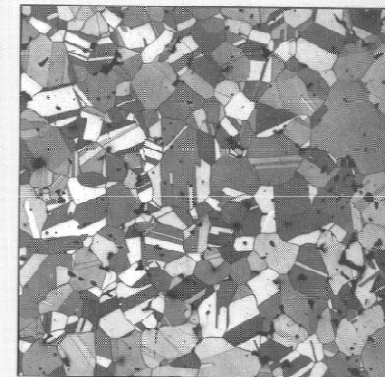


Figure 2.36 (b)

0 0.25 mm



Figure 2.37 (a)

0 0.2 mm

Two sorts of cast iron.

(left) 'Grey' cast iron. The black areas are flakes of graphite. This iron is hard and wear-resistant but brittle — the flakes are a ready source of cracks.

(right) 'Spheroidal' cast iron. The addition of small amounts of magnesium or cerium (about 0.5%) leads to spherical particles of graphite rather than flakes. It is stronger than grey cast iron and has some ductility.

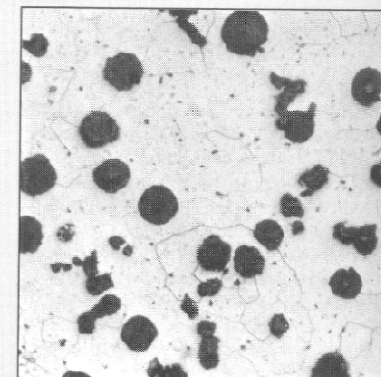


Figure 2.37 (b)

0 200 μm

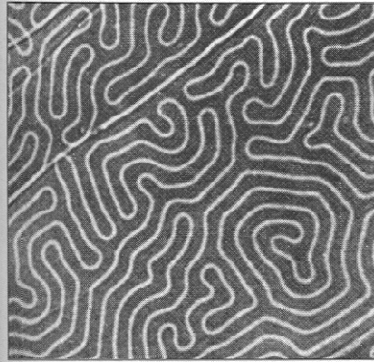
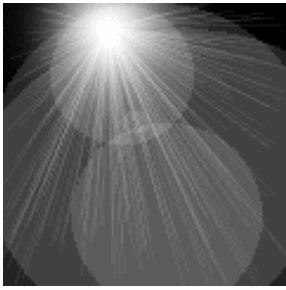


Figure 2.38 (a) 0 15 μm

(left) Magnetic domains in a ferromagnetic oxide ceramic viewed in polarized light.

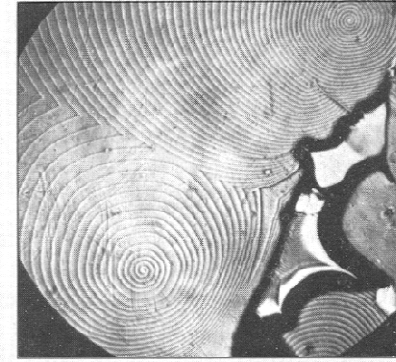


Figure 2.38 (b) 0 0.25mm

(right) Growth spirals on the surface of silicon carbide crystals grown from the vapour phase. The axes of the spirals are screw dislocations.

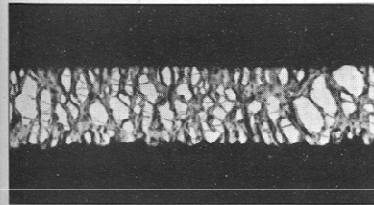


Figure 2.39 (a) 0 1 μm

Two transmission electron micrographs showing toughening mechanisms in polymers.

(left) Increased toughness is achieved by energy being absorbed in the crazes produced by the slow tearing apart of thin strands (micro-fibrils) of the polymer.

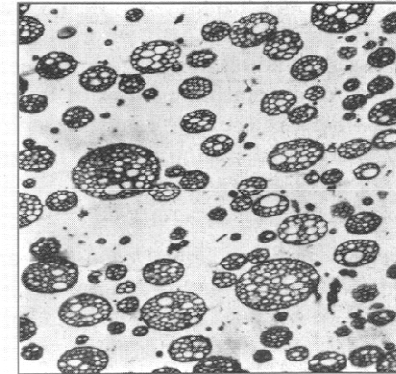


Figure 2.39 (b) 0 1 μm

(right) High impact polystyrene. Here energy is absorbed by very small particles of rubber.

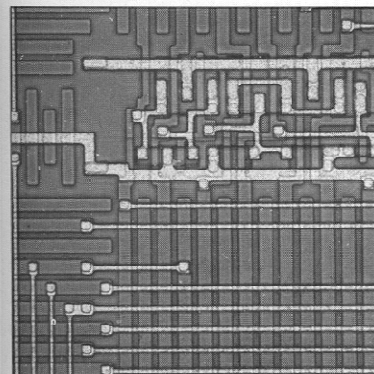


Figure 2.40 (a) 0 10 μm

(left) Part of an integrated circuit seen under an optical microscope.

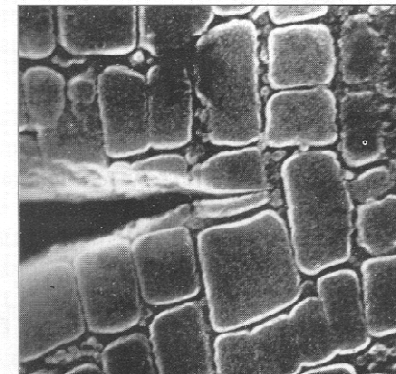
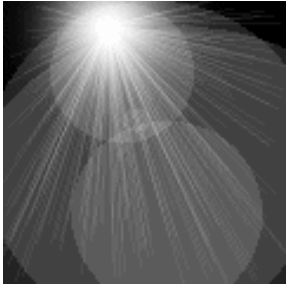


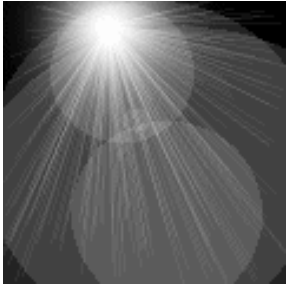
Figure 2.40 (b) 0 0.5 μm

(right) A crack in a nickel superalloy used in jet engine turbine blades. The neat pattern of particles is designed to give high-temperature strength.



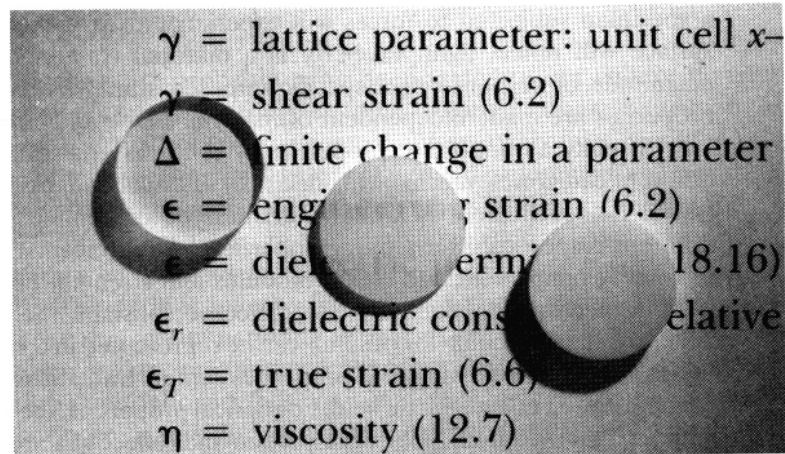
PROPRIEDADES DE UM MATERIAL

- Todo material exposto a um estímulo exerce uma resposta.
- As principais propriedades dos sólidos podem ser agrupadas em:
 - mecânicas
 - elétricas
 - térmicas
 - magnéticas
 - ópticas
 - de degradação (corrosão, oxidação, desgaste)

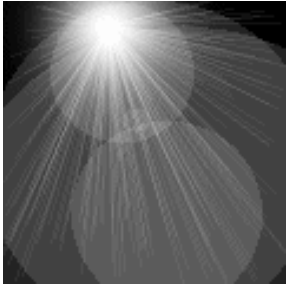


PROCESSAMENTO E DESEMPENHO

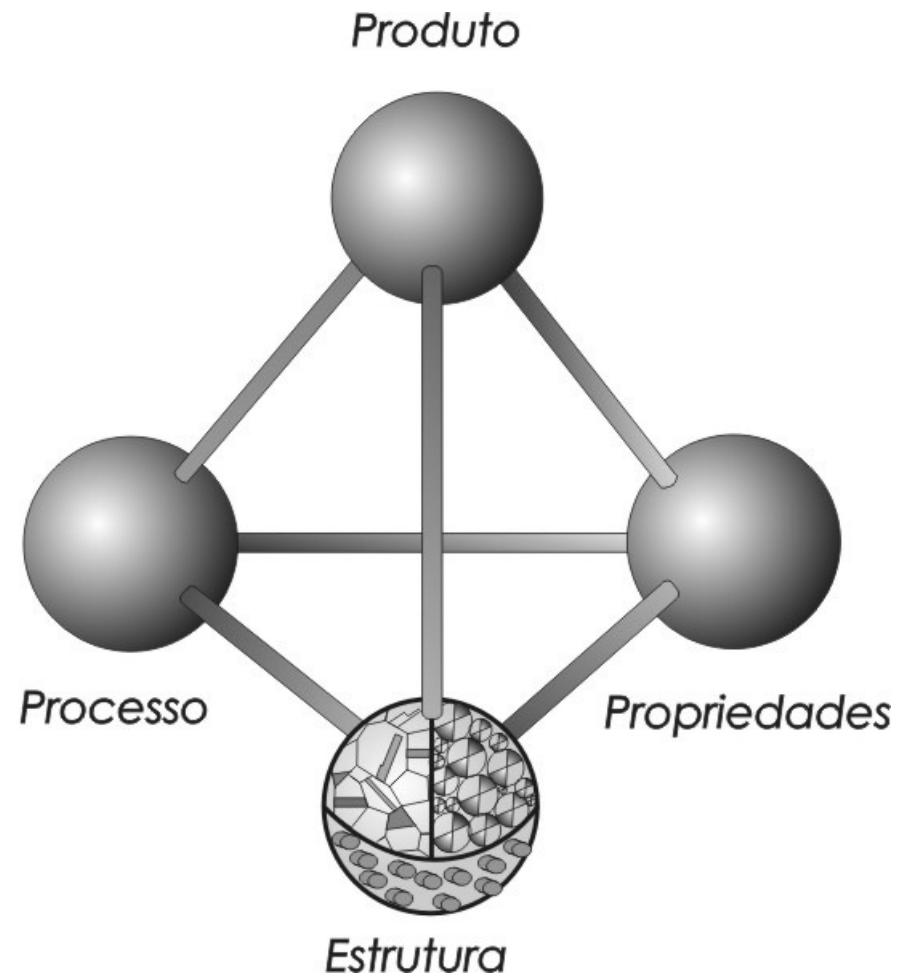
- Processamento: conjunto de técnicas para obtenção de materiais com formas e propriedades específicas.
- Desempenho: resposta do material a um estímulo externo.

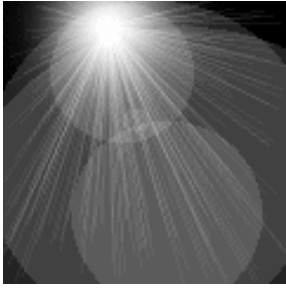


Três amostras de alumina (Al_2O_3) processadas por diferentes rotas. Da esquerda para a direita: (i) monocristal (transparente), (ii) policristal denso (translúcido) e (iii) policristal poroso (opaco).



RELAÇÃO ENTRE MICROESTRUTURA, PROCESSAMENTO, PROPRIEDADES E DESEMPENHO





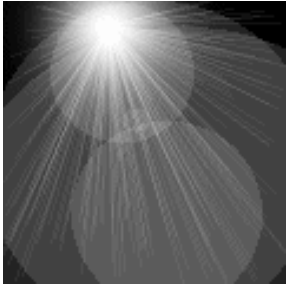
LIGAÇÕES QUÍMICAS

OBJETIVO

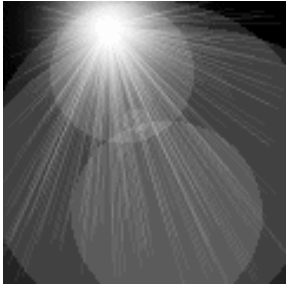
- Relacionar o tipo de ligação química com as principais propriedades dos materiais.

ROTEIRO

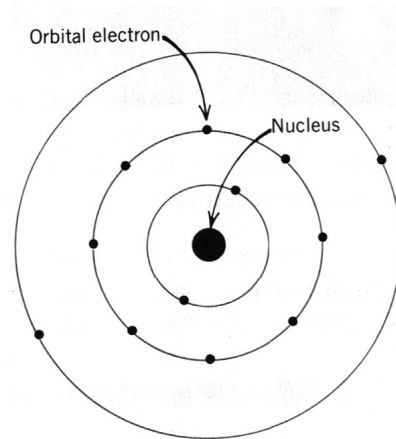
- Recordar conceitos básicos:
 - Conceitos fundamentais da estrutura atômica
 - Modelo atômico de Bohr e o da mecânica quântica.
 - Eletronegatividade
- Recordar os tipos de ligações químicas.
- Energia de Ligação
- Relacionar propriedades com os tipos de ligações químicas.



- Cada átomo é composto por:
 - Núcleo → prótons e nêutrons.
 - Elétrons, que circundam o núcleo.
- Elétrons e prótons são carregados eletricamente.
 - Elétrons tem carga *negativa*; prótons tem carga *positiva*; nêutrons não tem carga.
 - A magnitude da carga do próton e do elétron é $1,602 \times 10^{-19}\text{C}$.
- As massas são muito pequenas:
 - Prótons e nêutrons possuem massas quase iguais e que valem respectivamente $1,673 \times 10^{-27}\text{kg}$ e $1,675 \times 10^{-27}\text{kg}$.
 - Elétrons tem massa igual a $9,1095 \times 10^{-31}\text{kg}$.
- Cada elemento é caracterizado:
 - Pelo seu *número atômico* → número de prótons dentro do núcleo.
 - Pela sua *massa atômica* → soma do número de prótons e do número de nêutrons dentro do núcleo.



Modelos atômicos



Modelo de Bohr

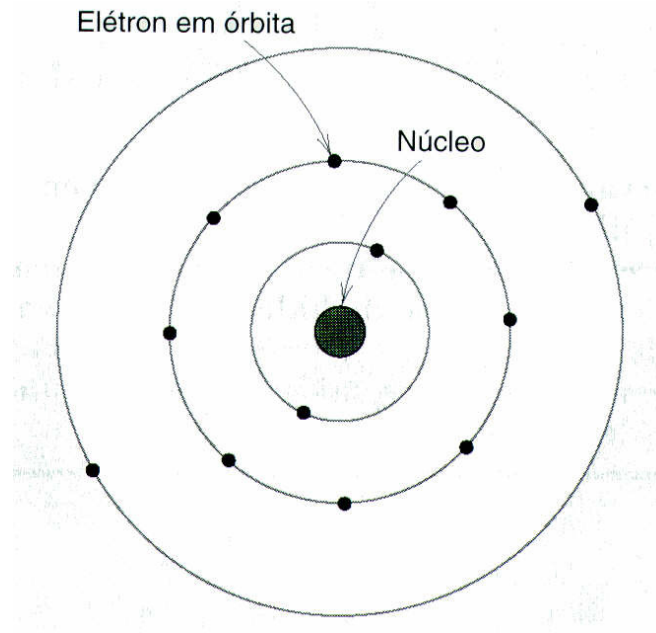
$$E = \frac{-2\pi^2me^4}{n^2h^2} = \frac{-13.6}{n^2} \text{ eV} \quad (\text{where } n = 1, 2, 3, \dots)$$

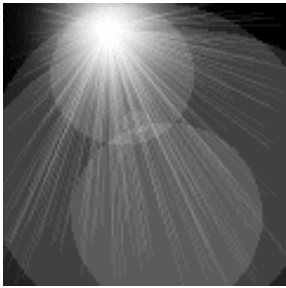
O modelo de Bohr apresenta limitações significativas, não servindo para explicar vários dos fenômenos nos quais estão envolvidos elétrons.



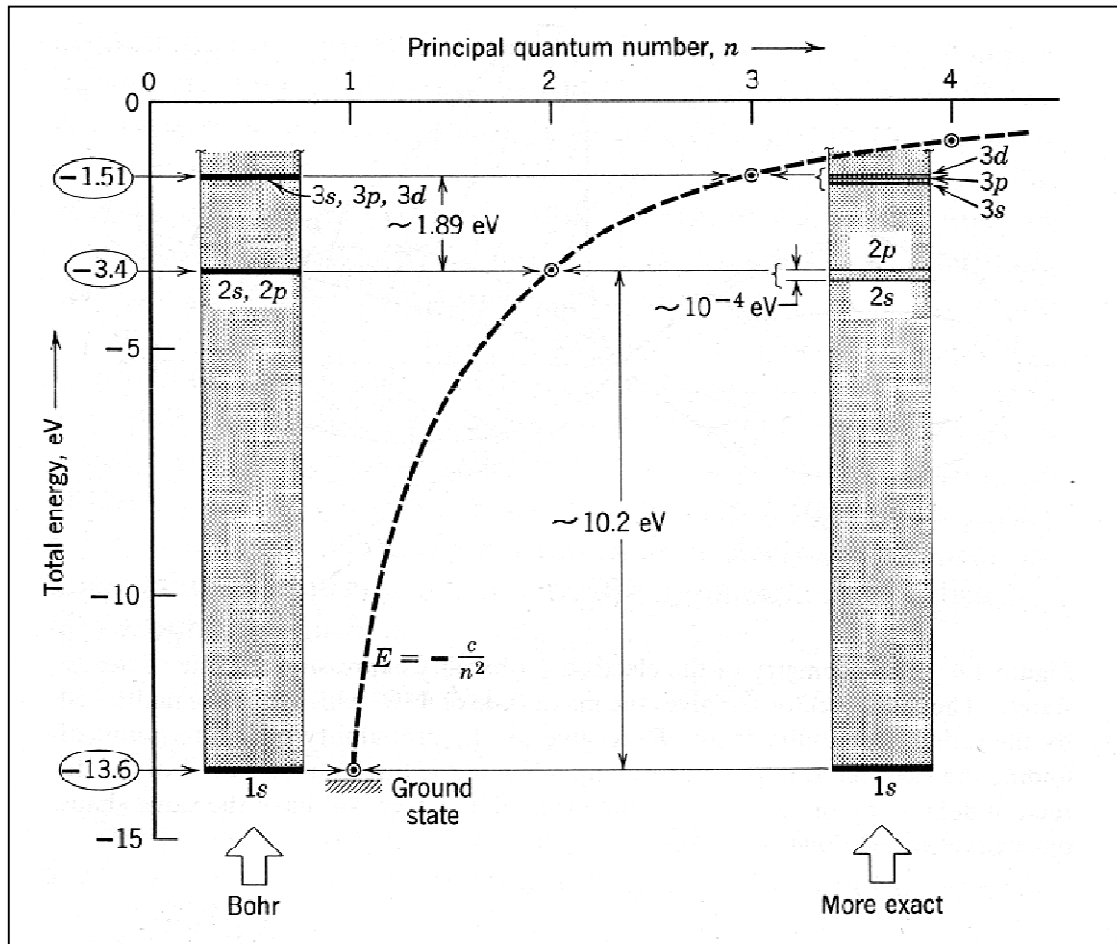
Átomo de Bohr

- Posição de cada elétron em particular é mais ou menos bem definida em termos do seu orbital.
- Energias dos elétrons são quantizadas → mudança de orbital é possível, com absorção (maior energia) ou emissão (menor energia) de energia.
- Estados adjacentes são separados por energias finitas.
- O modelo de Bohr apresenta limitações significativas, não servindo para explicar vários fenômenos envolvendo os elétrons.





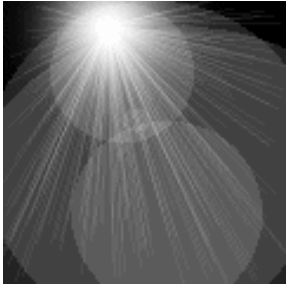
Modelo atômico da mecânica quântica



As deficiências do modelo de Bohr foram supridas pelo **modelo atômico da mecânica quântica**.

Neste modelo o elétron apresenta características tanto de onda quanto de partícula.

O elétron não é mais tratado como uma partícula que se movimenta num orbital discreto. Sua posição passa a ser considerada como a probabilidade de se encontrar um elétron em um local próximo do núcleo.

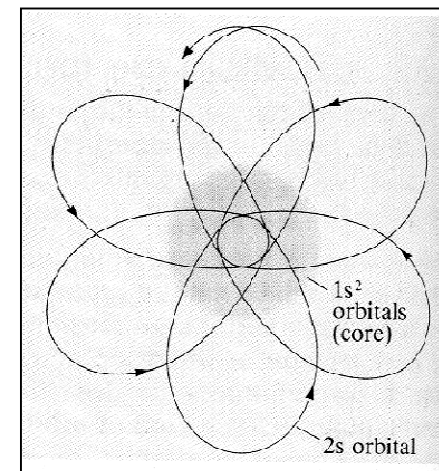
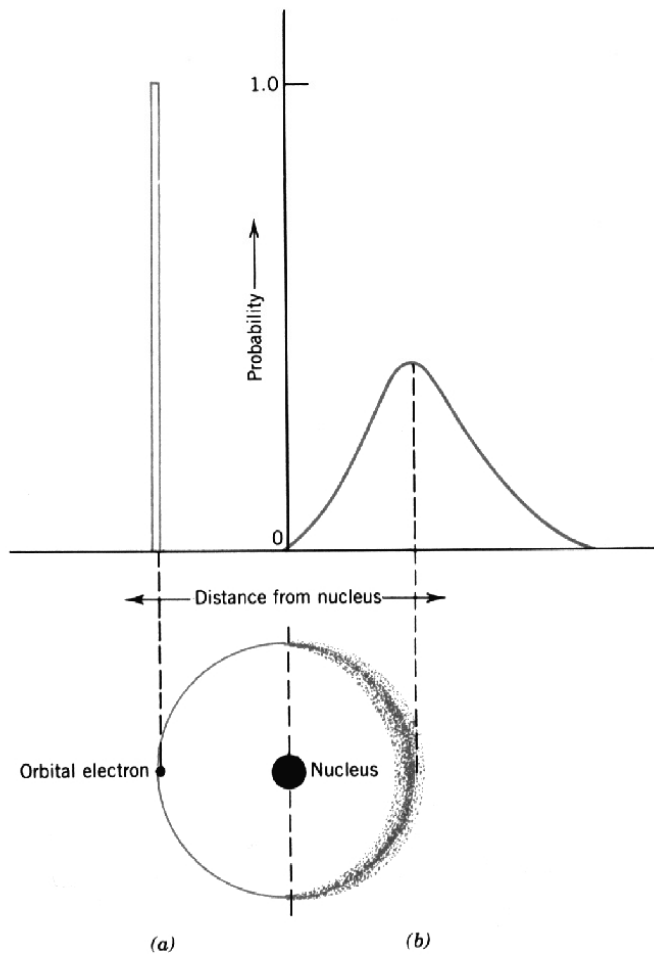


Modelo atômico da mecânica quântica

Distribuição eletrônica, segundo:

(a) modelo atômico de Bohr

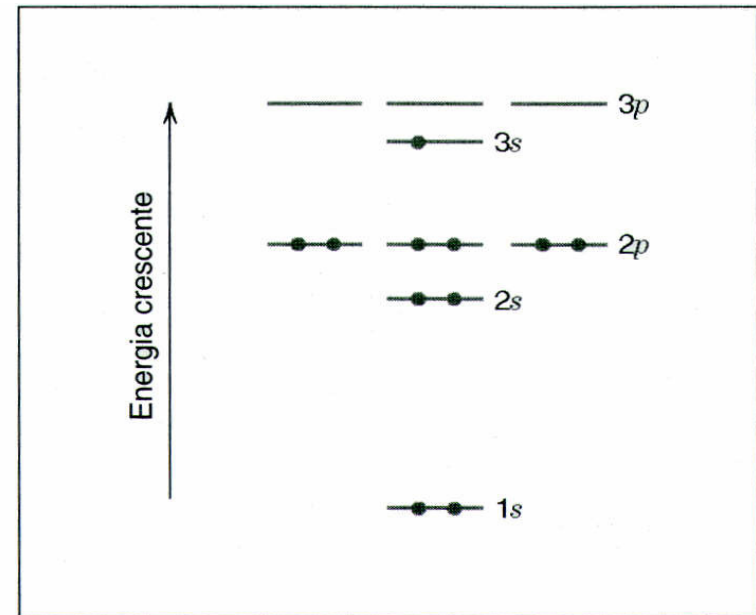
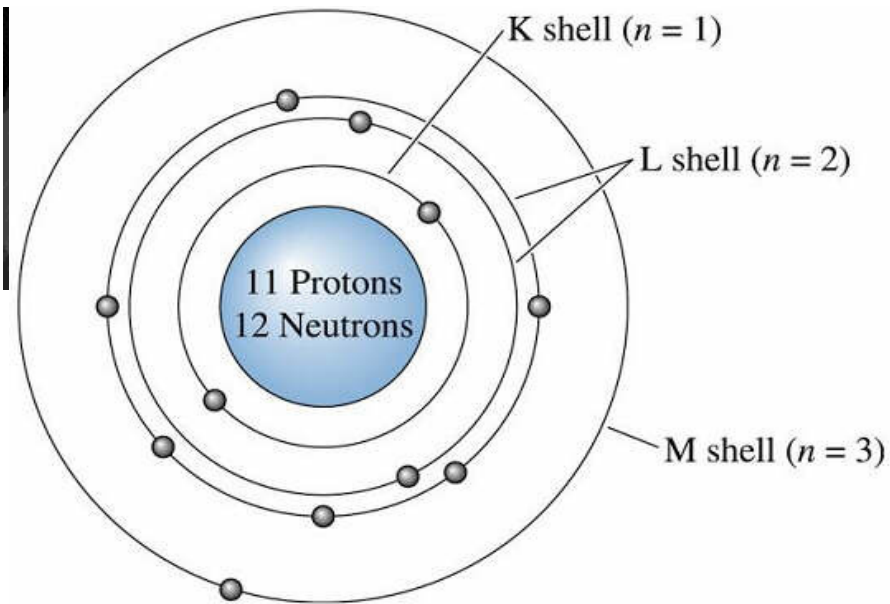
(b) mecânica quântica





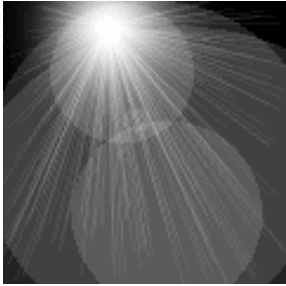
Números quânticos

- Cada elétron em um átomo é caracterizado por quatro parâmetros → os números quânticos.
- Não existem dois elétrons com os mesmos números quânticos.
- Número quântico principal n
 $n = 1, 2, 3, 4, 5, \dots$ (ou K, L, M, N, O,.....)
- Número quântico orbital (ou secundário) ℓ → subcamadas s, p, d, f, ...
 $\ell = 0, 1, 2, 3, 4, \dots, (n - 1)$
- Número quântico orbital magnético (ou terceiro) m_ℓ
 $m_\ell = -\ell, (-\ell + 1), \dots, (\ell - 1), \ell$
- Número quântico de spin (ou quarto) → $m_s = -1/2, +1/2$.



