Estructuras y su determinación.

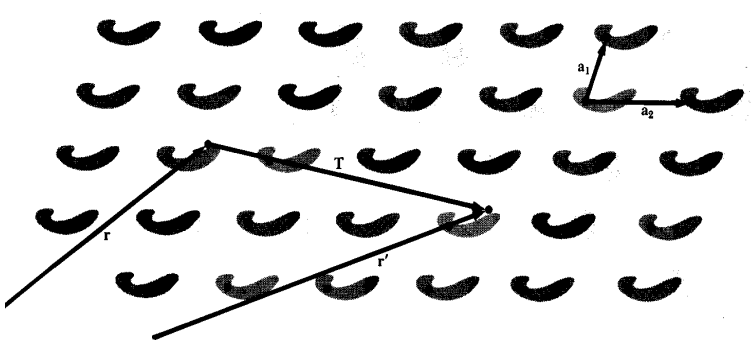
-Periodicidad. Simetrías. Definiciones.
-Estructuras Cristalinas.
-Otros tipos de ordenamientos.
-Difracción de ondas en cristales:
    -Condición de Bragg
    -Red recíproca.

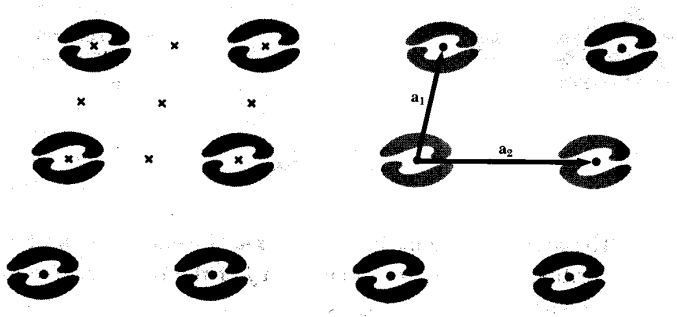
Estructura:

Red + Base = Estructura Cristalina

Simetría: La estructura es invariante (no cambia) bajo determinadas operaciones.

- Traslaciones: $\mathbf{T} = u_1\,\mathbf{a_1} + u_2\,\mathbf{a_2} + u_3\,\mathbf{a_3}$
- Puntuales: rotaciones y reflexiones.

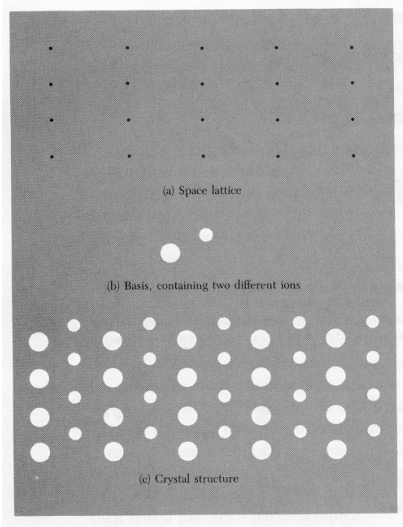




Base: conjunto de átomos ligados a cada sitio de la red

$\mathbf{r_j} = x_j\, \mathbf{a_1} + y_j\, \mathbf{a_2} + z_j\, \mathbf{a_3}$

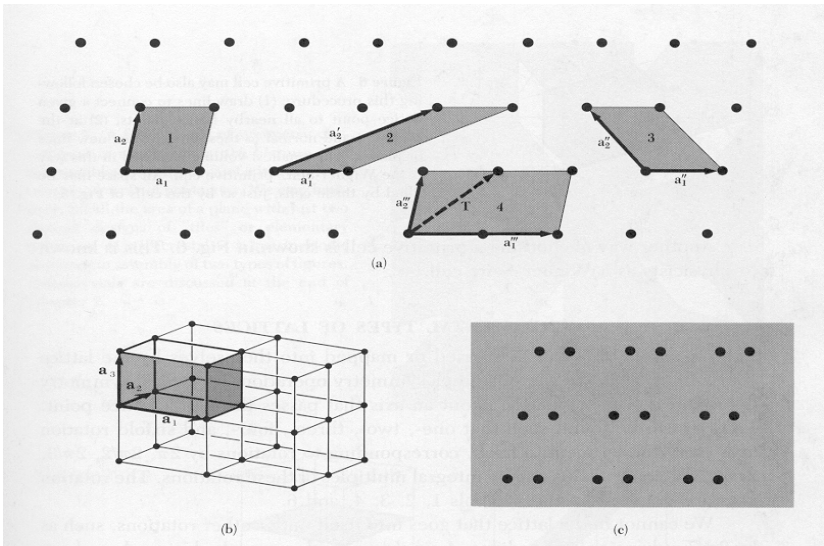