$3s^1$	electron 11	$n = 3, l = 0, m_l = 0, m_s = +\frac{1}{2}$ or $-\frac{1}{2}$
$2p^6$	electron 10	$n = 2, l = 1, m_l = +1, m_s = -\frac{1}{2}$
	electron 9	$n = 2, l = 1, m_l = +1, m_s = +\frac{1}{2}$
	electron 8	$n = 2, l = 1, m_l = 0, m_s = -\frac{1}{2}$
	electron 7	$n = 2, l = 1, m_l = 0, m_s = +\frac{1}{2}$
	electron 6	$n = 2, l = 1, m_l = -1, m_s = -\frac{1}{2}$
	electron 5	$n = 2, l = 1, m_l = -1, m_s = +\frac{1}{2}$
$2s^2$	electron 4	$n = 2, l = 0, m_l = 0, m_s = -\frac{1}{2}$
	electron 3	$n = 2, l = 0, m_l = 0, m_s = +\frac{1}{2}$
$1s^2$	electron 2	$n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$
	electron 1	$n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$

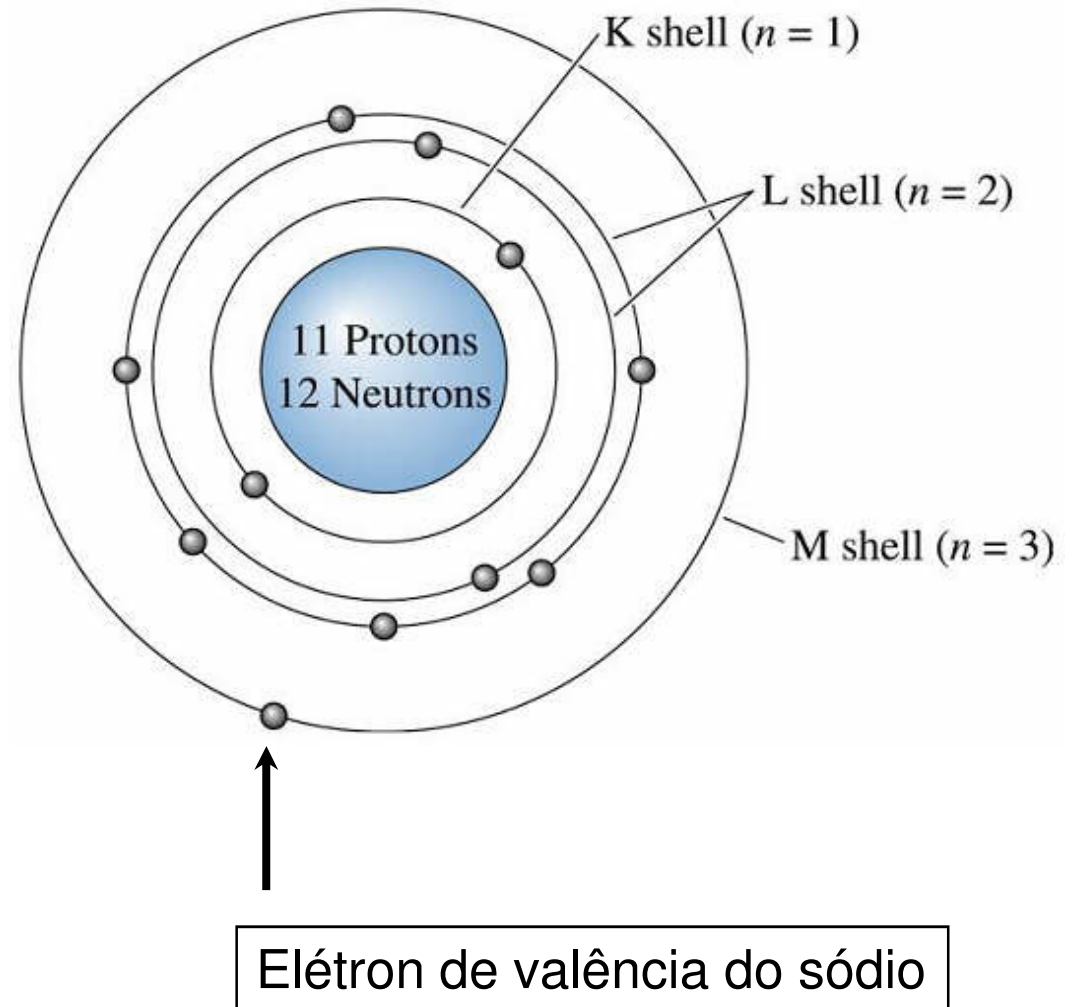
EXEMPLO
Configuração Eletrônica do Átomo de Sódio



Elétrons de Valência

Configurações Estáveis

- **Elétrons de Valência**
 - São aqueles que ocupam a camada eletrônica mais externa.
- **Configurações Eletrônicas Estáveis**
 - As camadas eletrônicas mais externas estão completamente preenchidas.





Mecânica quântica

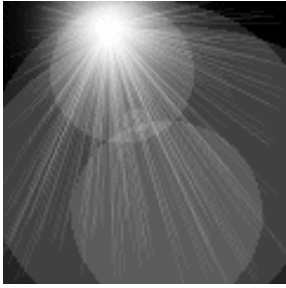
Equação de Einstein
(~ 1910)

$$\Delta E = E_2 - E_1 = h\nu \quad (1.1)$$

Princípio da incerteza

$$\Delta p_x \Delta x \geq \frac{h}{2\pi} \quad (1.2)$$

$$\Delta E \Delta t \geq \frac{h}{2\pi} \quad (1.3)$$



Mecânica ondulatória e mecânica quântica

De Broglie (1924)

$$\lambda = \frac{h}{p} \quad (1.4)$$

Equação da corda vibrante

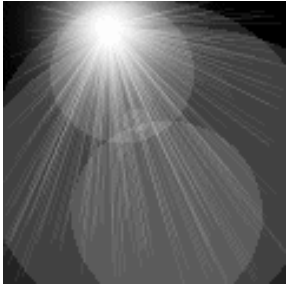
$$\frac{d^2u}{dx^2} + \frac{4\pi^2}{\lambda^2} u = 0 \quad (1.5)$$

Equação de Schrödinger (1926)

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - V)\psi = 0 \quad (1.6)$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2m}{h^2} (E - V)\psi = 0 \quad (1.7)$$

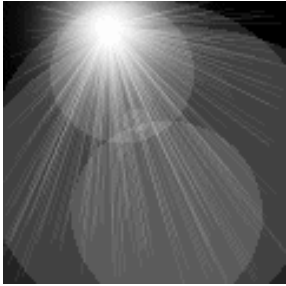
$$\nabla^2\psi + \frac{8\pi^2m}{h^2} (E - V)\psi = 0$$



Números quânticos

Table 1.1 Permissible Values of the Three Quantum Numbers

QUANTUM NUMBER	PERMISSIBLE VALUES
n	1, 2, 3, 4, 5, 6, . . . (n)
l	0(<i>s</i>), 1(<i>p</i>), 2(<i>d</i>), 3(<i>f</i>), . . . ($n - 1$)
m	+ l , . . . , +1, 0, -1, . . . , - l



6 Electrons and Bonding

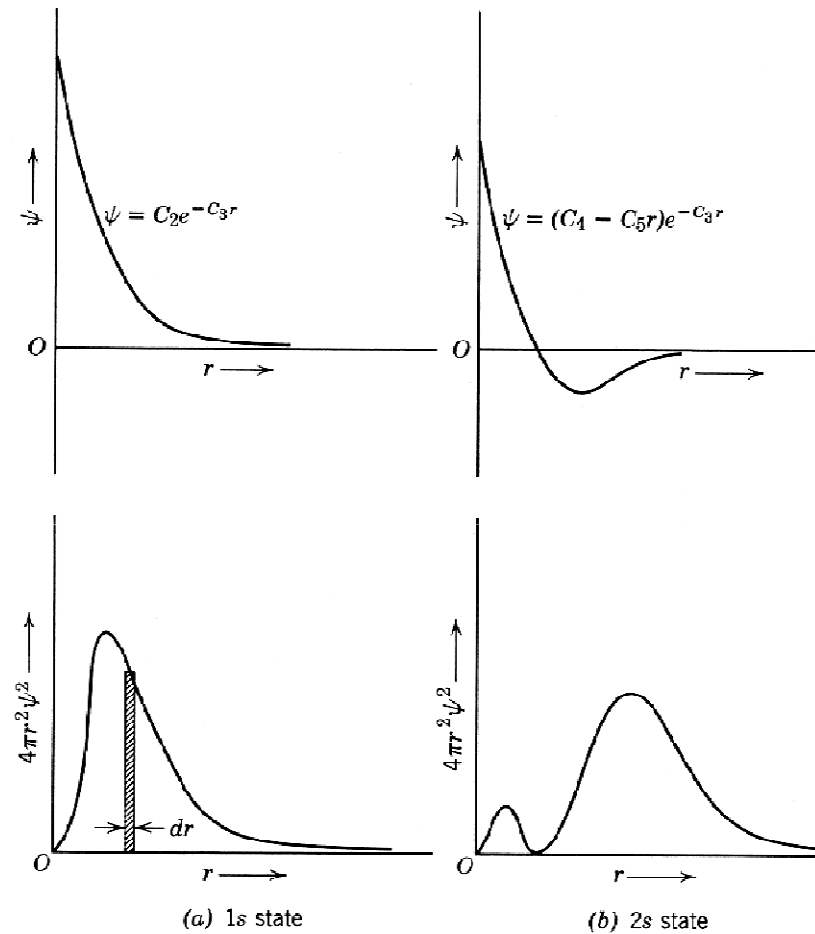
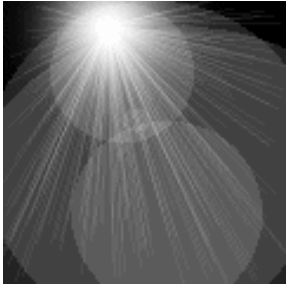


Figure 1.2 Qualitative curves of ψ and of $4\pi r^2 \psi^2 dr$ versus r for single electrons in the 1s ($n = 1$) state and the 2s ($n = 2, l = 0$) state. The cross-hatched strip in (a) has the area $(4\pi r^2 \psi^2)(dr)$ and is thus the probability of finding the electron between r and $r + dr$. The values of the constants, C_2 to C_6 , are determined by the boundary conditions imposed on the wave equation.



Soluções da Equação de Schrödinger

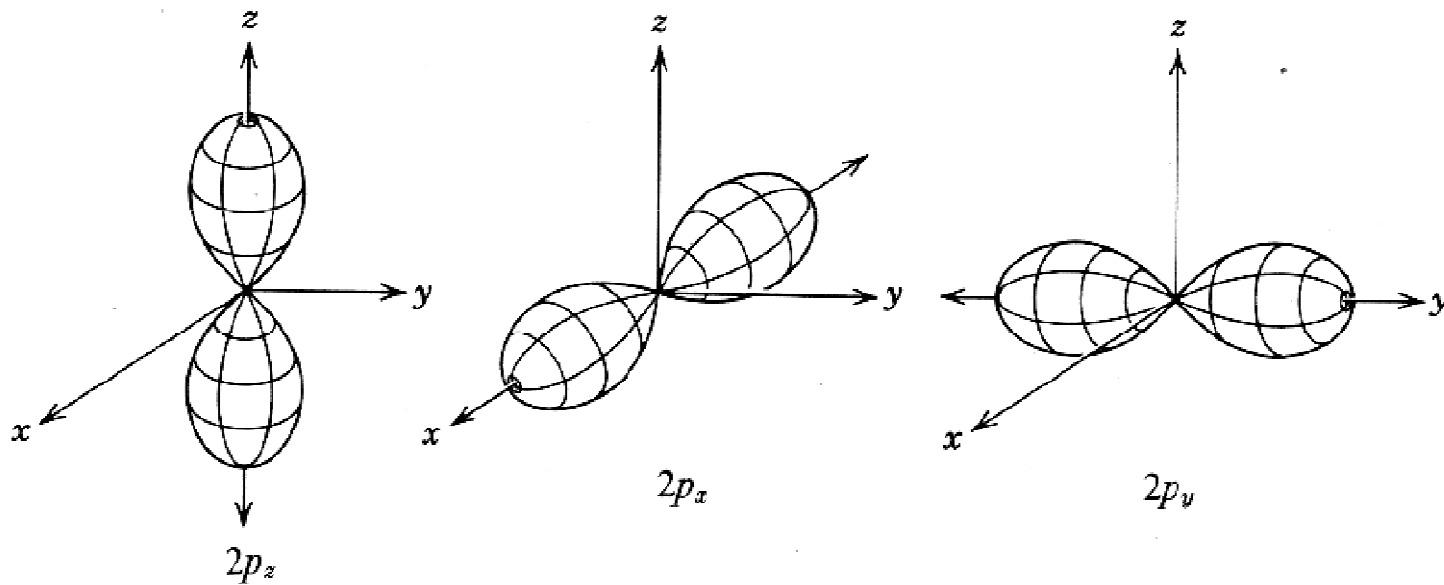
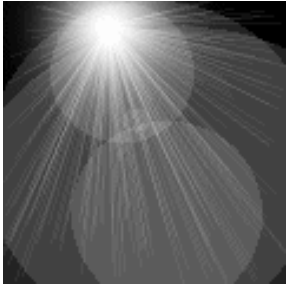


Figure 1.3 The angular dependent probability factors for the three $2p$ states often used in atomic bonding.



Soluções da Equação de Schrödinger

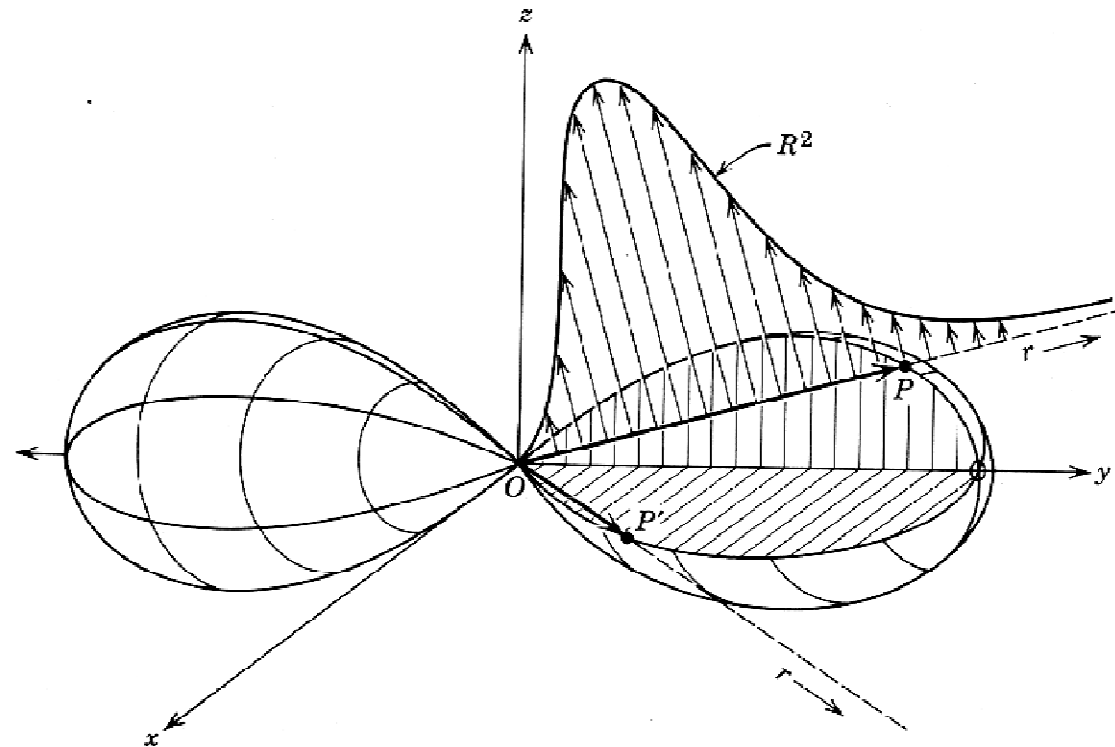
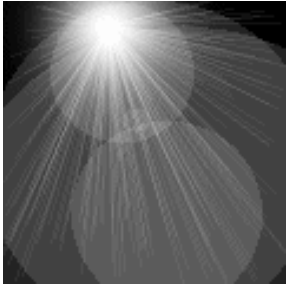


Figure 1.4 The geometry of the electron probability expression for one of the $2p$ states. The radius vector \overline{OP} gives the magnitude of $\Phi^2\Theta^2$ which must be multiplied by the radial probability factor R^2 to give ψ^2 , the probability per unit volume of finding the electron at any radius r along a line in the direction of \overline{OP} . For the direction defined by the vector $\overline{OP'}$, the probability curve will have the same shape but will be scaled down since $|\overline{OP'}| < |\overline{OP}|$.



Soluções da Equação de Schrödinger

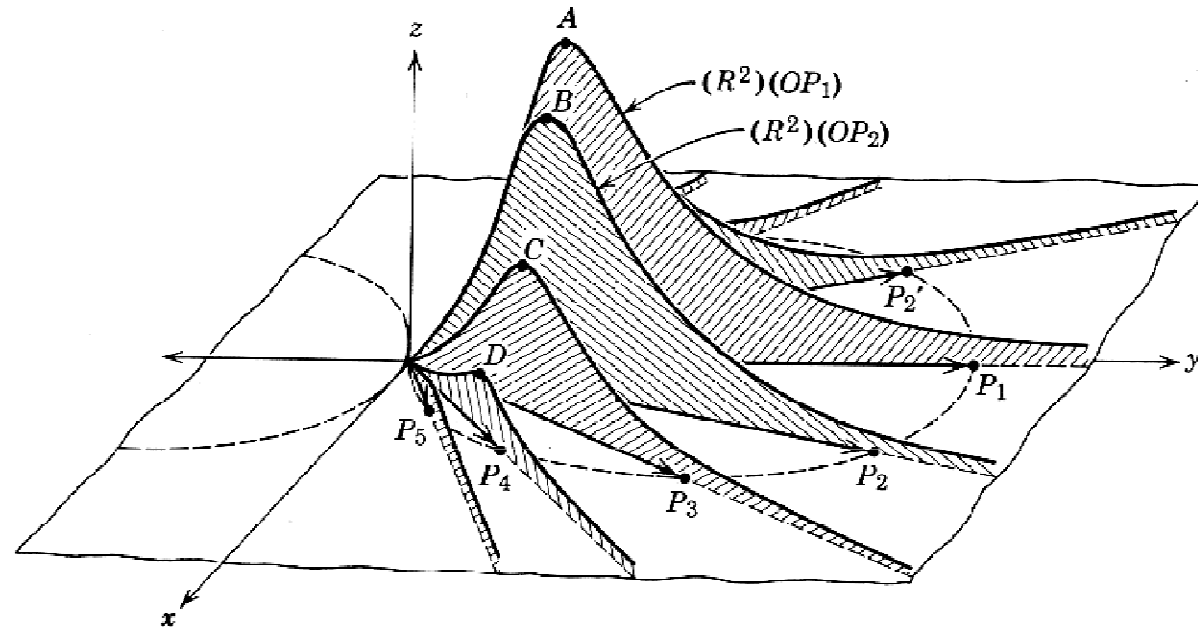
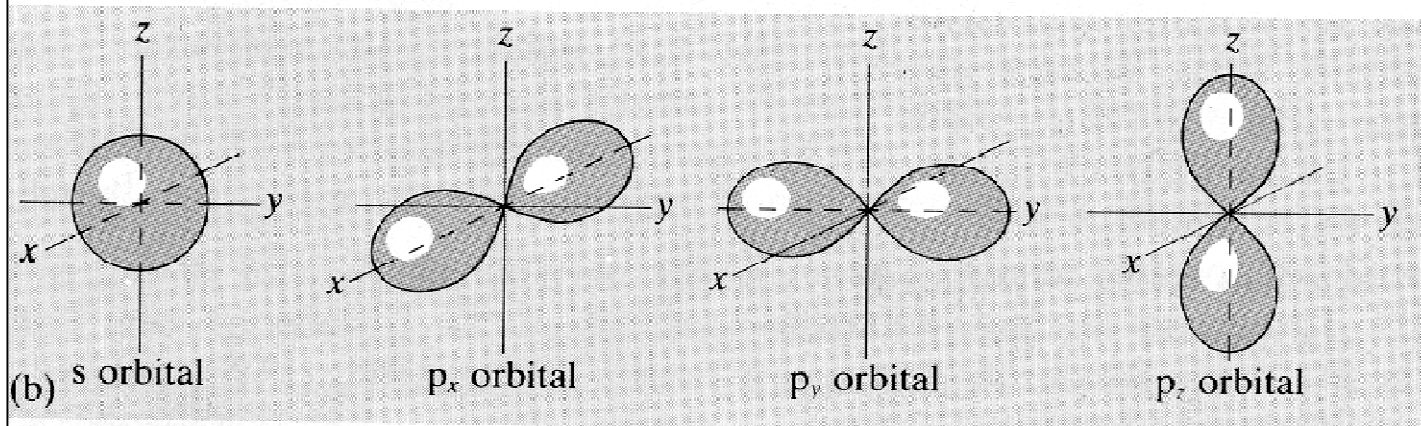
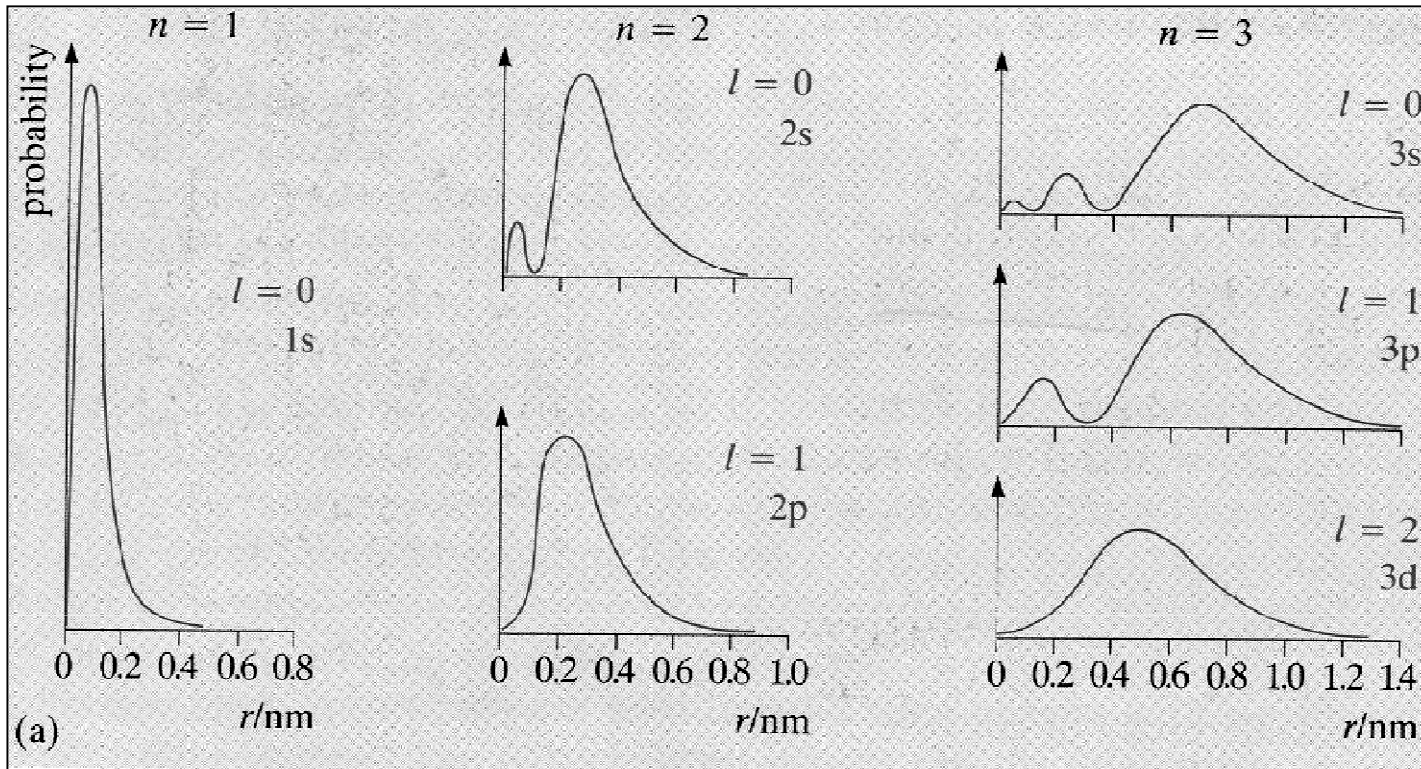
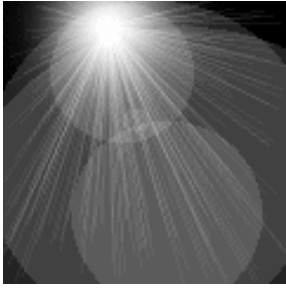


Figure 1.5 Representation of ψ^2 on the xy plane for the $2p$ state in Figure 1.4. The ordinate of the curves gives the probability per unit volume (ψ^2) of finding the electron at various points on the xy plane. The ratios of heights of the ordinates $A:B:C:D$ are the same as the ratios of the lengths $|\overline{OP}_1| : |\overline{OP}_2| : |\overline{OP}_3| : |\overline{OP}_4|$ because the radial probability factor R^2 is the same for all curves. The dashed curve is the angular dependent probability factor, $\Phi^2\Theta^2$.



Átomo de hidrogênio

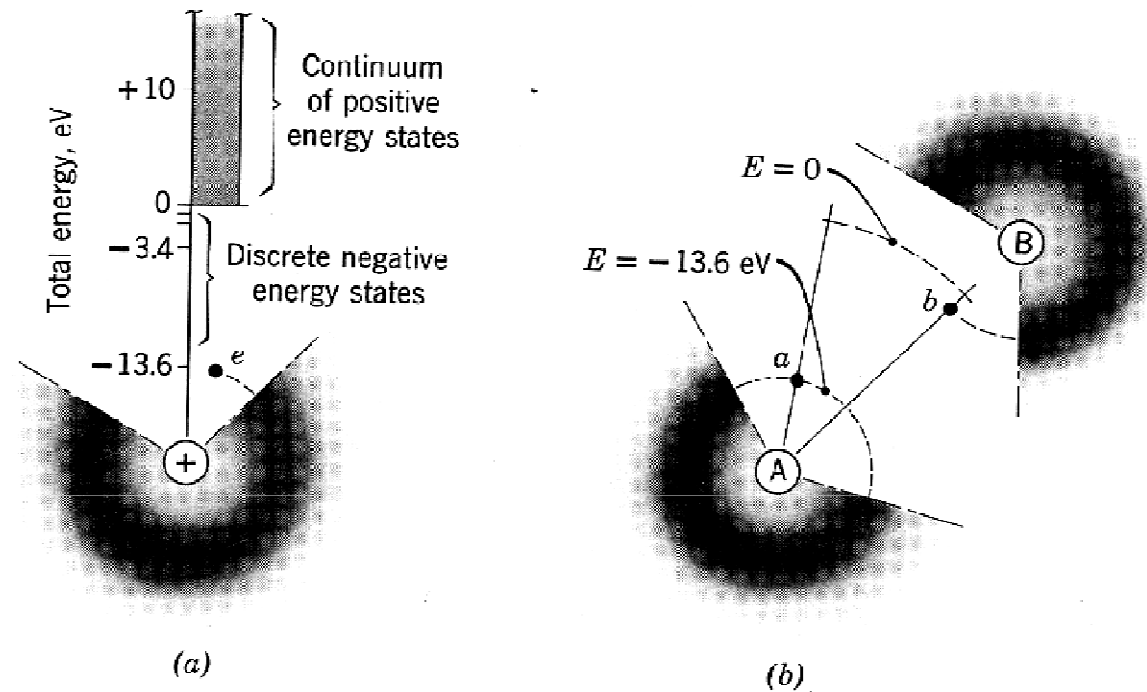
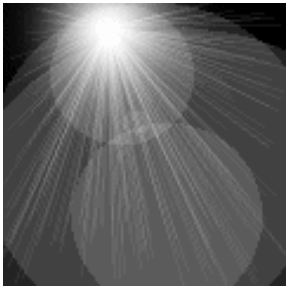


Figure 1.7 Energy levels for the hydrogen atom. (a) The free atom; the total energy of the electron is at a minimum with respect to its nucleus. (b) A pair of hydrogen atoms with electron clouds just starting to overlap. Electron *a* has minimum energy with respect to nucleus **A** but can lower its energy with respect to nucleus **B** if it moves closer to it. Simultaneously, the energy of electron *b* with respect to nucleus **A** will be lowered if the atoms move closer together.



Molécula de hidrogênio

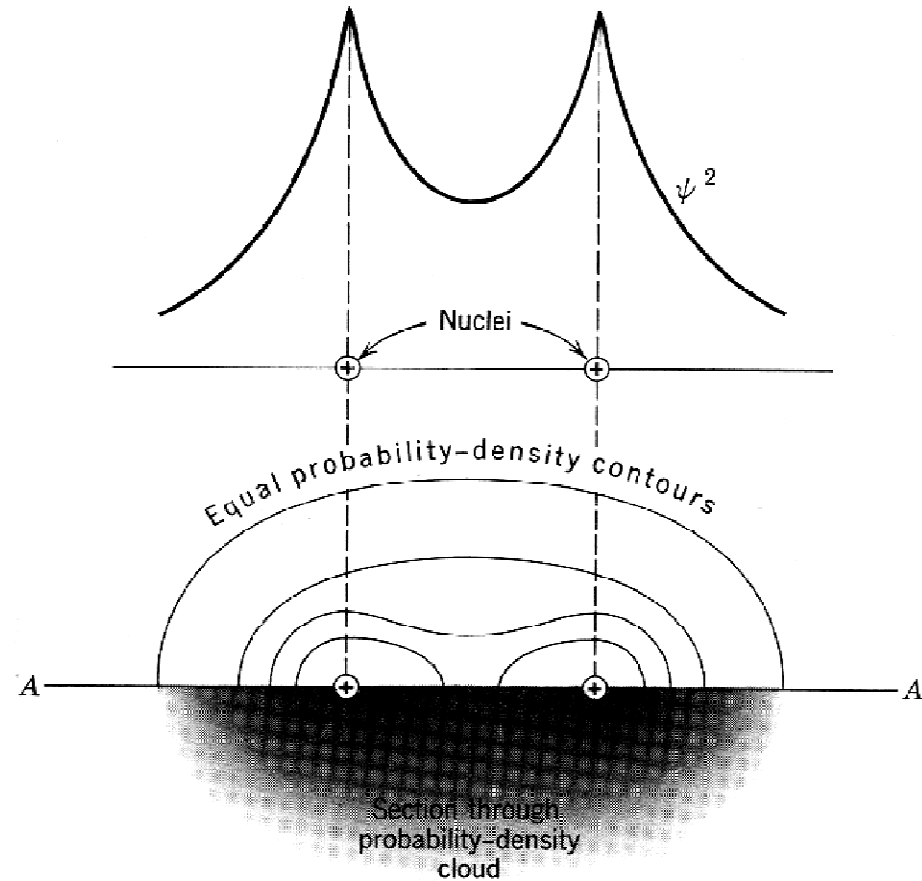
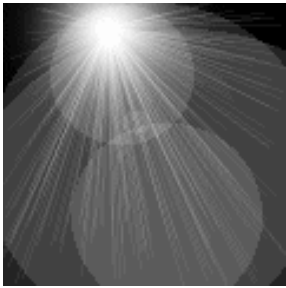
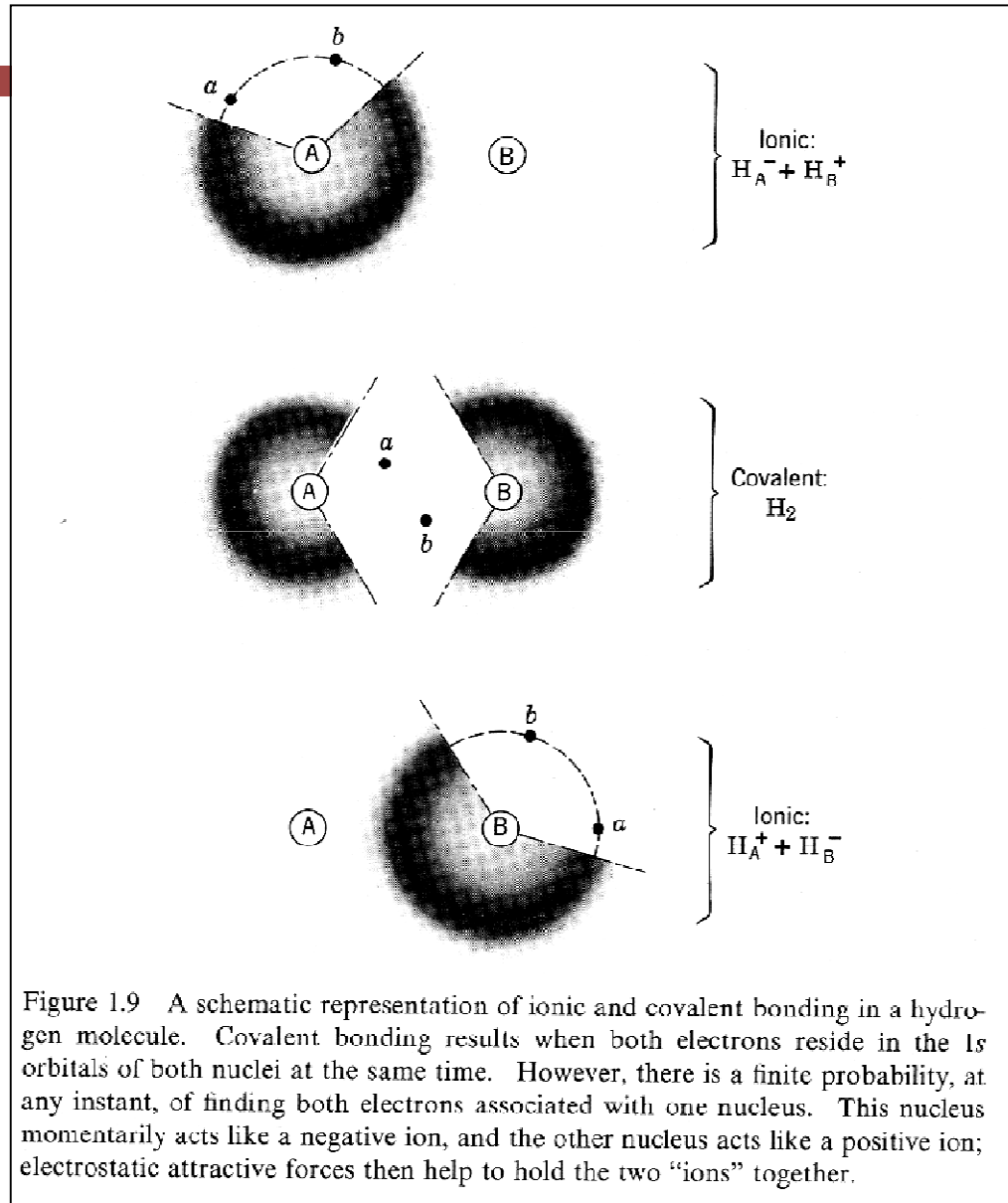
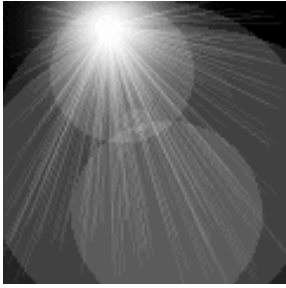


Figure 1.8 The probability density (probability per unit volume), ψ^2 , along the line joining two nuclei of a hydrogen molecule (upper curve), and contours of equal probability density for a section through the nuclei. The probability density is rotationally symmetric around the line $A-A$ passing through the nuclei.

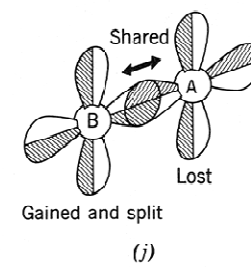
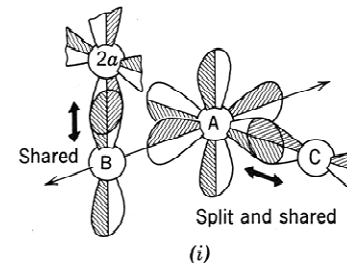
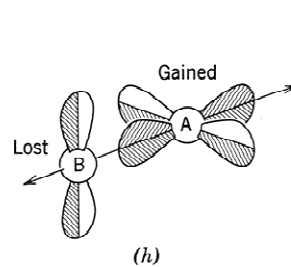
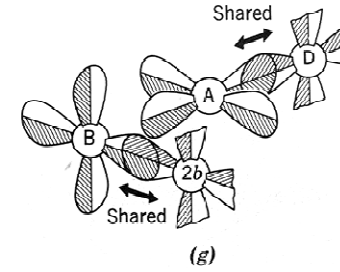
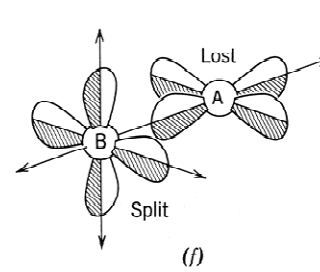
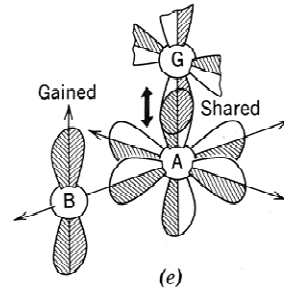
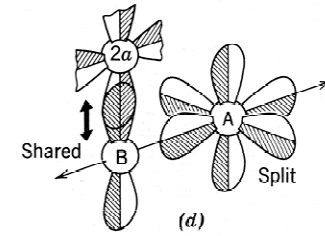
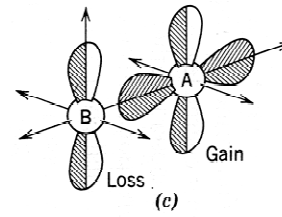
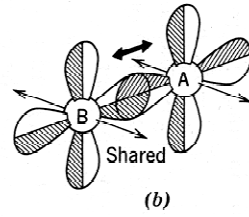
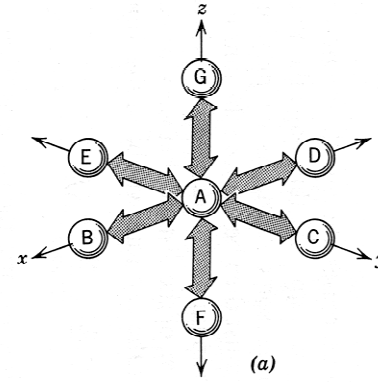


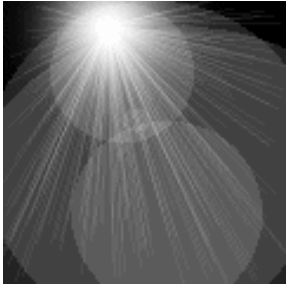
Ligação iônica e covalente





Ligação metálica





Transição contínua entre tipos de ligação

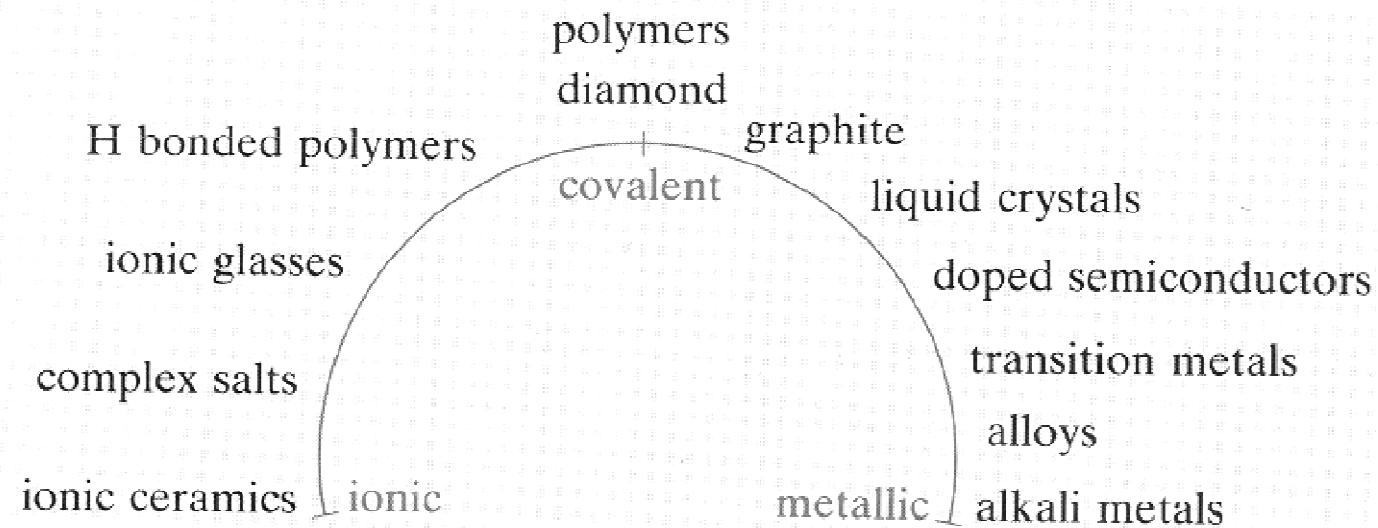
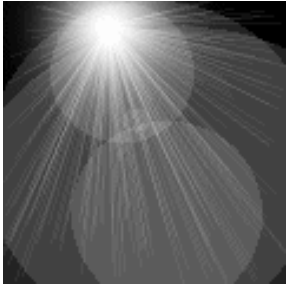
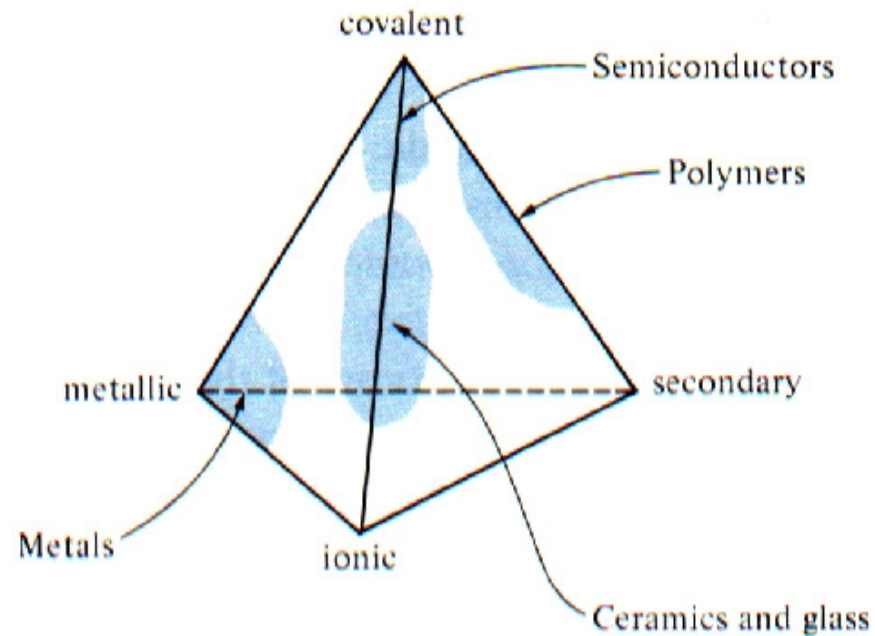


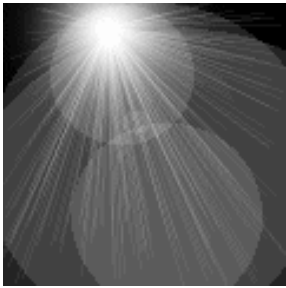
Figure 3.9 A continuum of bonding types



MATERIAIS SEGUNDO O TIPO DE LIGAÇÃO



Tetraedro que representa a contribuição relativa dos diferentes tipos de ligação para as quatro categorias fundamentais de materiais de engenharia (metais, cerâmicas, polímeros e semicondutores)



Distância de equilíbrio entre átomos ou íons

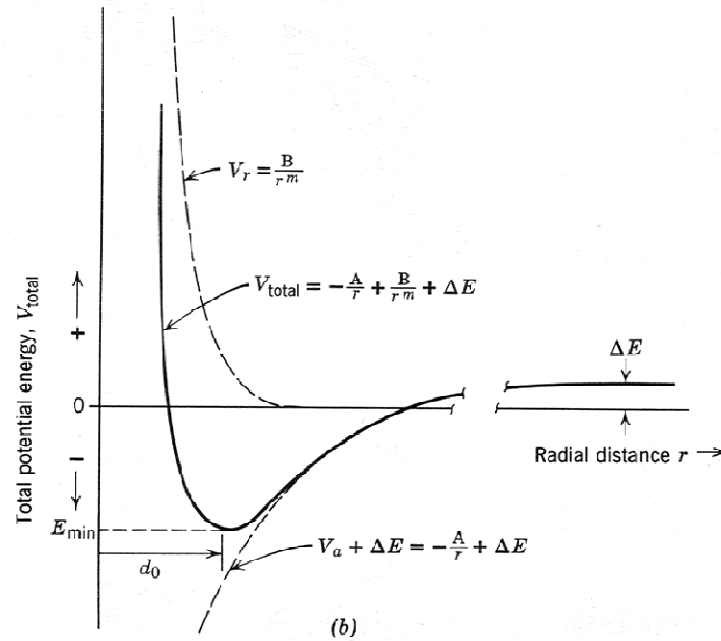
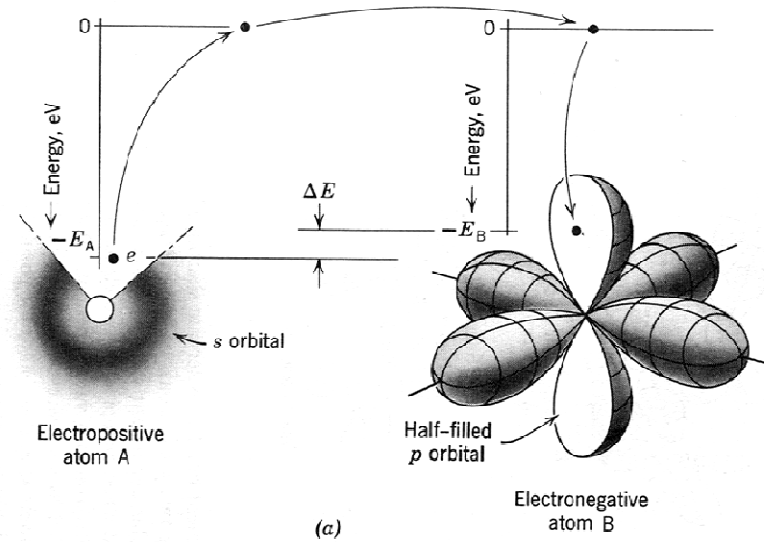
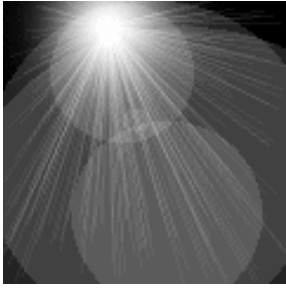
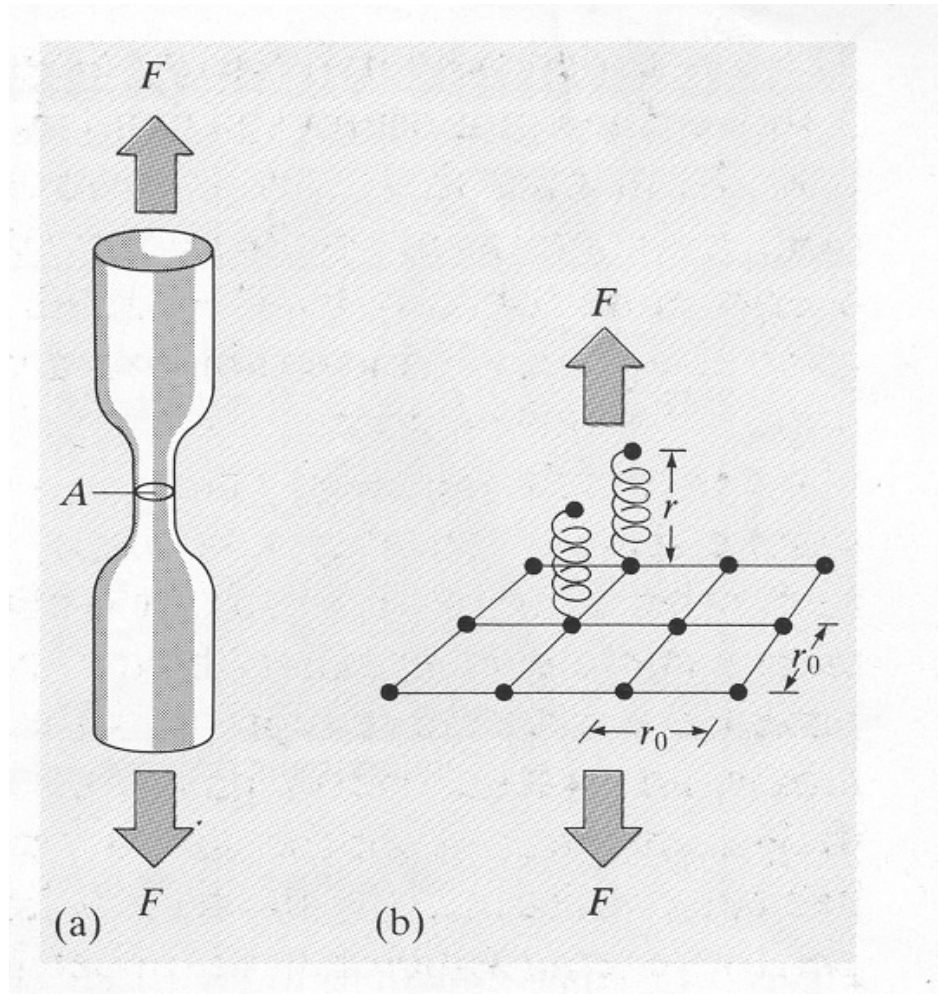
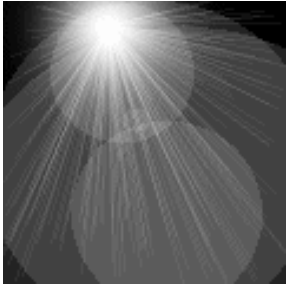


Figure 1.11 Over-all energy changes associated with the formation of a pair of ions from the free atoms and with the formation of an ionic bond. (a) The energy level changes in the formation of a pair of ions from free atoms. (b) The total potential of an ion pair as a function of radial distance from one ion. The distance $|d_0|$ is the equilibrium distance between the two ions.

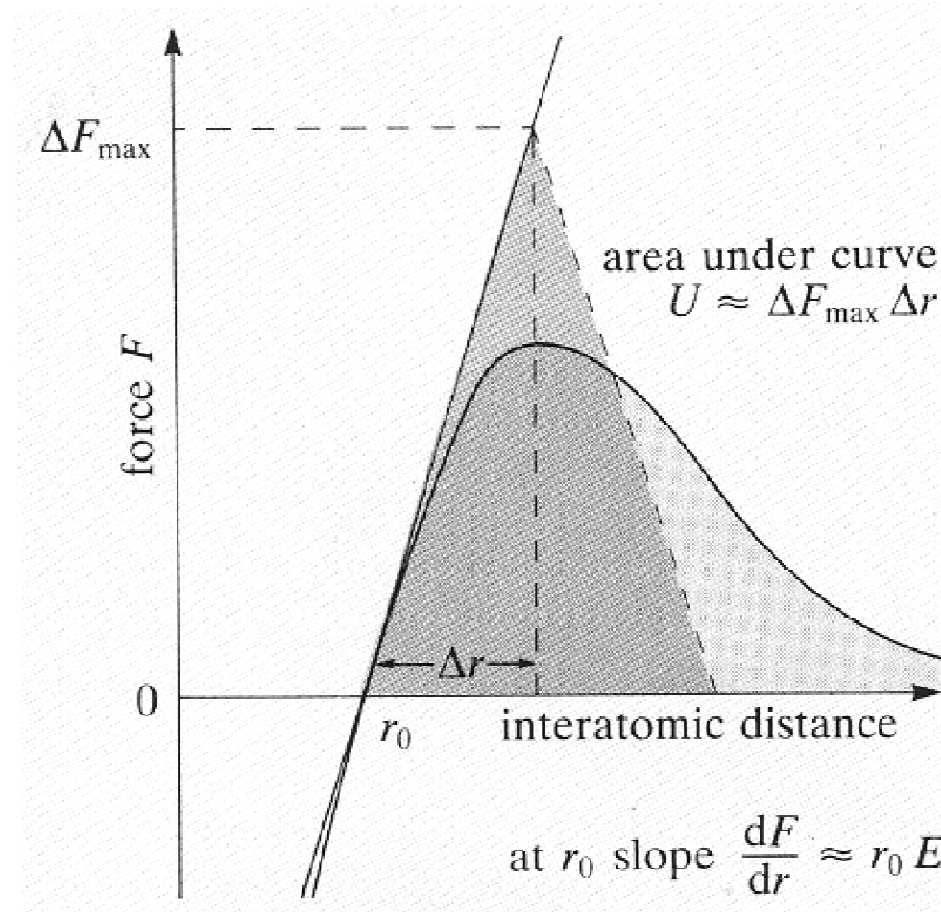


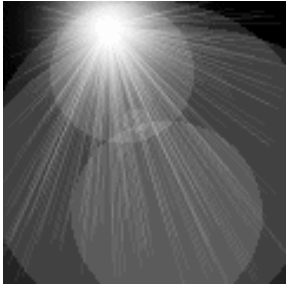
VISÃO ATÔMICA DO MÓDULO DE ELASTICIDADE





VISÃO ATÔMICA DA FRATURA





Algumas propriedades de materiais

Table 3.1

Substance	Young's modulus $E/\text{GN m}^{-2}$	Melting temperature T/K	Surface energy $\gamma/\text{J m}^{-2}$	Atom spacing r_0/nm	Tensile strength $\sigma/\text{GN m}^{-2}$	
					observed (in buk)	calcula
alumina	345	2320	1.0	0.22	0.7	
copper	190	1360	1.7	0.21	0.4*	
diamond	1200	> 4000	5.4	0.16†	50	
glass (pristine fibre)	70	1400	0.5	0.35	3.6	
graphite	200	> 3770	0.07‡	0.36‡	0.1	
iron (wrought)	200	1810	2.0	0.29	0.20*	
salt (NaCl)	44	1073	0.12	0.27	0.1	
silicon (single crystal)	190	1680	1.2	0.22	3.3	
tungsten	360	3650	3.0	0.16	1.5*	

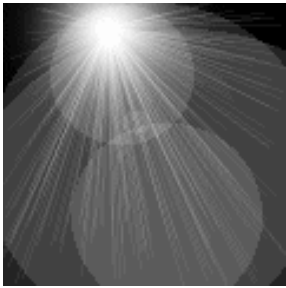





TABELA PERIÓDICA

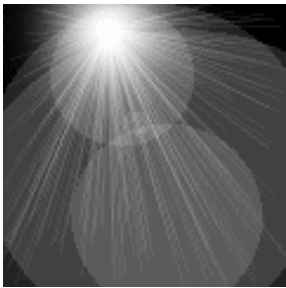
Os elementos químicos são classificados de acordo com a sua configuração eletrônica.

Key

- Atomic number
- Symbol
- Atomic weight

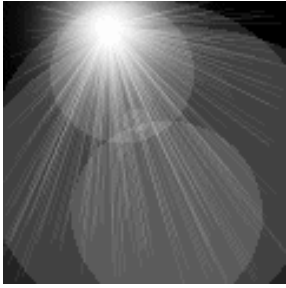
 Metal
 Nonmetal
 Intermediate

IA																	0				
1 H 1.0080																	2 He 4.0026				
3 Li 6.939	4 Be 9.0122															5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.183
11 Na 22.990	12 Mg 24.312															13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.54	30 Zn 65.37	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.91	36 Kr 83.80				
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30				
55 Cs 132.91	56 Ba 137.34	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)				
87 Fr (223)	88 Ra (226)	Actinide series																			
Rare earth series		57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97					
Actinide series		89 Ac (227)	90 Th 232.04	91 Pa (231)	92 U 238.03	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lw (257)					



A eletronegatividade dos elementos

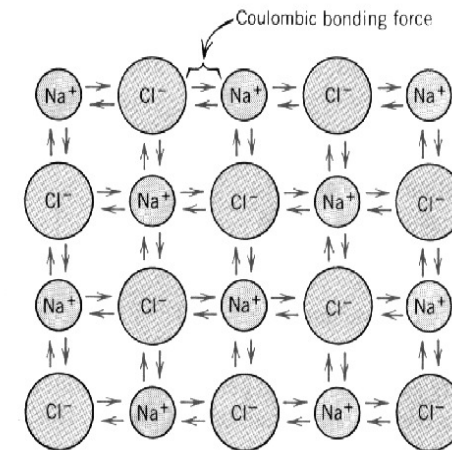
IA												IIIA					IVA	VA	VIA	VIIA	0
1 H 2.1												5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne -				
IIA												III A	IV A	V A	VI A	VII A	0				
3 Li 1.0	4 Be 1.5											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar -				
11 Na 0.9	12 Mg 1.2	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar -				
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr -				
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe -				
55 Cs 0.7	56 Ba 0.9	57-71 La-Lu 1.1-1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn -				
87 Fr 0.7	88 Ra 0.9	89-102 Ac-No 1.1-1.7																			



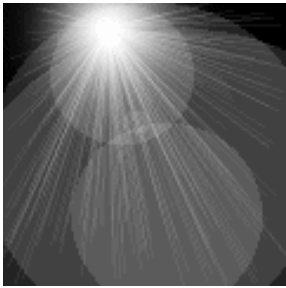
LIGAÇÕES PRIMÁRIAS

LIGAÇÃO IÔNICA

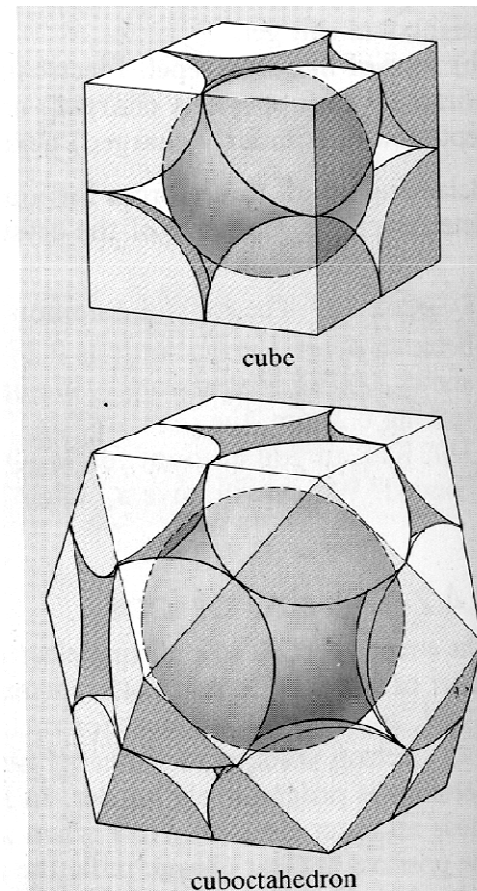
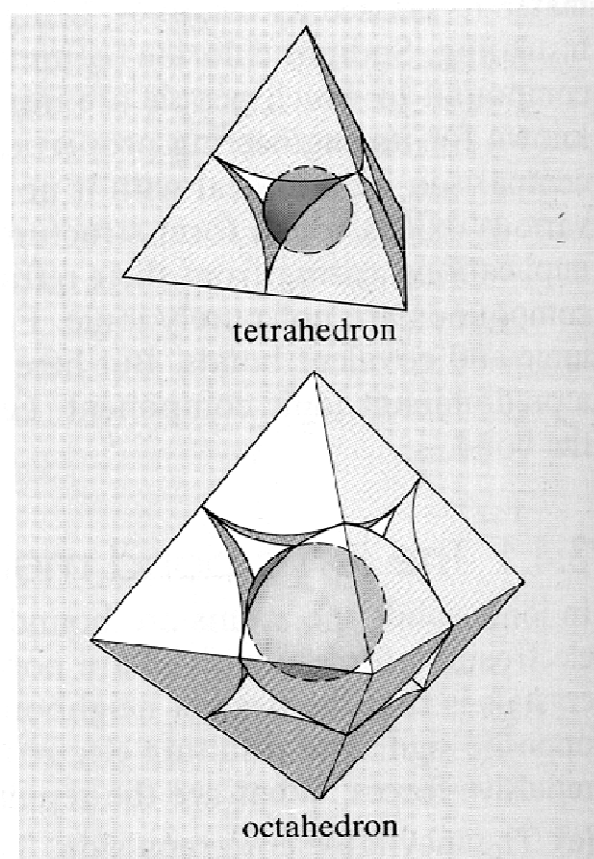
- envolve a transferência de elétrons de um átomo para outro
- a ligação é não-direcional
- a ligação iônica resulta da atração eletrostática entre dois íons de cargas opostas

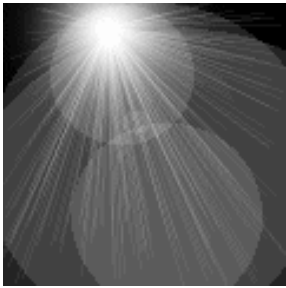


Exemplo: Para o cloreto de sódio, tanto o cátion Na^+ quanto o ânion Cl^- ficam com seus orbitais externos completos.

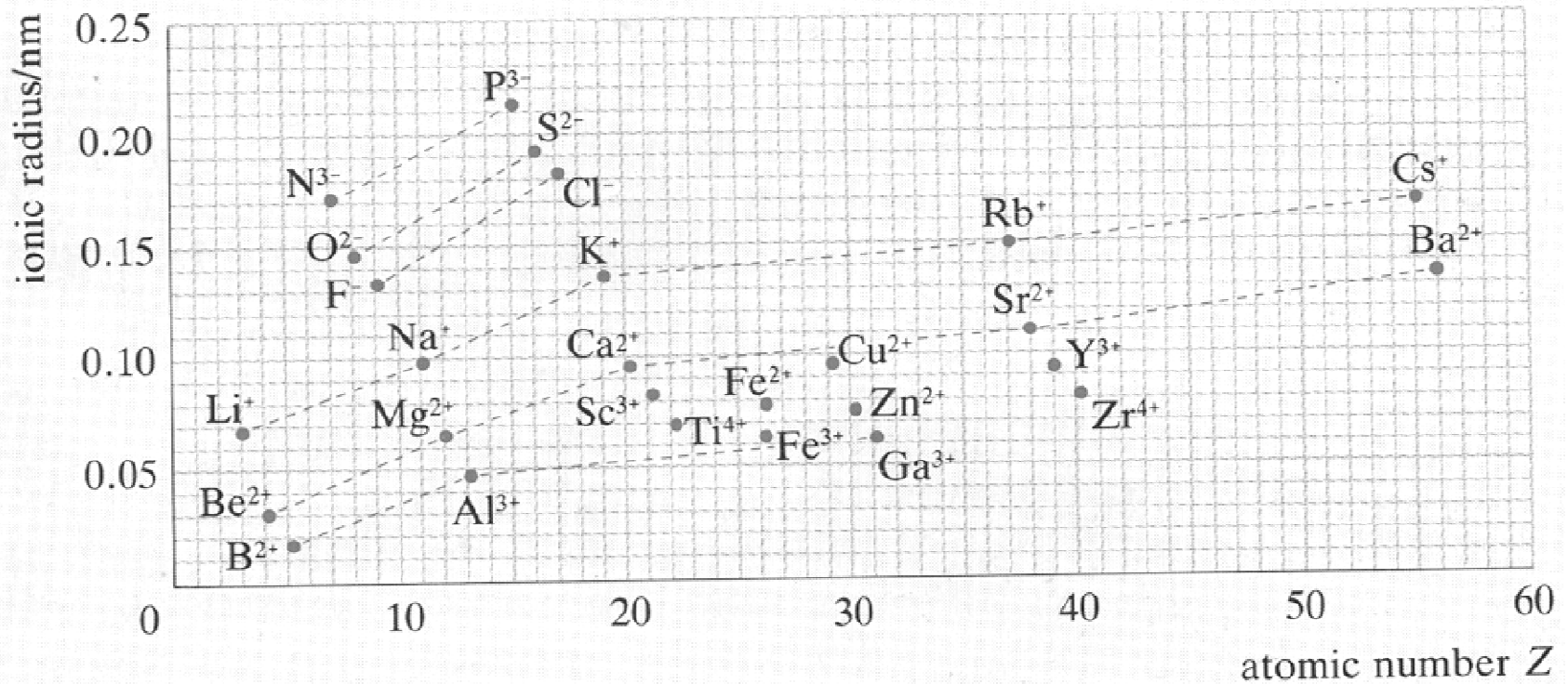


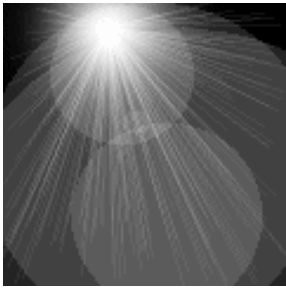
CRISTAIS IÔNICOS





CRISTAIS IÔNICOS

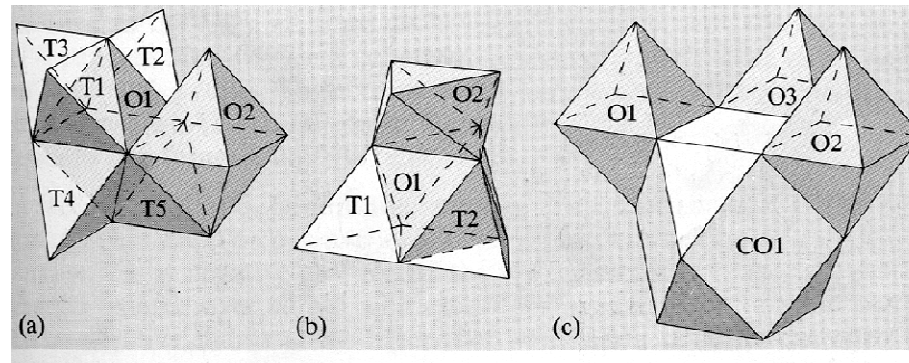


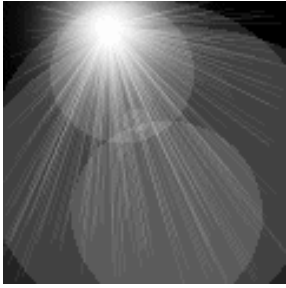


CRISTAIS IÔNICOS

Table 3.2

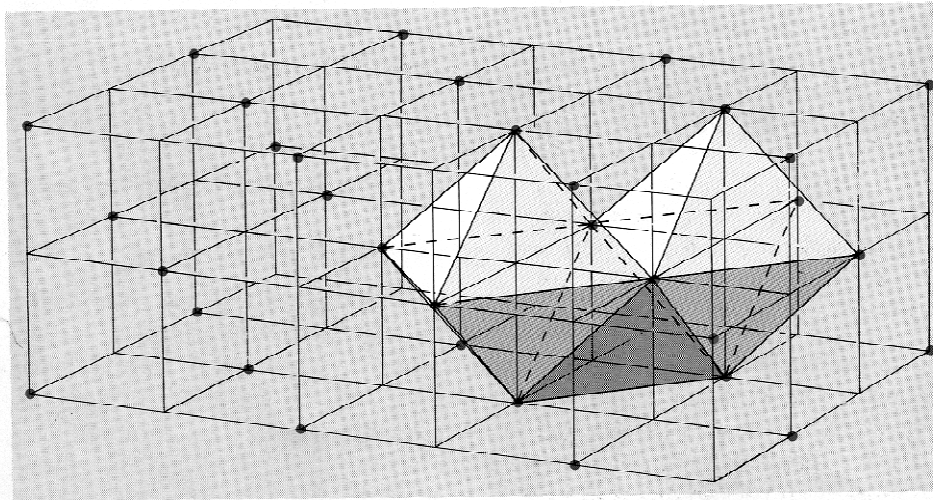
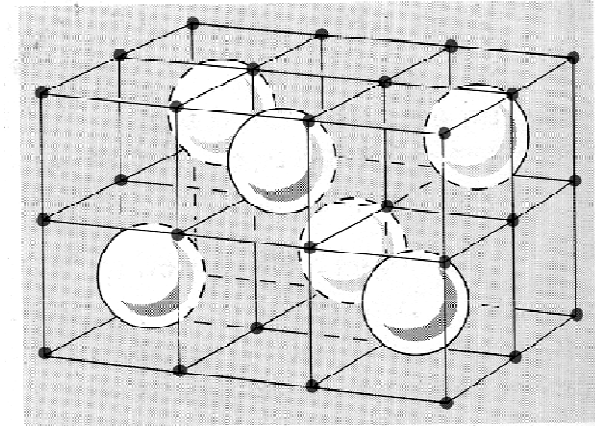
Coordination number	Cage size	Geometry
4	$0.22 R$	tetrahedron
6	$0.41 R$	octahedron
8	$0.73 R$	cube
12	$1.0 R$	cuboctahedron



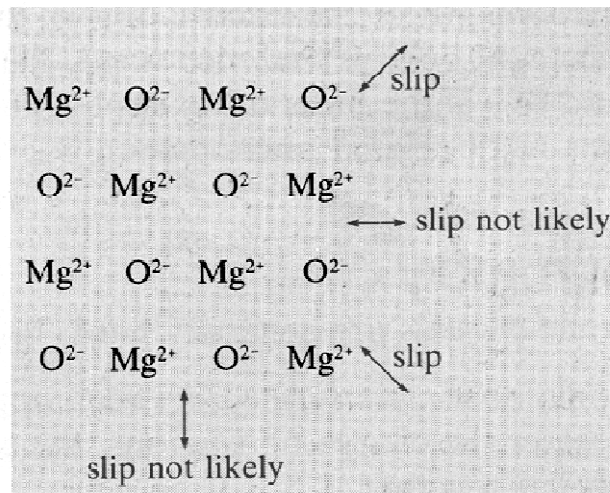


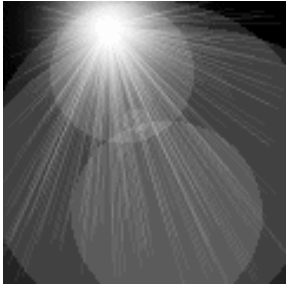
CRISTAIS IÔNICOS

Óxido de urânio



Óxido de magnésio





LIGAÇÕES PRIMÁRIAS

LIGAÇÃO COVALENTE

- compartilhamento dos elétrons de valência de dois átomos adjacentes
- a ligação resultante é altamente direcional

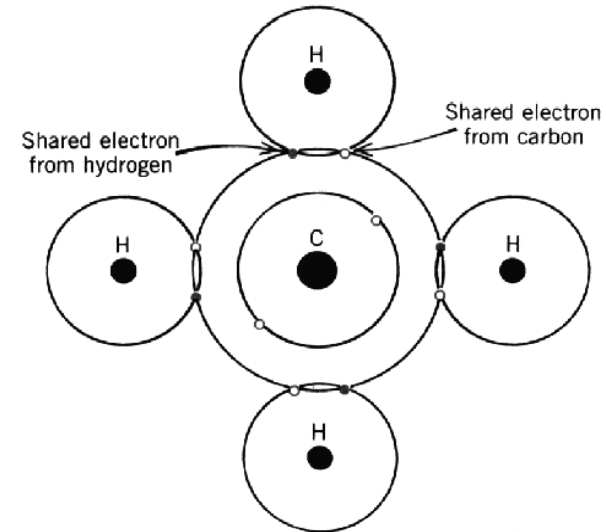
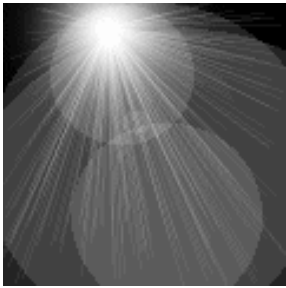
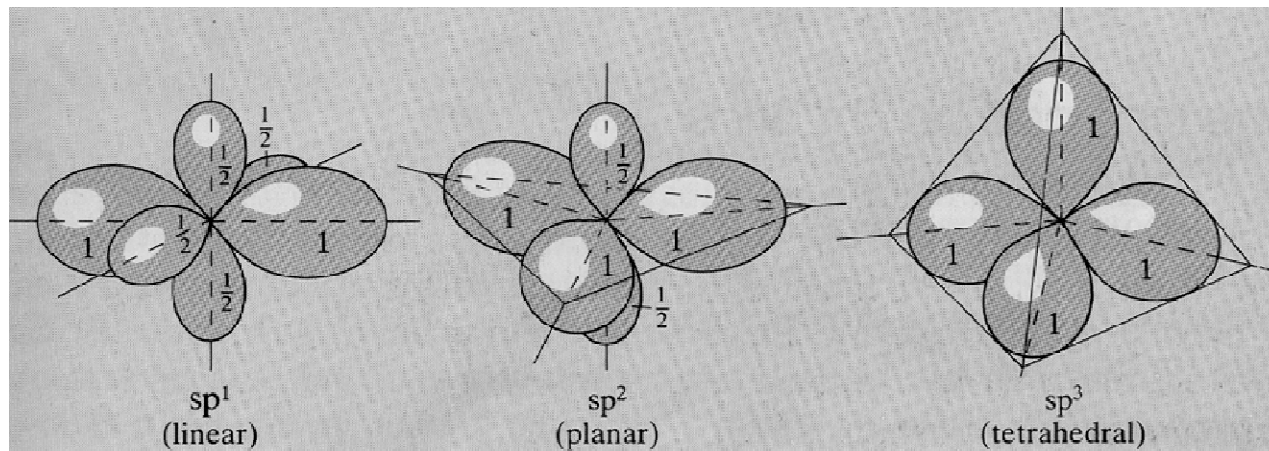
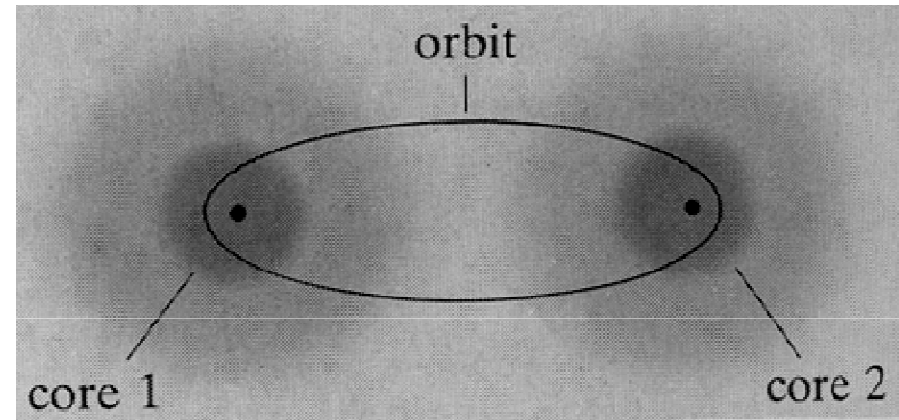


FIGURE 2.10 Schematic representation of covalent bonding in a molecule of methane (CH_4).

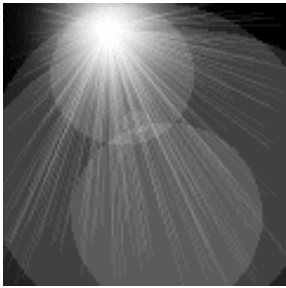


COVALÊNCIA

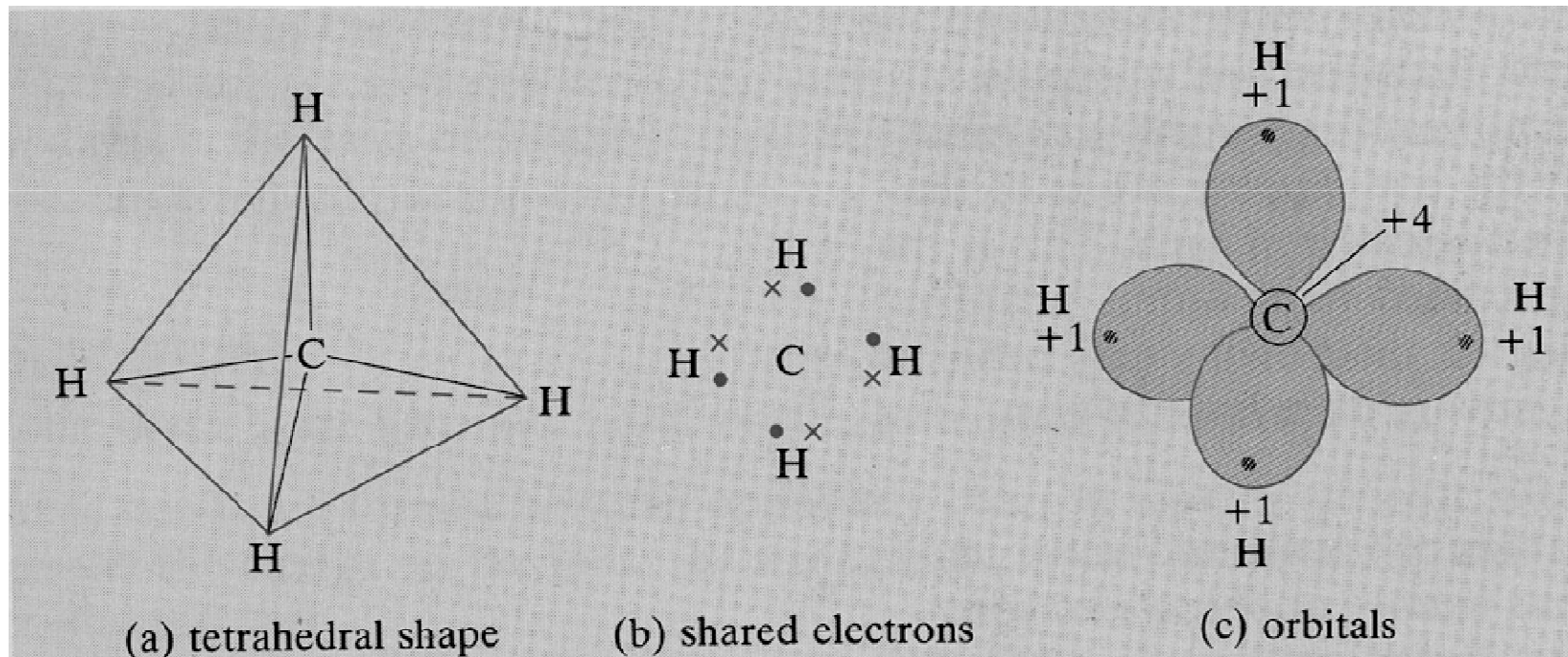
Orbital que penetra dois núcleos



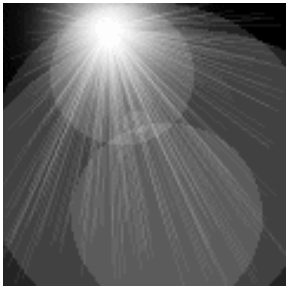
Orbitais híbridos



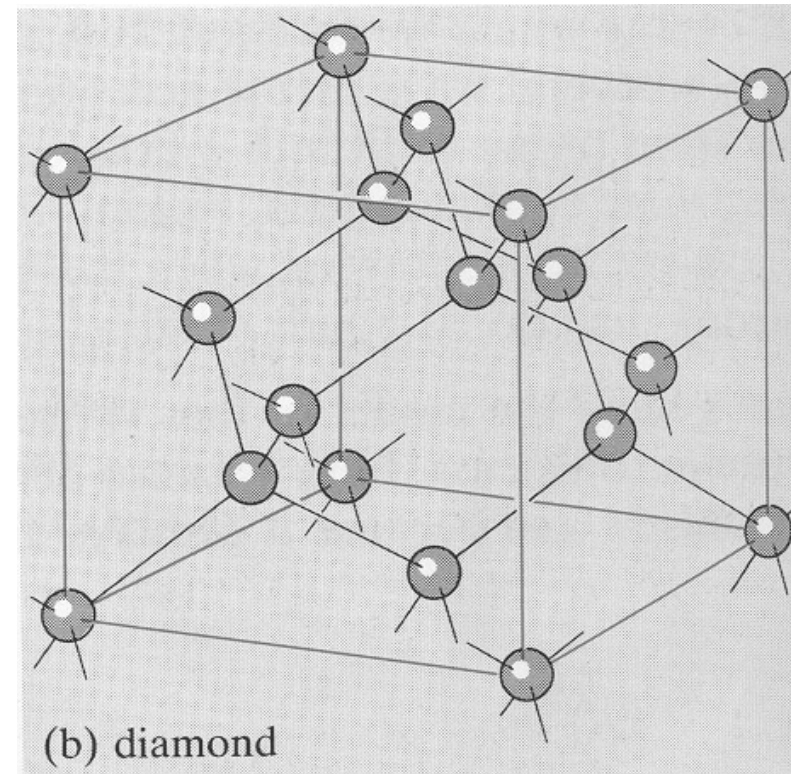
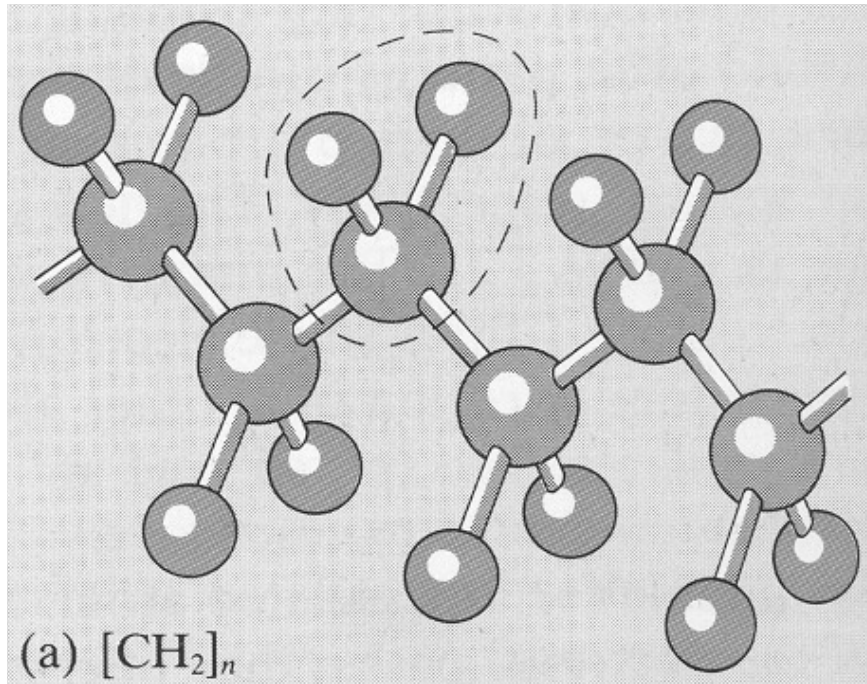
HIBRIDIZAÇÃO sp^3

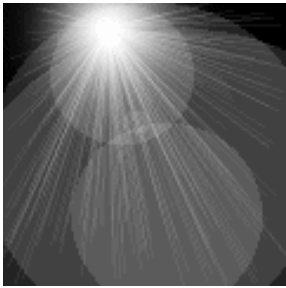


Molécula de metano

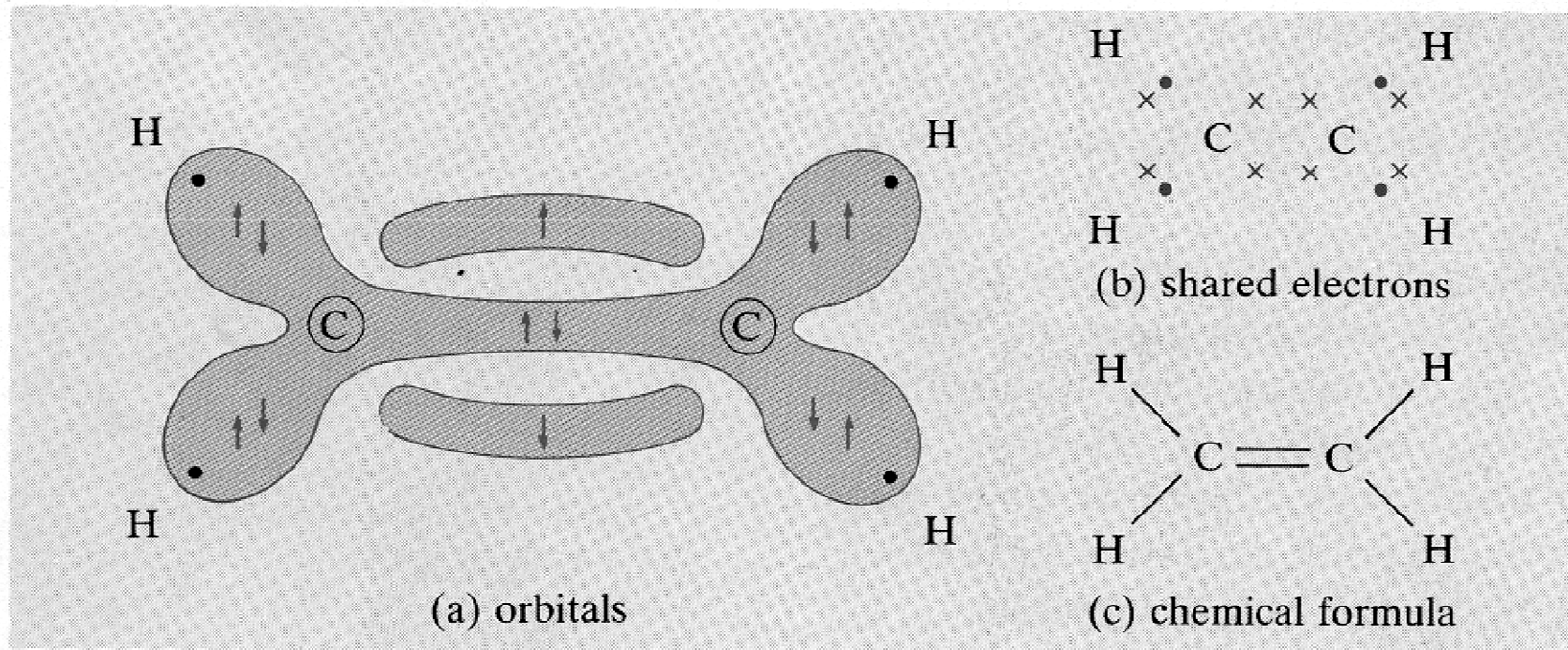


HIBRIDIZAÇÃO sp^3

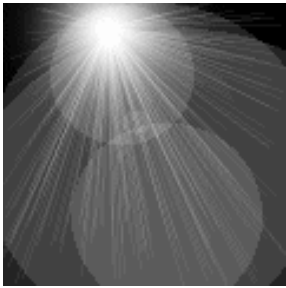




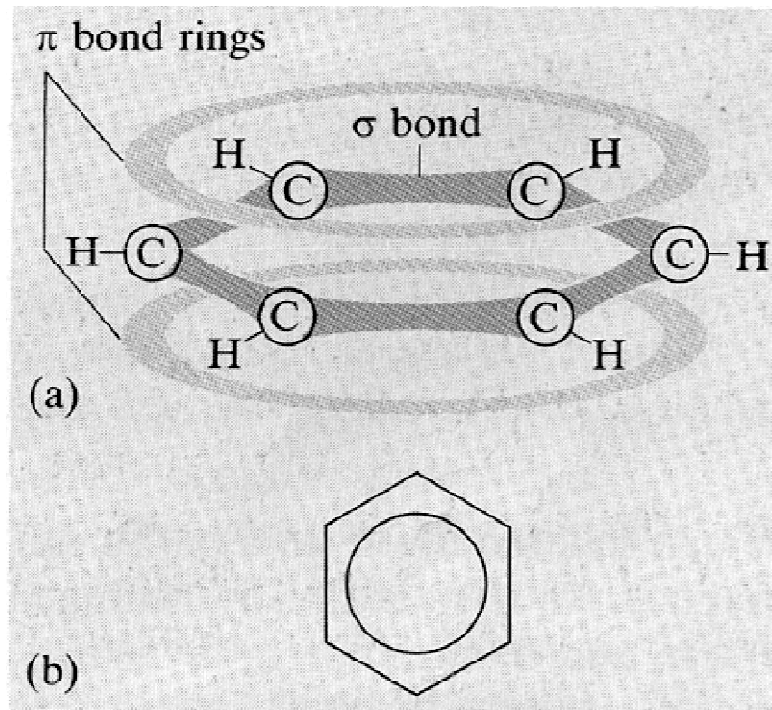
HIBRIDIZAÇÃO sp^2



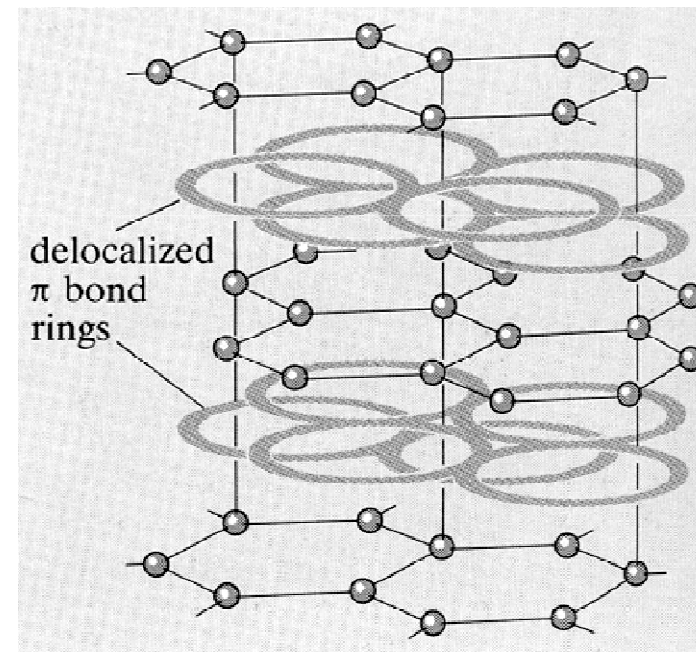
Molécula de etileno



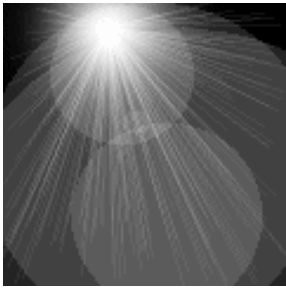
HIBRIDIZAÇÃO sp^2



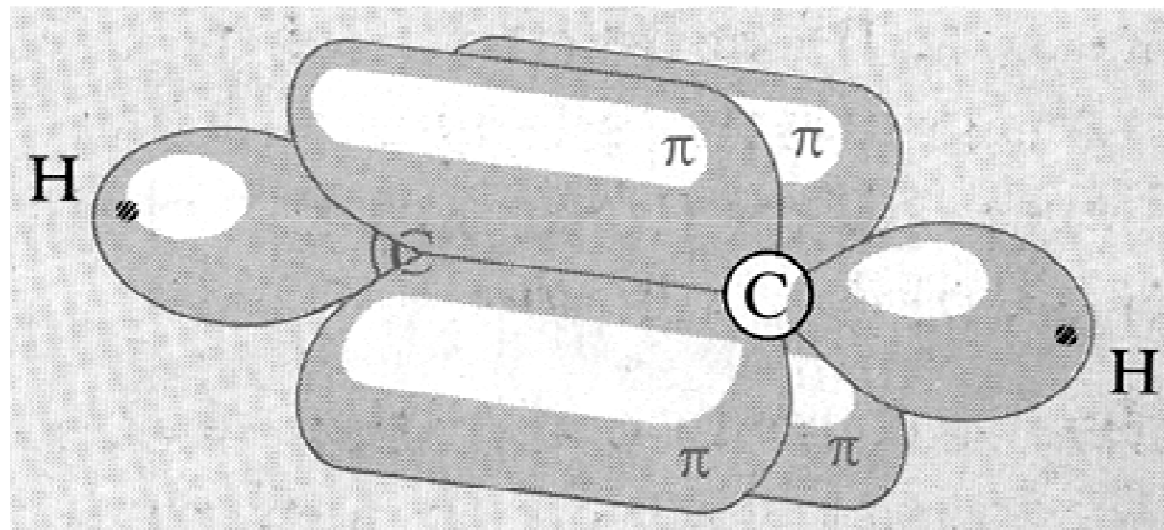
Anel de benzeno



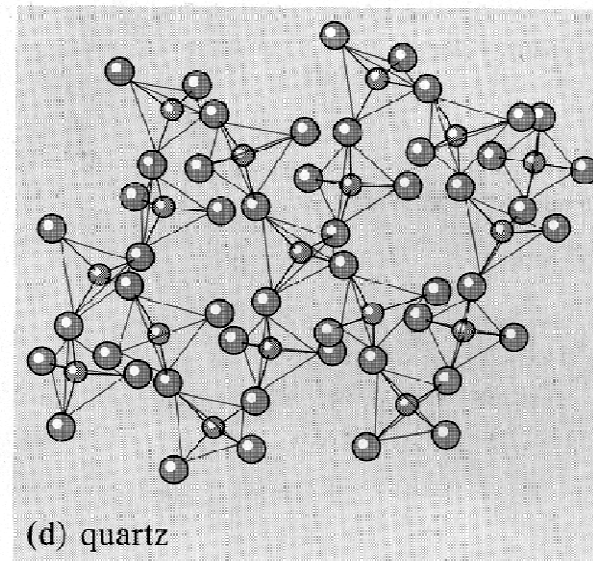
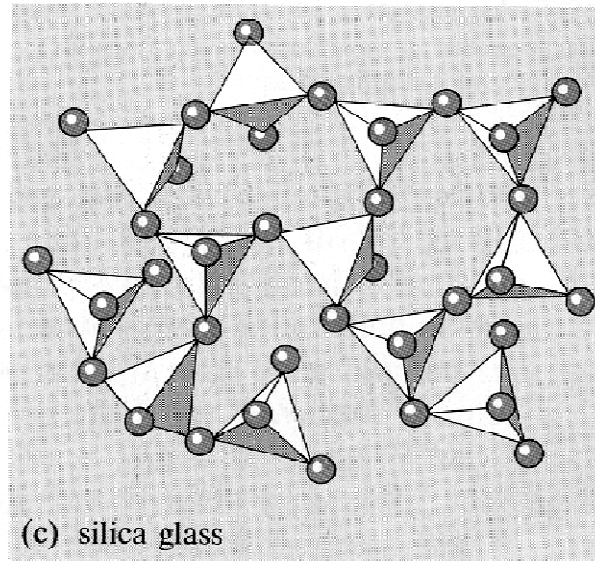
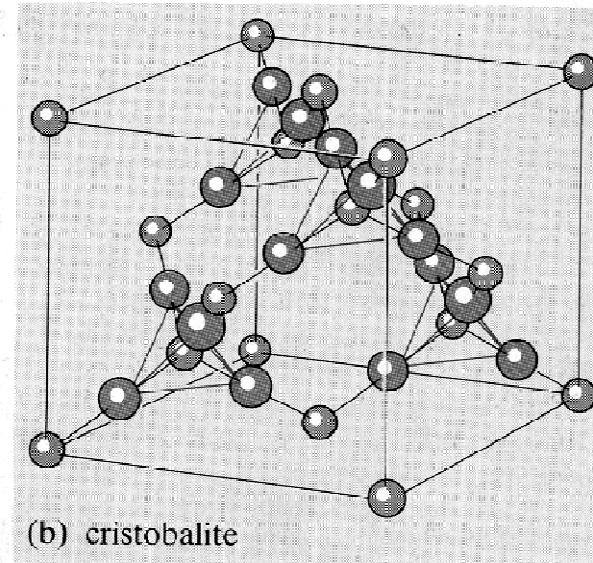
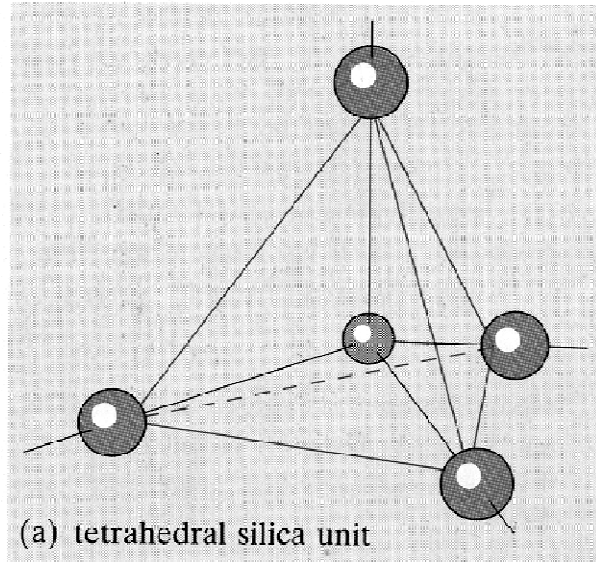
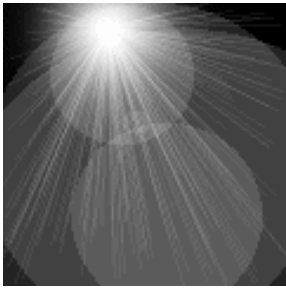
Grafita



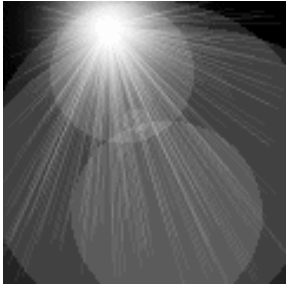
HIBRIDIZAÇÃO sp^1



Molécula de acetileno



ESTRUTURAS DA SÍLICA



LIGAÇÕES PRIMÁRIAS

LIGAÇÃO METÁLICA

- envolve compartilhamento de elétrons
- não direcional
- metais possuem de um a três elétrons de valência
- os elétrons de valência passam a ser elétrons “livres”, que (i) apresentam a mesma probabilidade de se associar a um grande número de átomos vizinhos e (ii) formam uma nuvem eletrônica

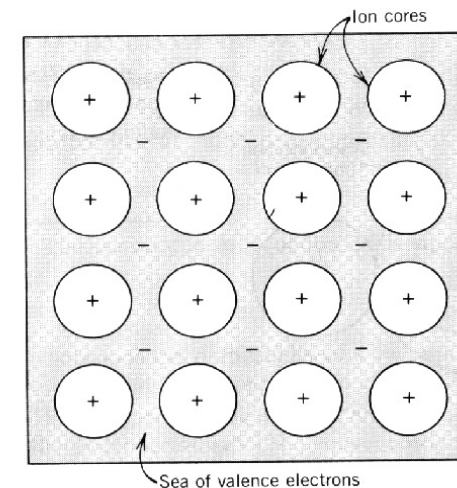
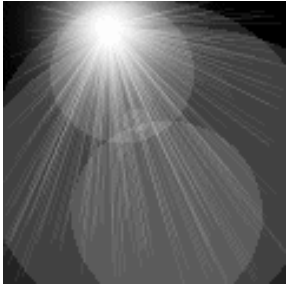
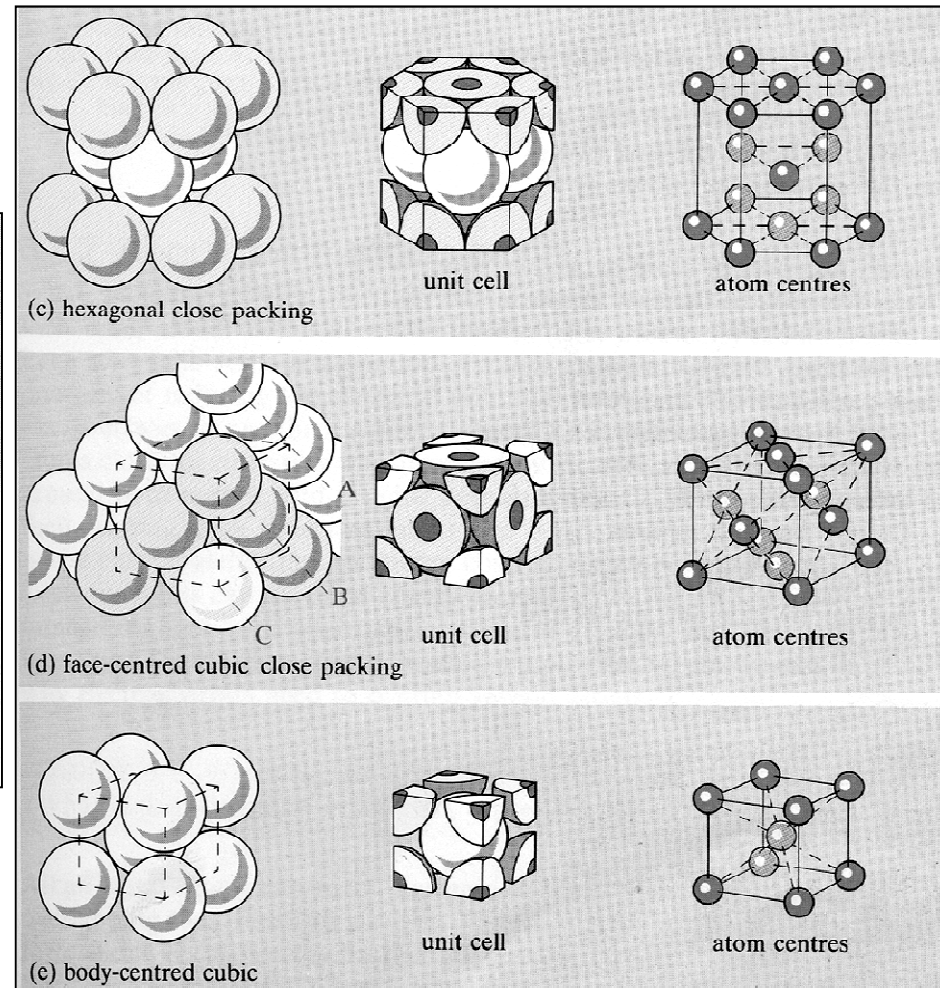
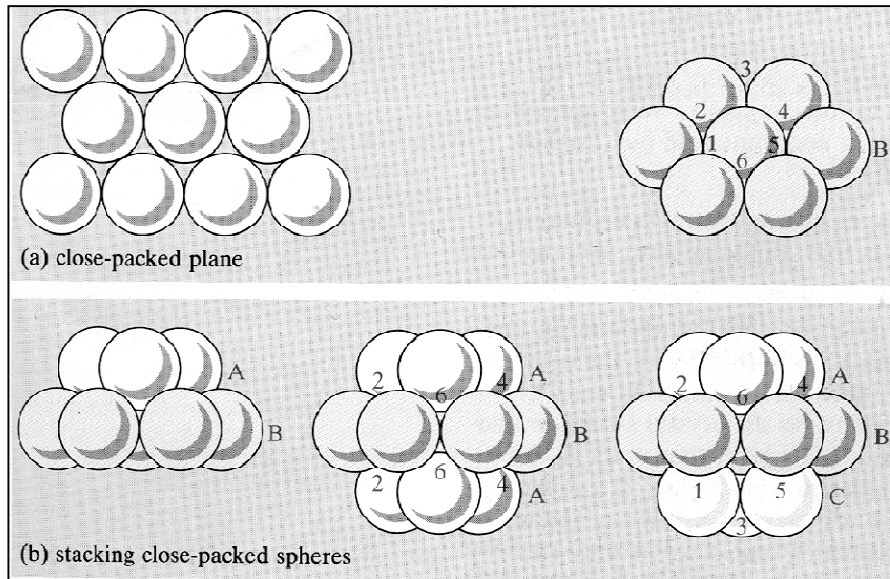
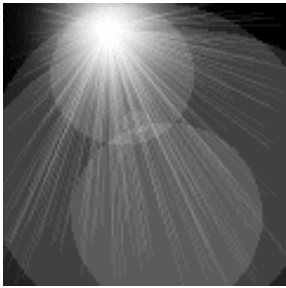


FIGURE 2.11 Schematic illustration of metallic bonding.

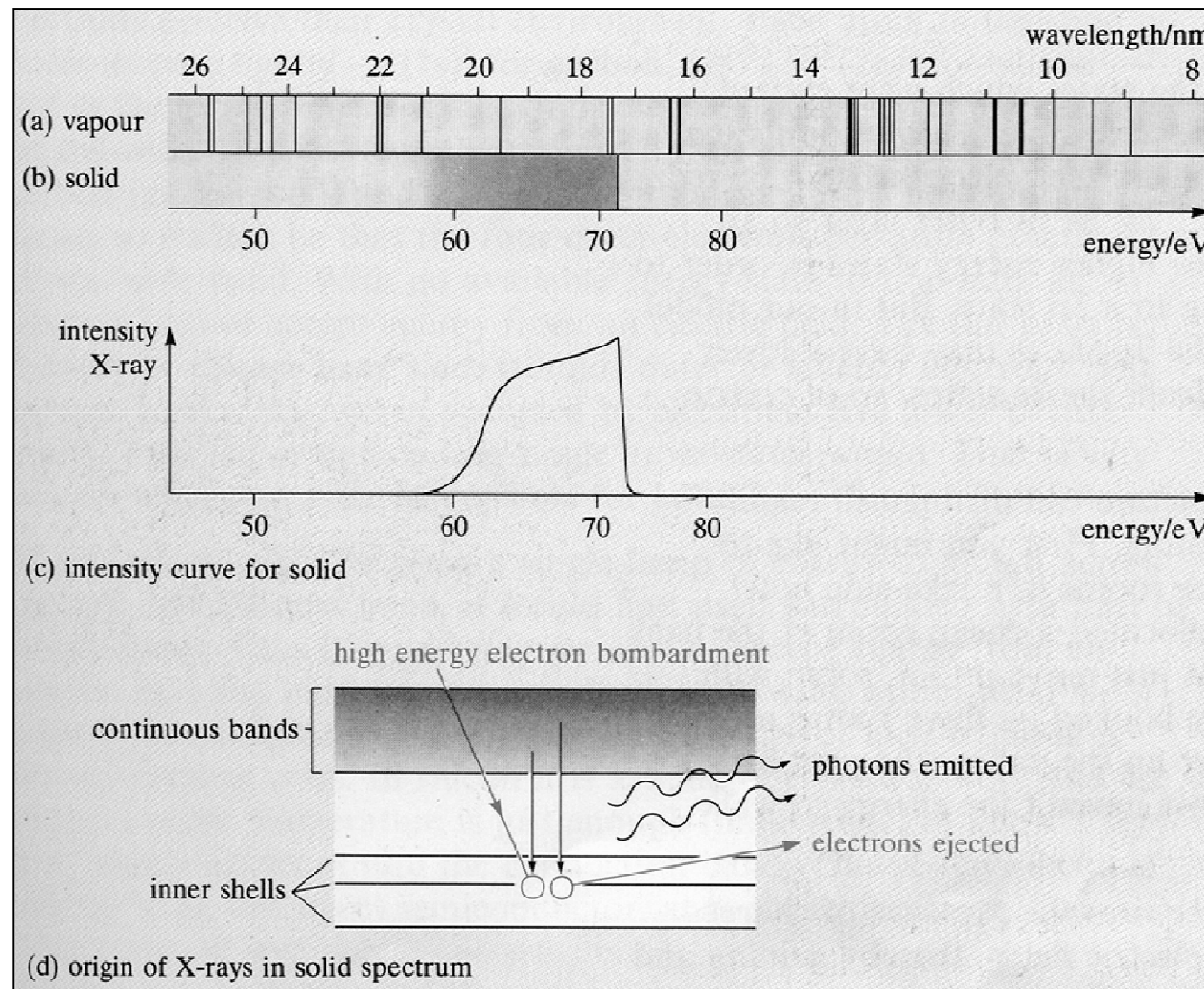


CRISTAIS METÁLICOS





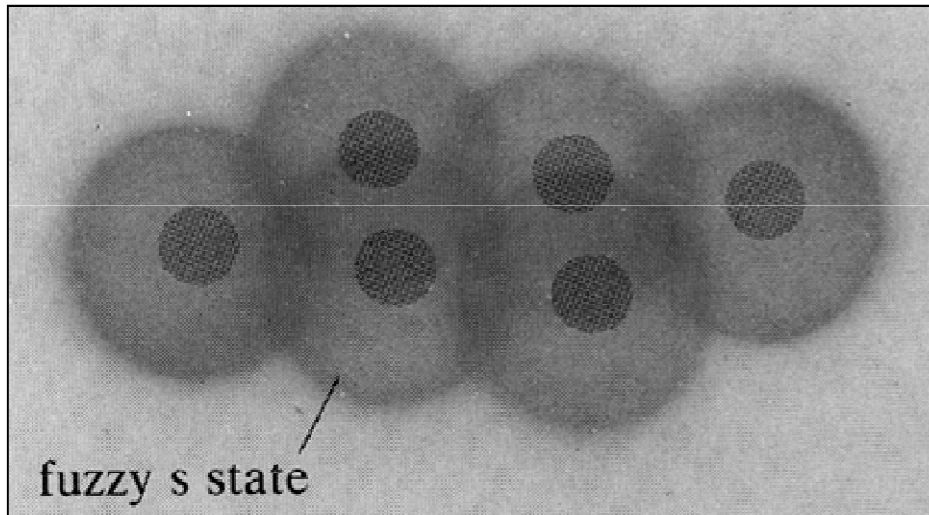
Elétrons nos sólidos



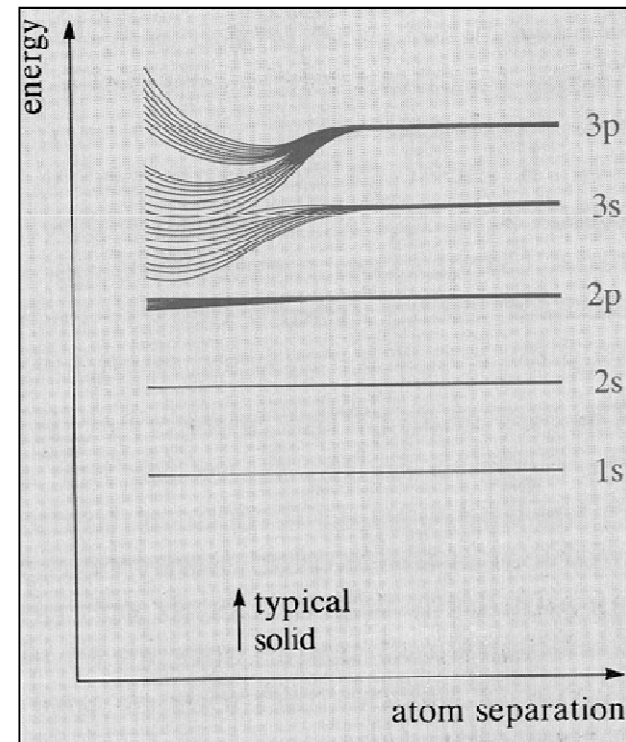
Raios X e bandas de energia



Elétrons nos sólidos



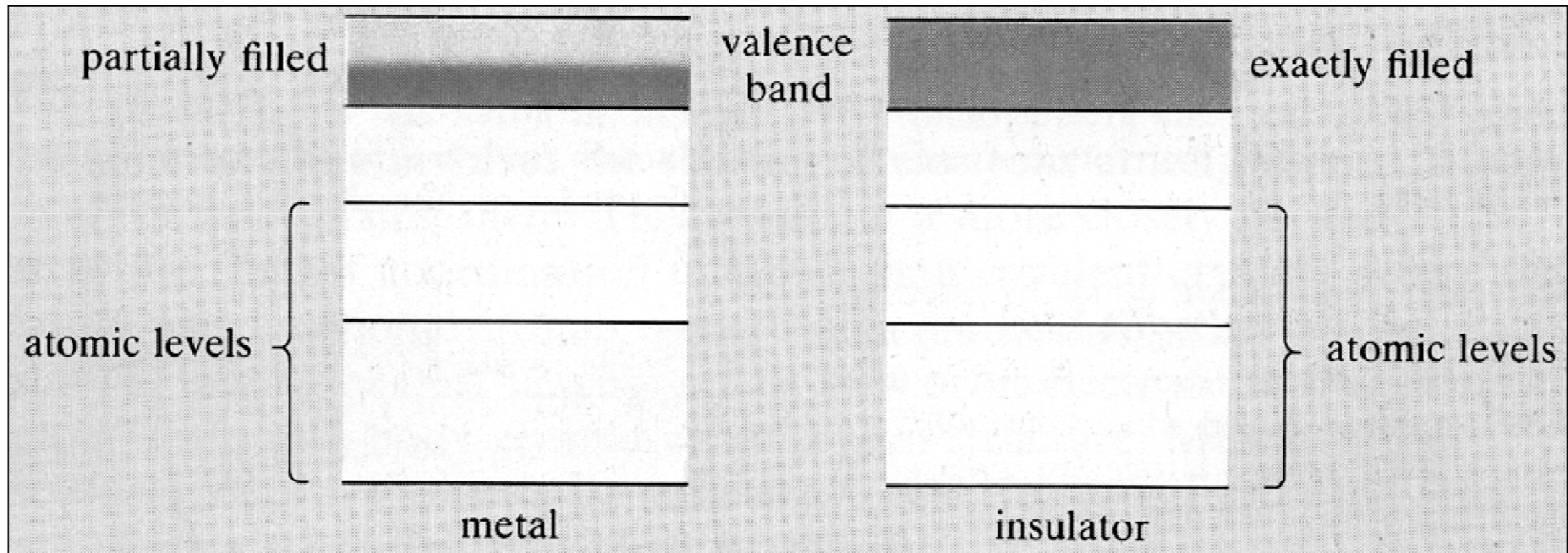
Superposição de estados S



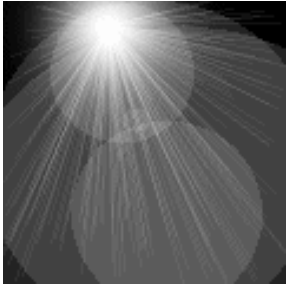
Níveis de energia e separação atômica



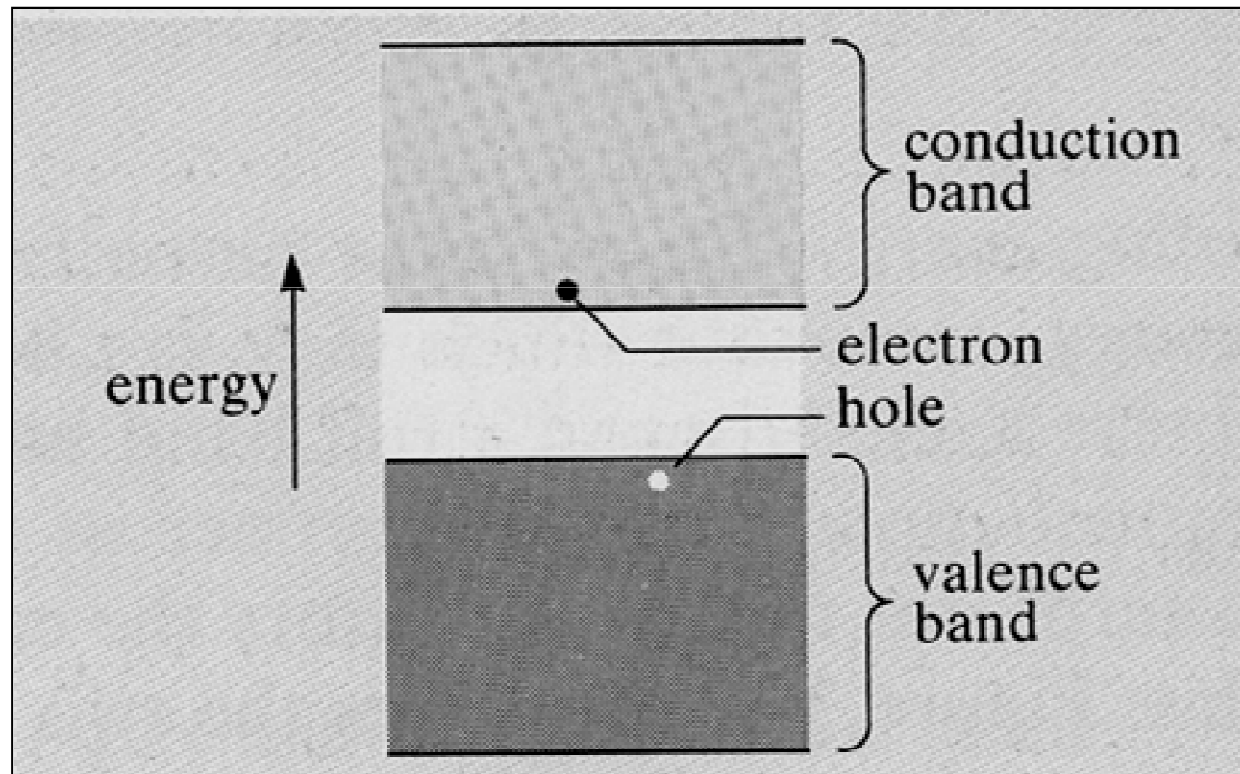
Elétrons nos sólidos



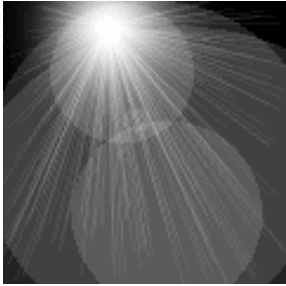
Bandas de energia para metais (condutores) e isolantes



Elétrons nos sólidos

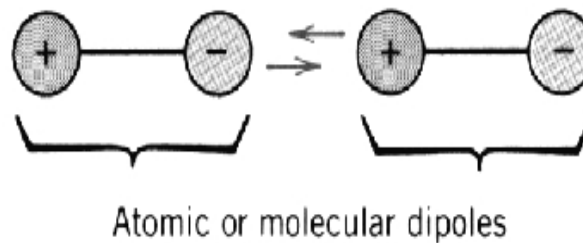


Bandas de energia para materiais semi-condutores

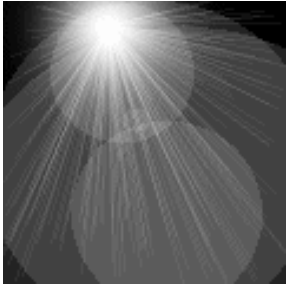


Ligações secundárias ou de Van der Waals

- Ocorrem atrações entre dipolos gerados pela assimetria de cargas.
- O mecanismo dessas ligações é similar ao das ligações iônicas, porém não existem elétrons transferidos.

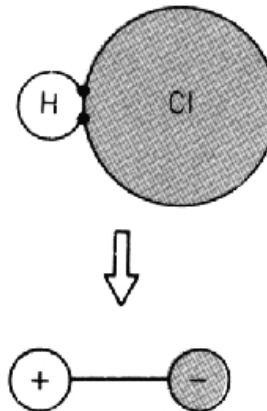
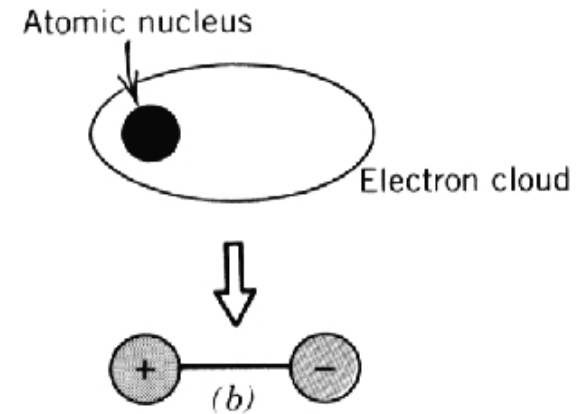
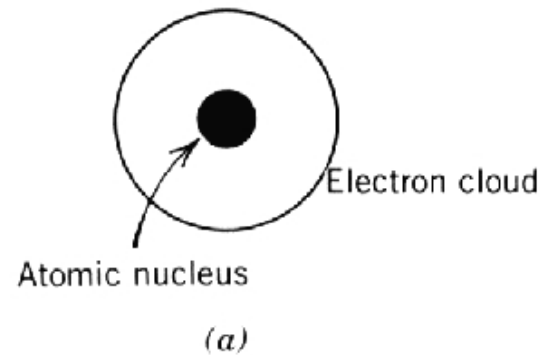


As ligações dipolares podem ser entre: (i) dipolos induzidos flutuantes, (ii) dipolos permanentes e induzidos, (iii) dipolos permanentes.

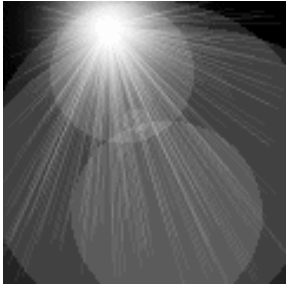


Ligações secundárias ou de Van der Waals

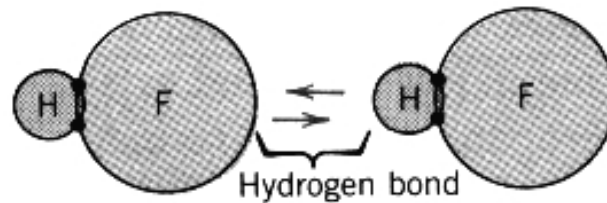
Representação esquemática de (a) um átomo eletricamente simétrico e (b) um dipolo atômico flutuante.



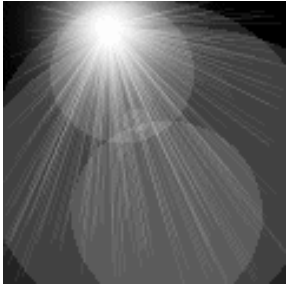
dipolo permanente



PONTE DE HIDROGÊNIO

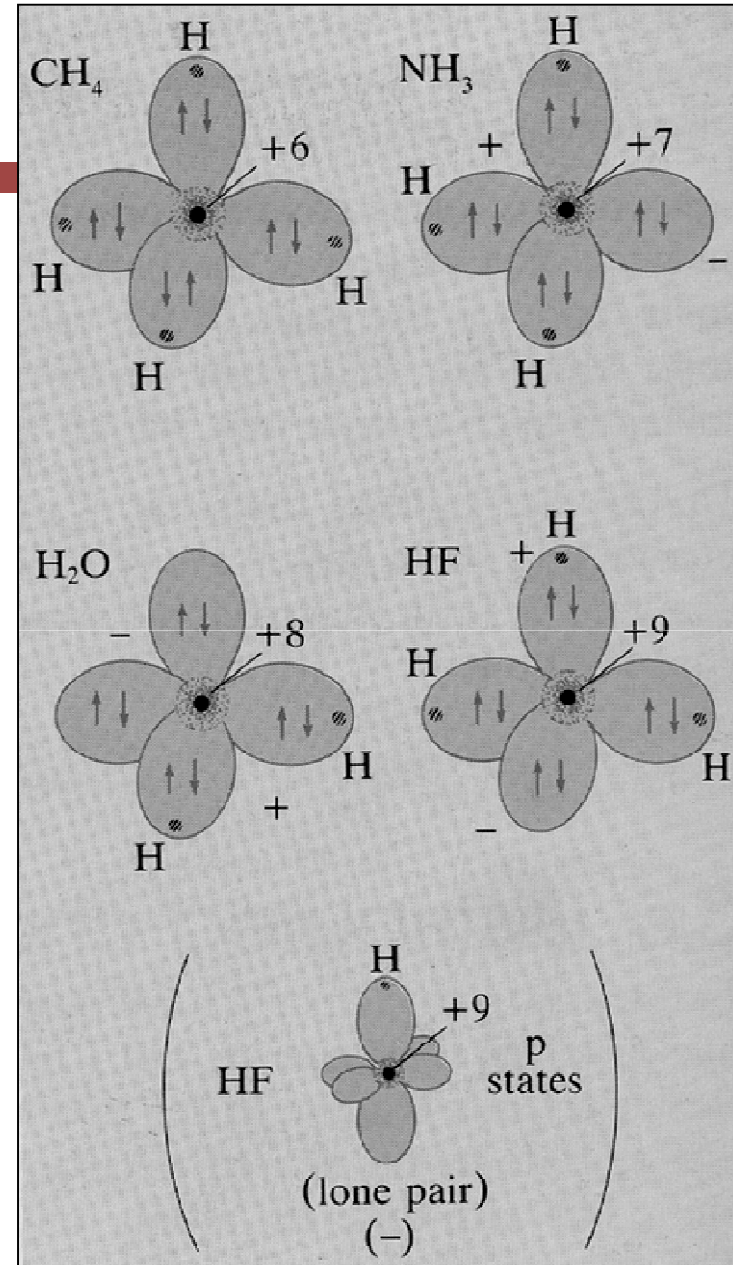


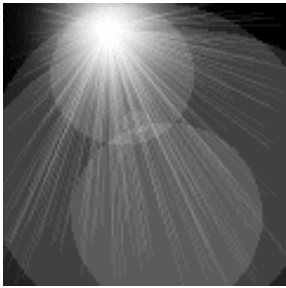
- É um caso especial de ligação entre moléculas polares.
- É o tipo de ligação secundária mais forte.
- Ocorre entre moléculas em que o H está ligado covalentemente ao F (HF), O (H₂O) ou N (NH₃).



MOLÉCULAS POLARES

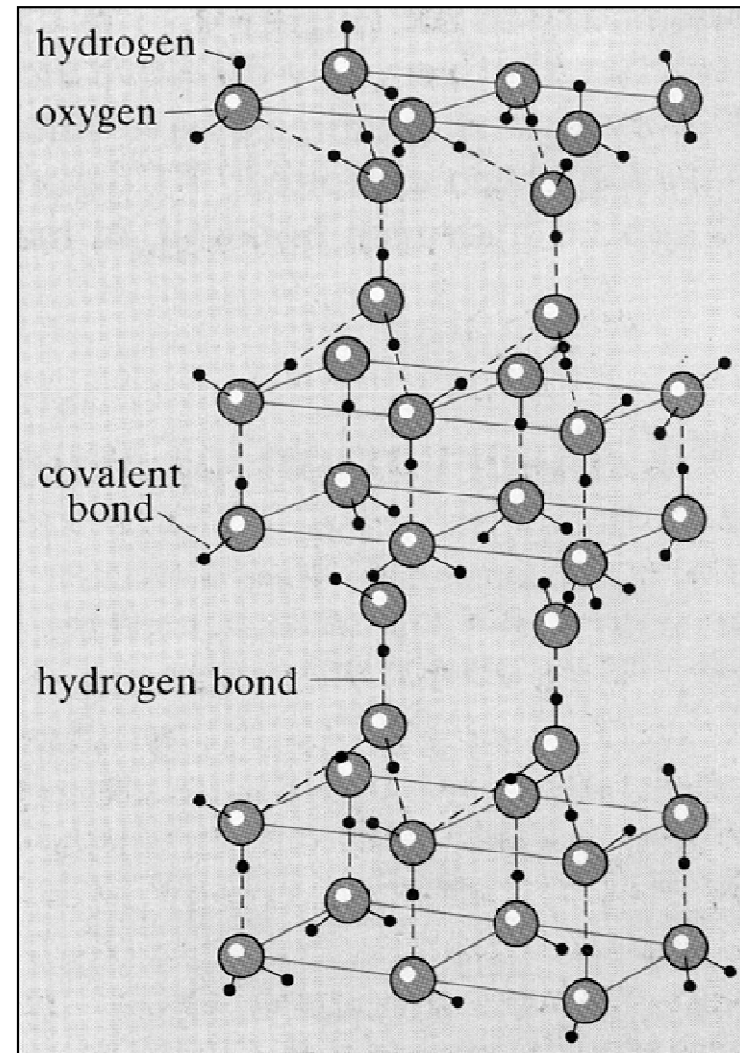
Distribuição de carga em diferentes de moléculas

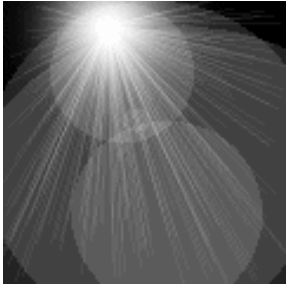




PONTES DE HIDROGÊNIO

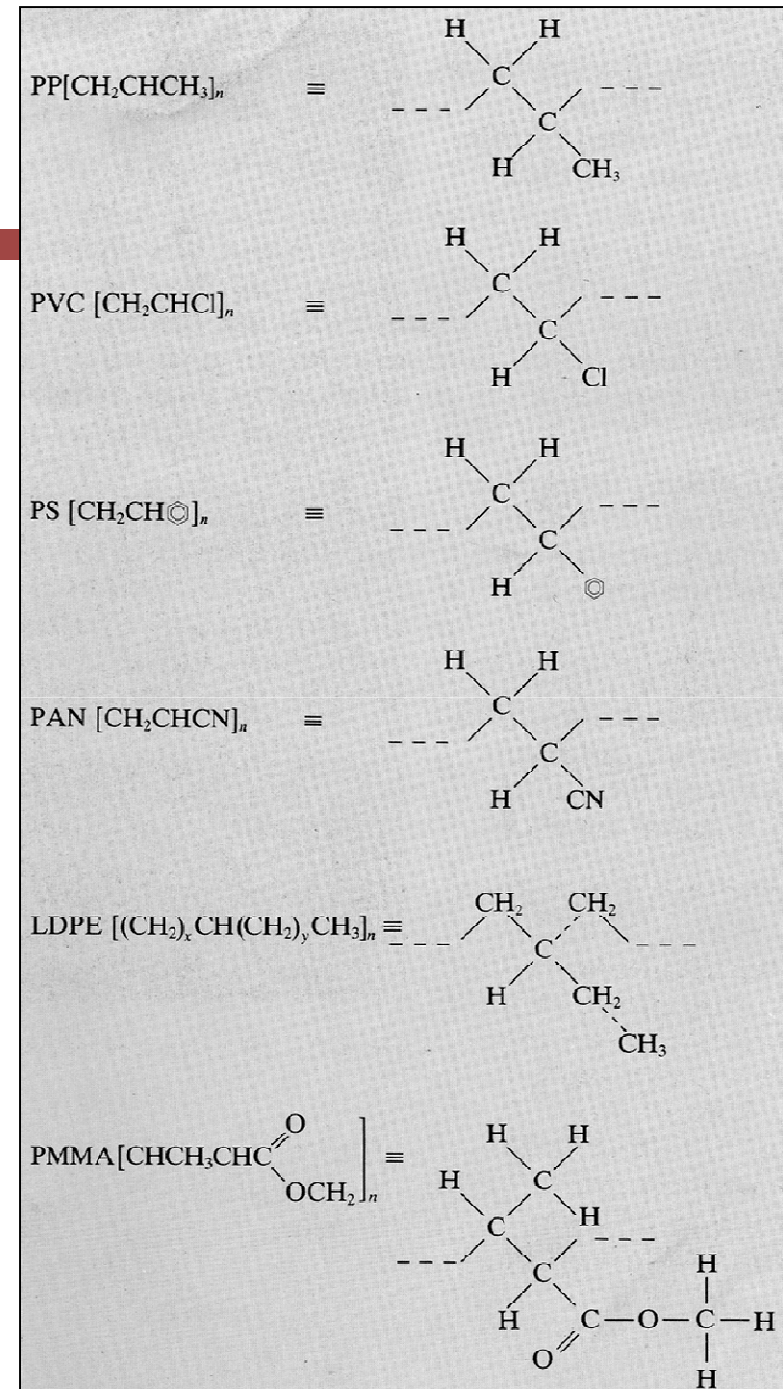
Pontes de hidrogênio formando a estrutura cristalina do gelo.

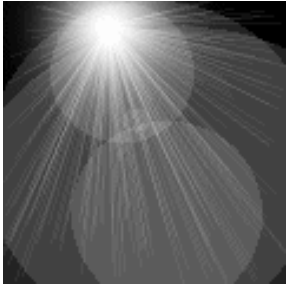




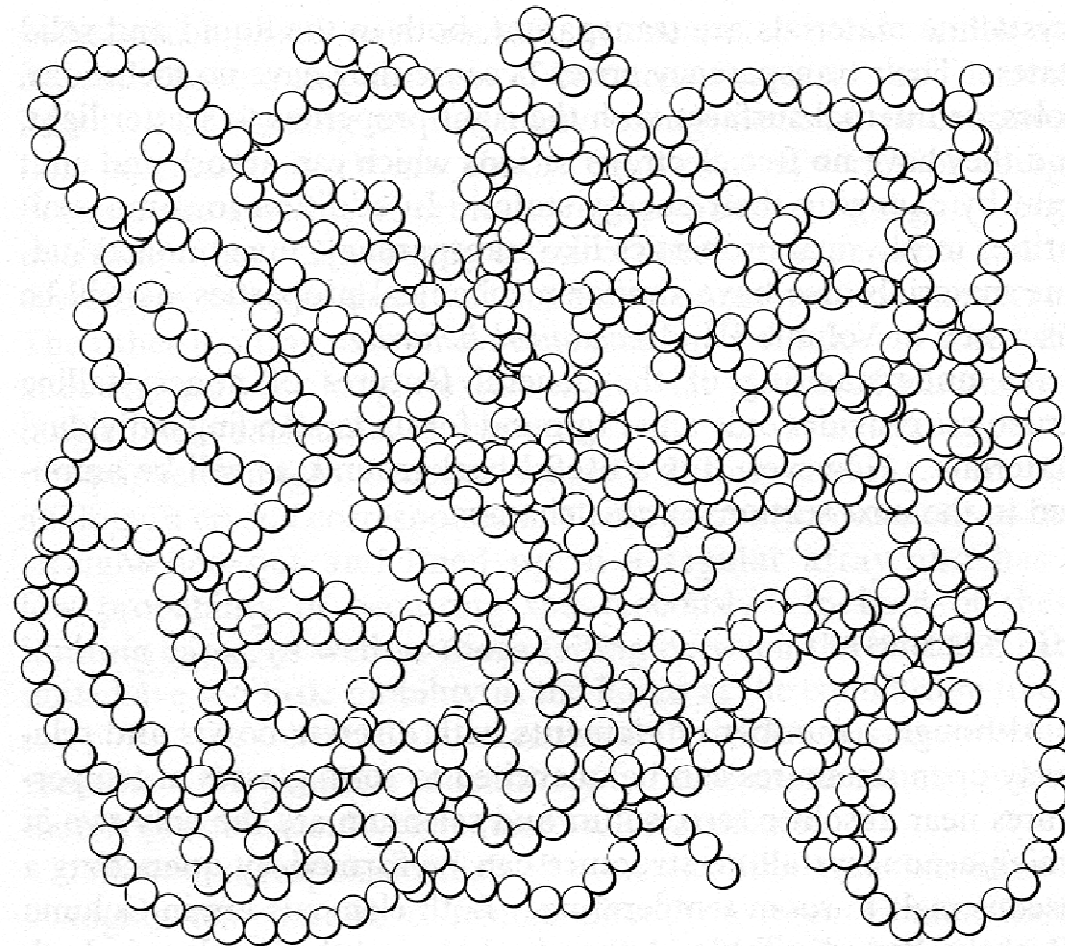
MACROMOLÉCULAS POLÍMEROS

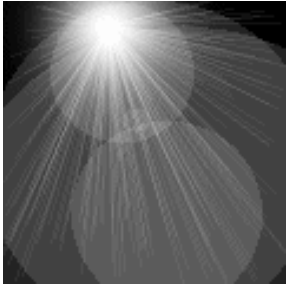
Polímeros ramificados lisos
ou que formam caroço



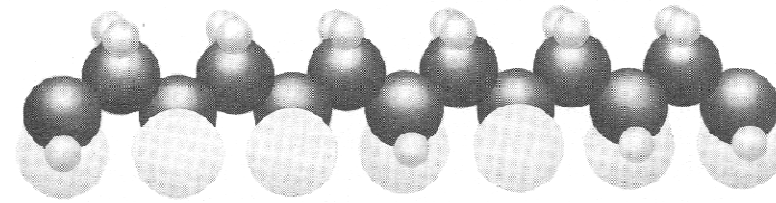


POLÍMEROS AMORFOS

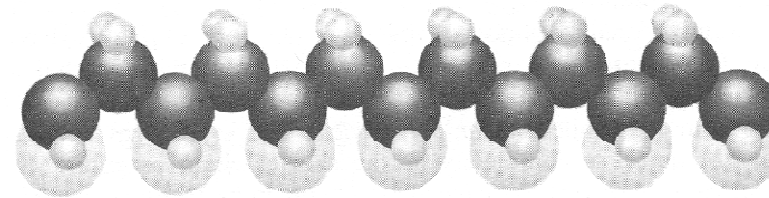




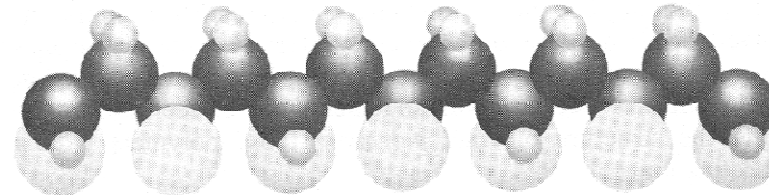
Polímeros parcialmente cristalinos



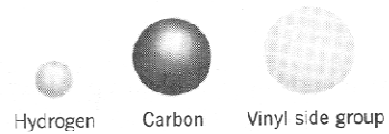
Atactic (random)

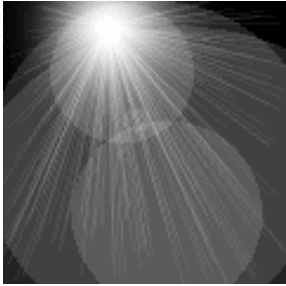


Isotactic (same side)

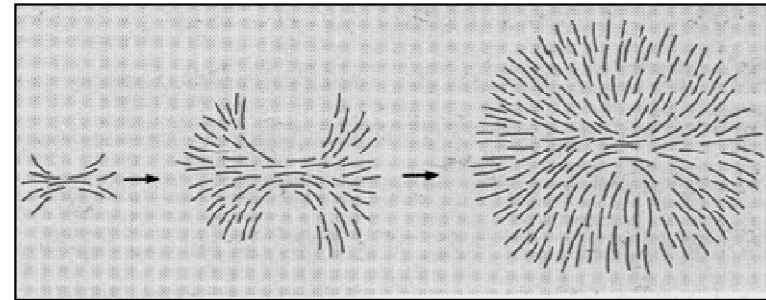
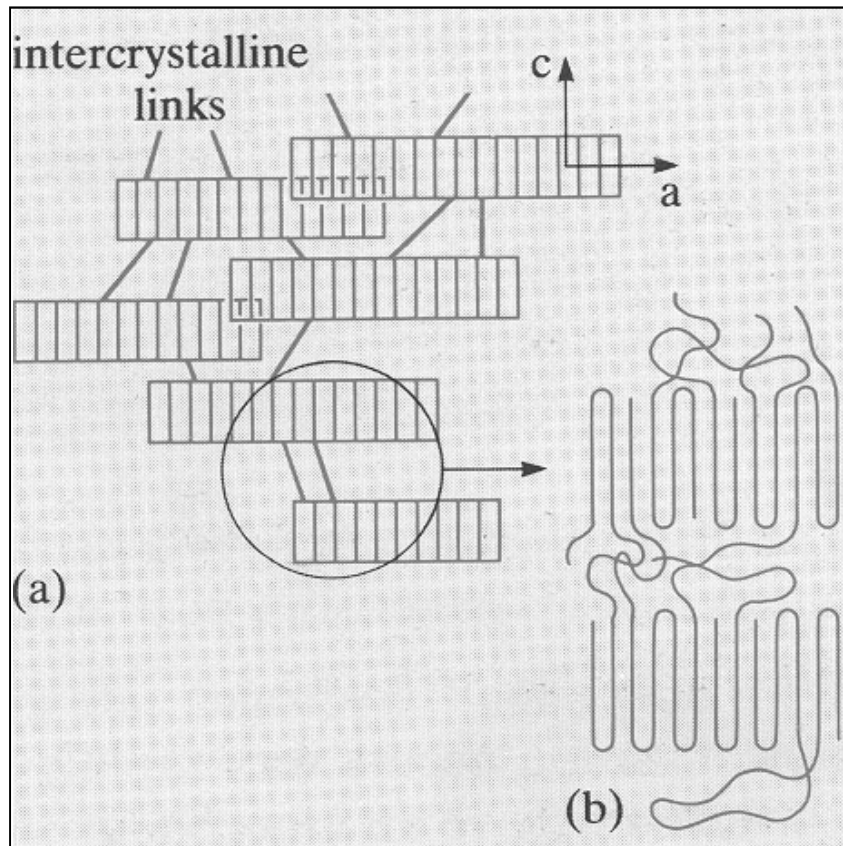


Syndiotactic (regularly alternating)

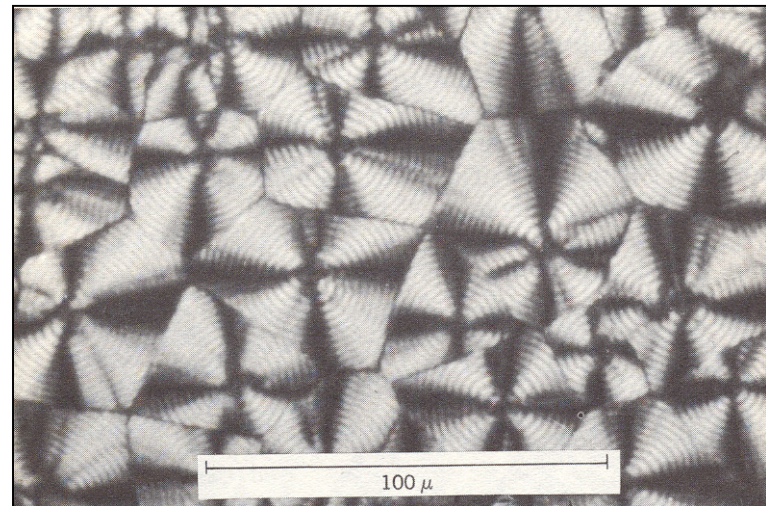


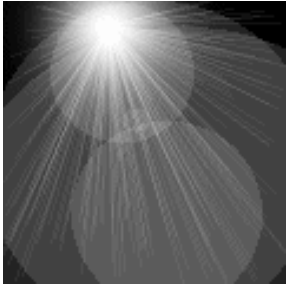


Polímeros parcialmente cristalinos

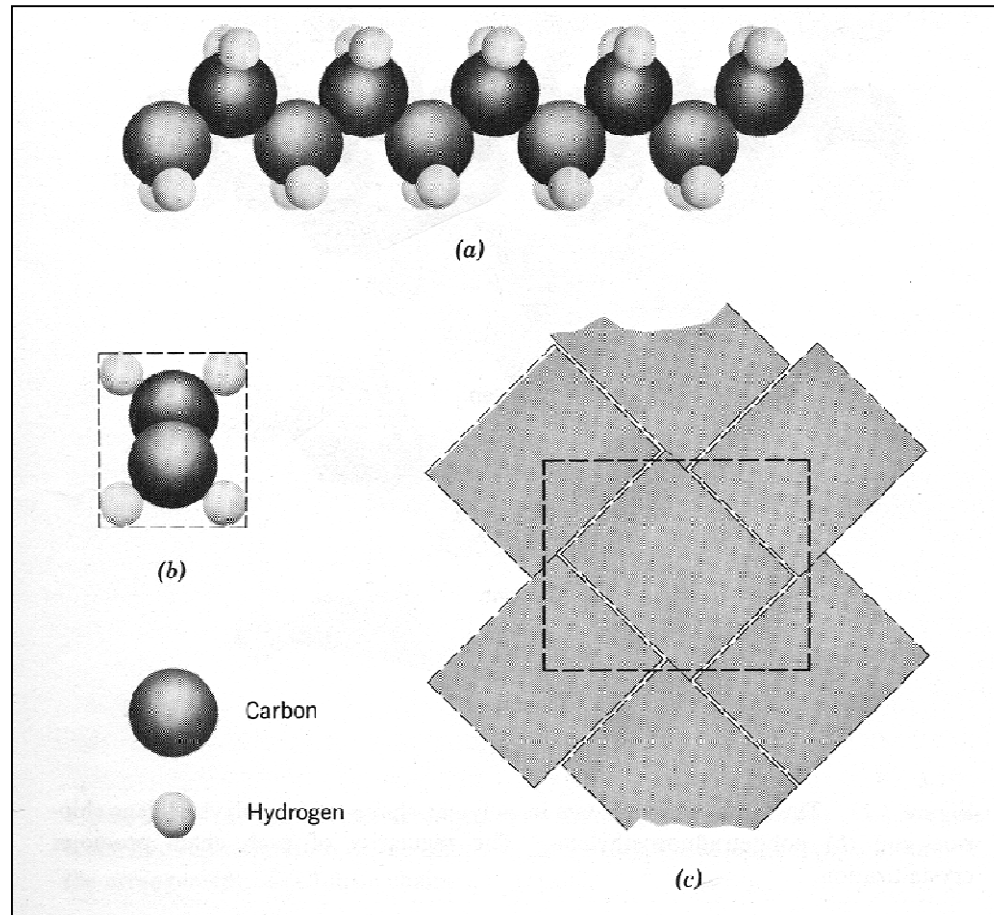


Esferulitos

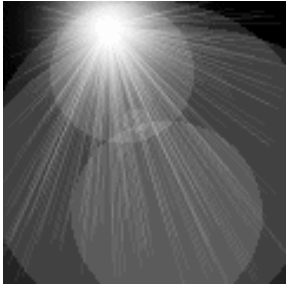




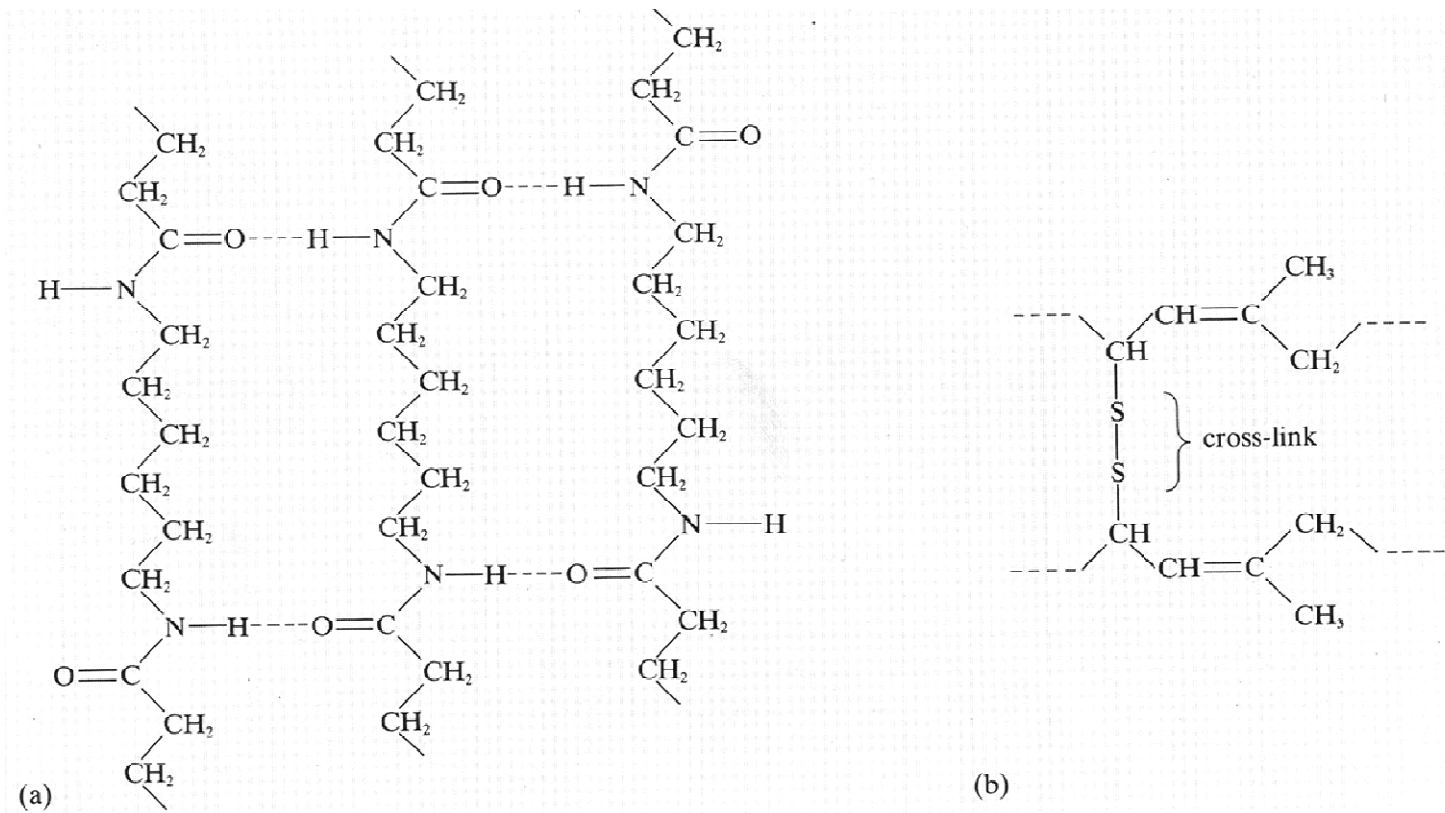
Polímeros parcialmente cristalinos



Estrutura do polietileno de alta densidade

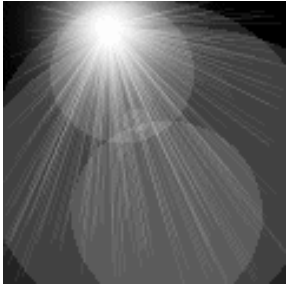


LIGAÇÕES CRUZADAS - Elastômeros

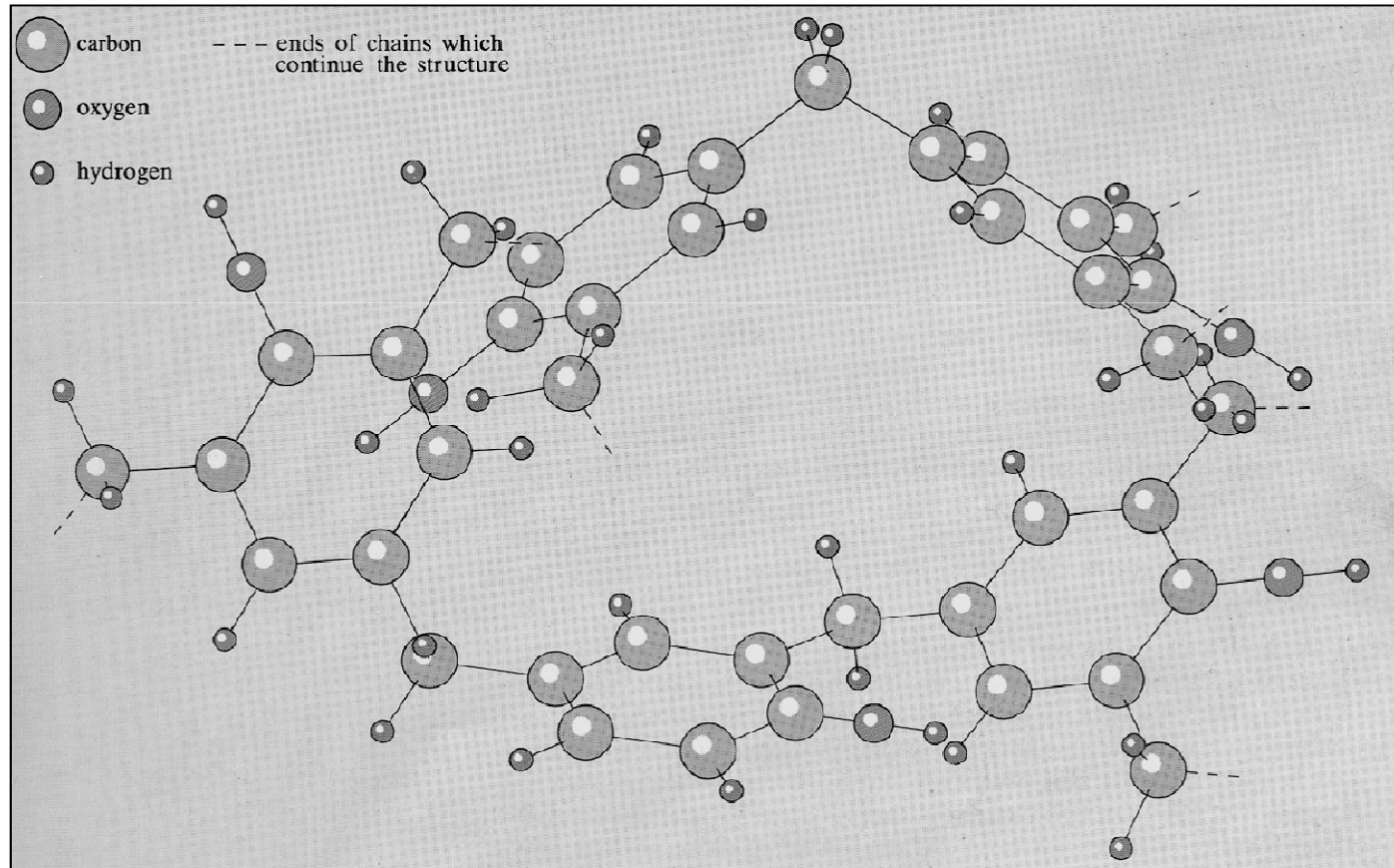


Nylon

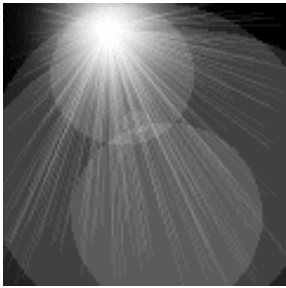
Borracha



LIGAÇÕES CRUZADAS



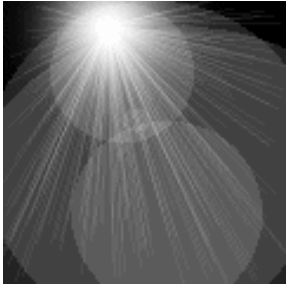
Baquelite (formaldeído fenólico)



ENERGIAS DE LIGAÇÃO

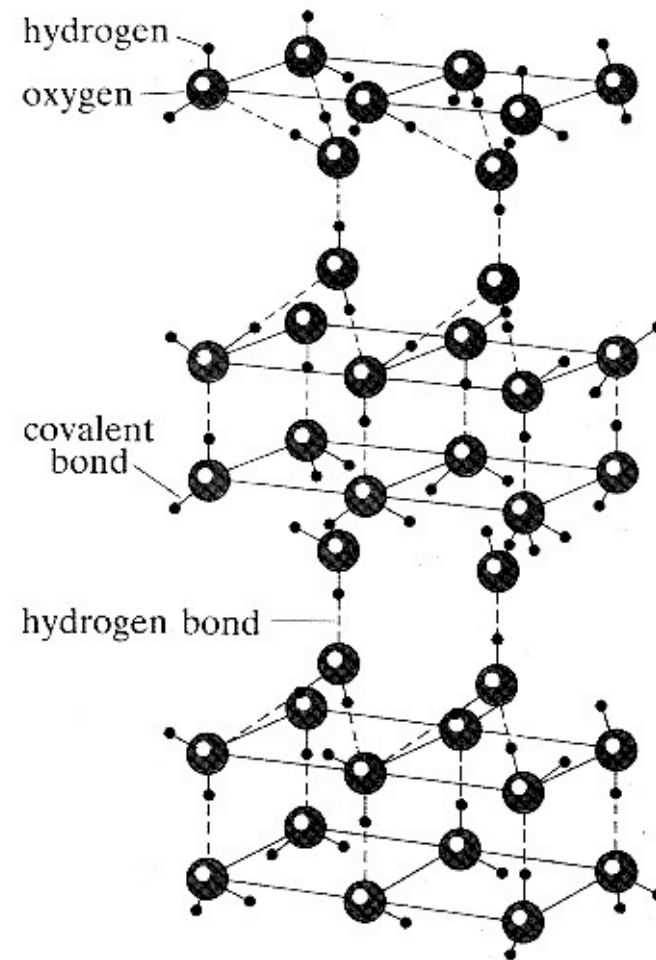
Table 2.3 Bonding Energies and Melting Temperatures for Various Substances

<i>Bonding Type</i>	<i>Substance</i>	<i>Bonding Energy</i>		<i>Melting Temperature</i> (°C)
		<i>kJ/mol</i> (<i>kcal/mol</i>)	<i>eV/Atom,</i> <i>Ion, Molecule</i>	
Ionic	NaCl	640 (153)	3.3	801
	MgO	1000 (239)	5.2	2800
Covalent	Si	450 (108)	4.7	1410
	C (diamond)	713 (170)	7.4	>3550
Metallic	Hg	68 (16)	0.7	-39
	Al	324 (77)	3.4	660
	Fe	406 (97)	4.2	1538
	W	849 (203)	8.8	3410
van der Waals	Ar	7.7 (1.8)	0.08	-189
	Cl ₂	31 (7.4)	0.32	-101
Hydrogen	NH ₃	35 (8.4)	0.36	-78
	H ₂ O	51 (12.2)	0.52	0

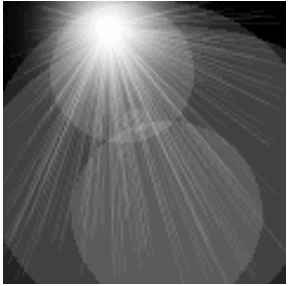


Relação entre estrutura e propriedades

- Densidade: peso atômico, raio atômico (iônico) e distribuição atômica espacial.
- Condutividades elétrica e térmica: estão associadas à mobilidade dos portadores de carga, que depende da distribuição eletrônica espacial.



Pontes de hidrogênio na água no estado sólido (gelo).



FORÇAS E ENERGIAS DE LIGAÇÃO

- Quando dois átomos se aproximam, eles exercem uma força um no outro:

$$F_N = F_A + F_R$$

onde:

$F_A \equiv$ força de atração

$F_R \equiv$ força de repulsão

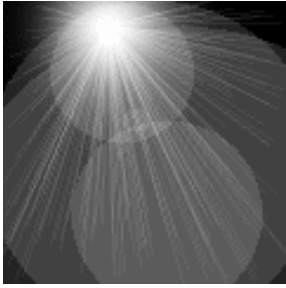
$F_N \equiv$ força resultante

- A energia potencial (E_N) será dada por:

$$E_N = \int_{\infty}^r F_N dr = \int_{\infty}^r F_A dr + \int_{\infty}^r F_R dr$$

onde:

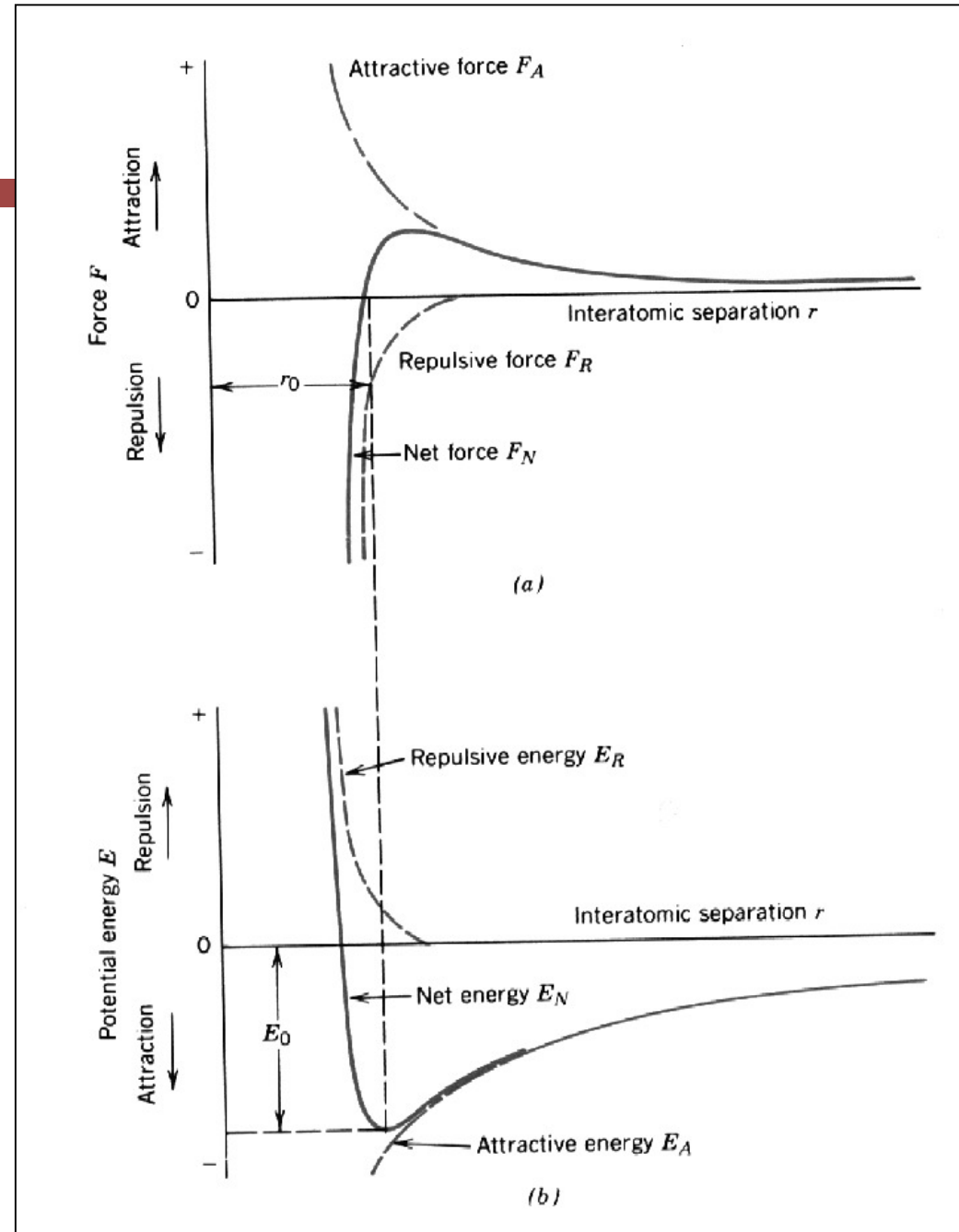
$r \equiv$ distância interatômica

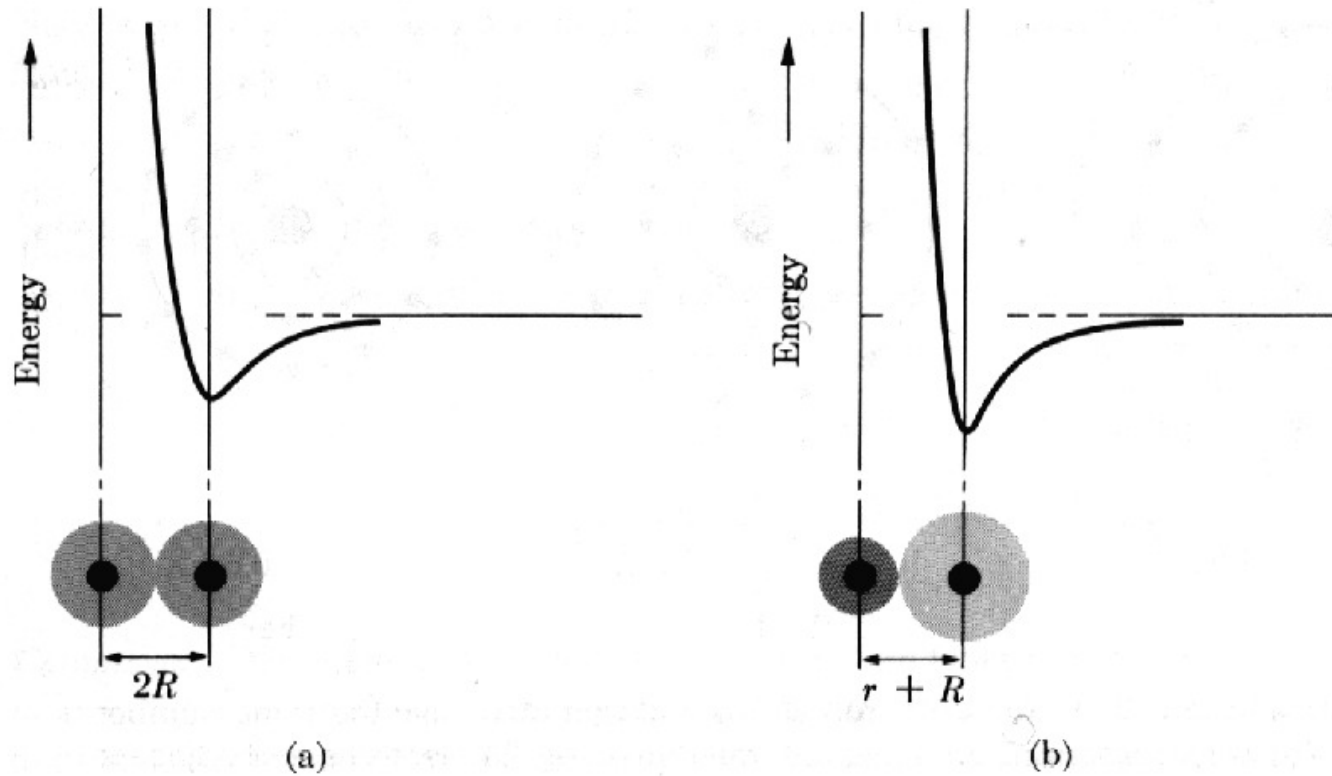
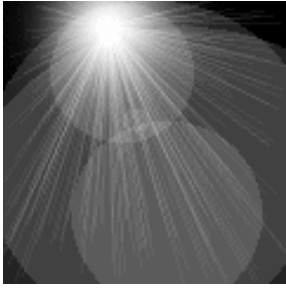


FORÇAS E ENERGIAS DE LIGAÇÃO

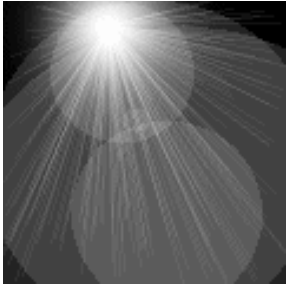
(a) Forças de atração e de repulsão em função da distância interatômica para dois átomos isolados

(b) Energia potencial em função da distância interatômica para dois átomos isolados



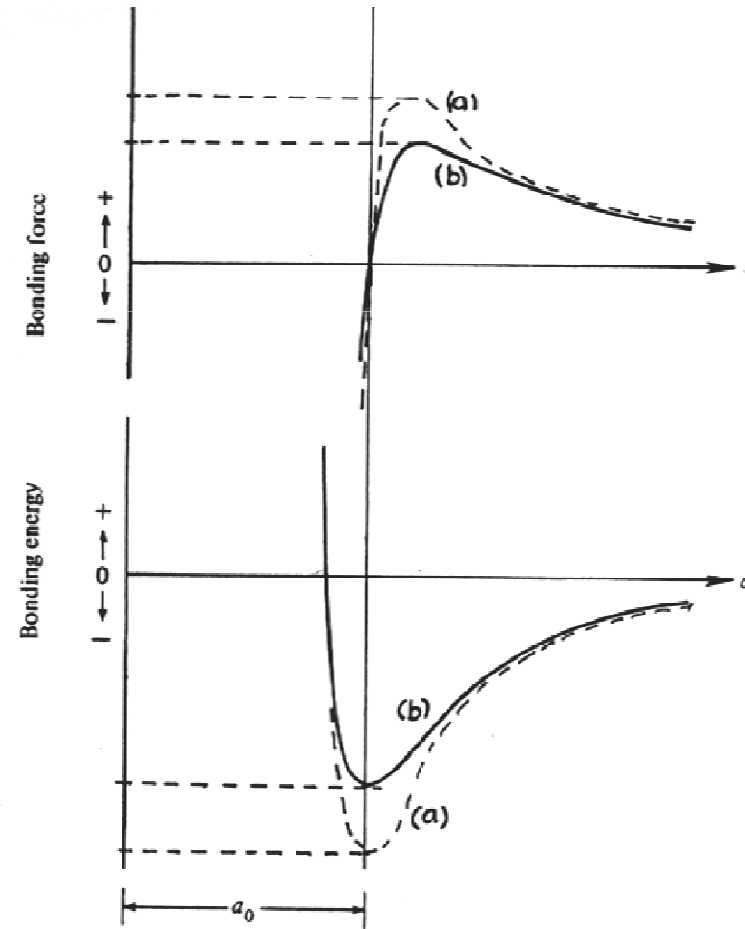


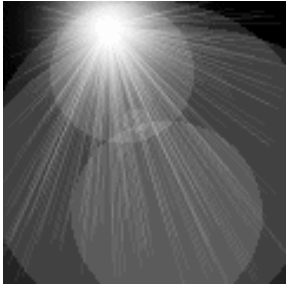
O comprimento da ligação entre dois átomos é a distância correspondente ao ponto de mínima energia (soma dos dois raios atômicos). (a) Para metais puros, todos os átomos têm o mesmo raio atômico. (b) Para sólidos iônicos, os raios atômicos são diferentes, uma vez que íons adjacentes nunca são idênticos.



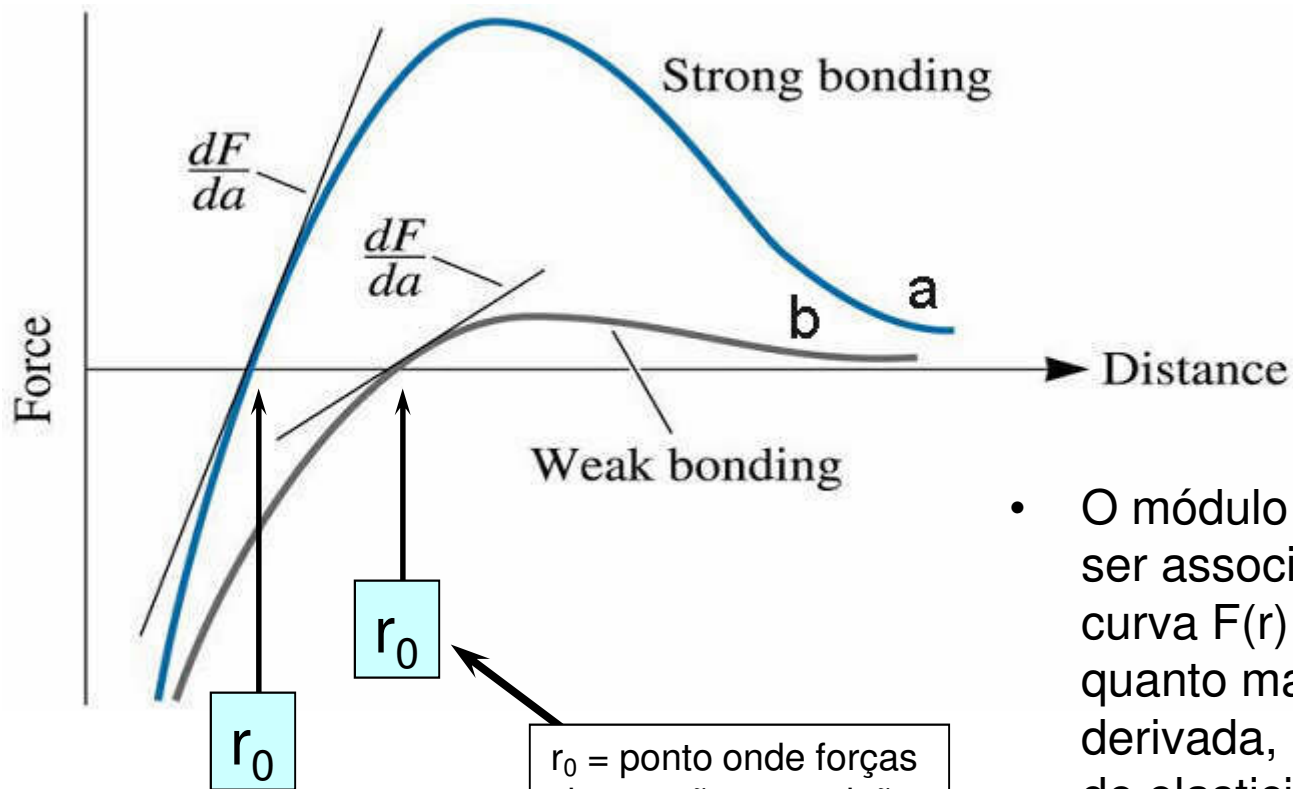
CORRELAÇÃO DAS PROPRIEDADES COM AS CURVAS DE FORÇA E DE ENERGIA DE LIGAÇÃO

- Resistência mecânica: aumenta com a força máxima e com a profundidade do poço da curva de energia de ligação.
- Pontos de fusão e de ebulição: aumentam com a profundidade do poço da curva de energia de ligação
- Coeficiente de expansão térmica: diminui com a profundidade do poço da curva de energia de ligação





Relação Entre Algumas Propriedades e Curvas de Força e Energia de Ligação

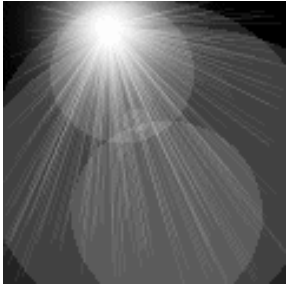


Módulo de Elasticidade

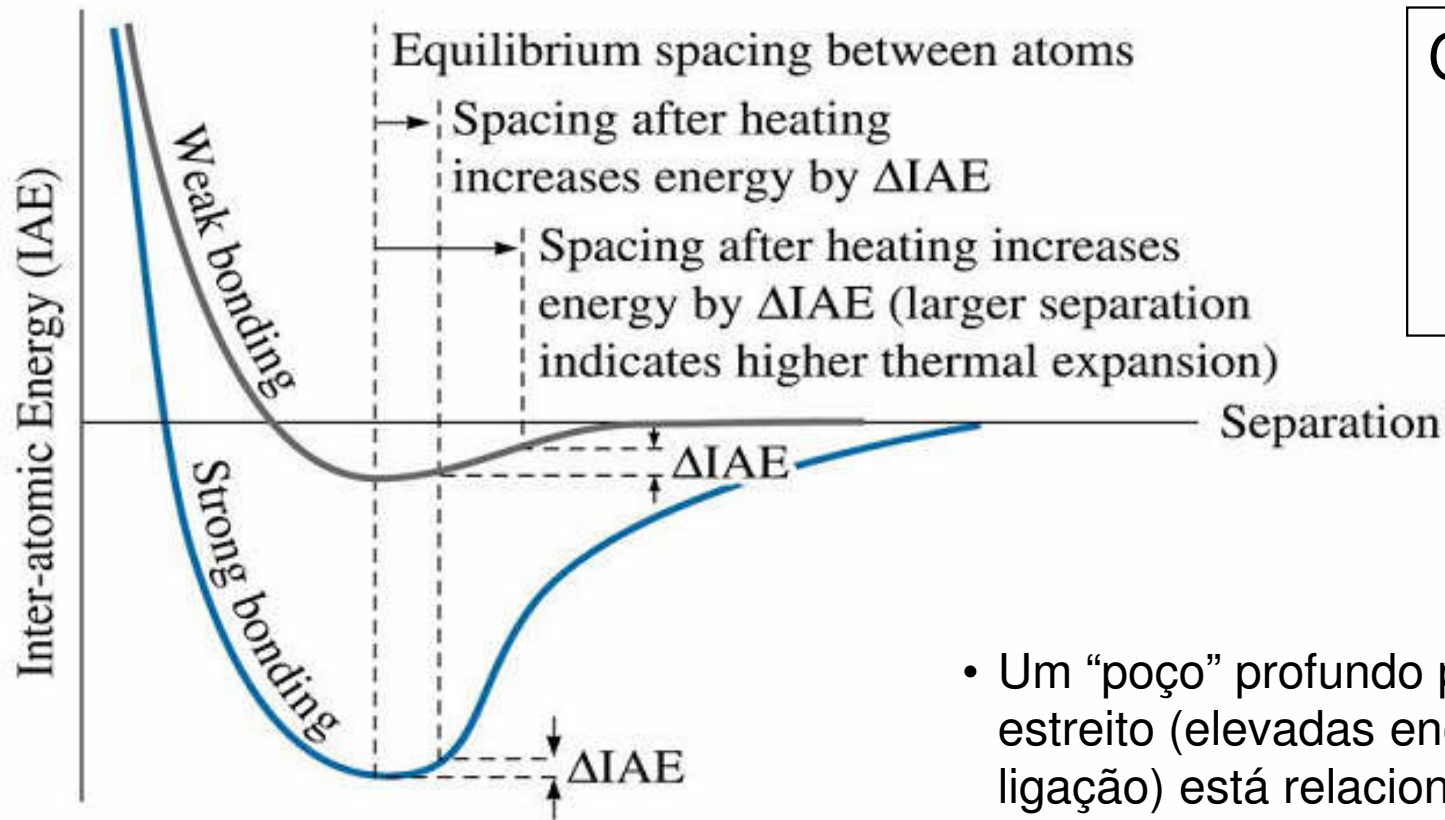
- O módulo de elasticidade pode ser associado à derivada da curva $F(r)$ no ponto $r = r_0$; quanto maior for o valor da derivada, maior será o módulo de elasticidade.
- O material a apresenta *maior rigidez* do que o material b.

r_0 = ponto onde forças de atração e repulsão são iguais

Obs.: o módulo de elasticidade é uma propriedade mecânica que será estudada em detalhe mais à frente no curso



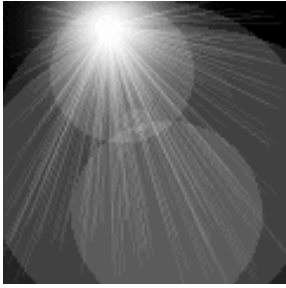
Relação Entre Algumas Propriedades e Curvas de Força e Energia de Ligação



Coeficiente de Expansão Térmica

- Um “poço” profundo e estreito (elevadas energias de ligação) está relacionado a um baixo coeficiente de expansão térmica.

Obs.: IAE = interatomic energy



CORRELAÇÃO DAS PROPRIEDADES COM AS CURVAS DE FORÇA E DE ENERGIA DE LIGAÇÃO

- Módulo de elasticidade: aumenta com a tangente da curva de força de ligação no ponto onde a força é nula, (dF_N/dr), para $F_N=0$

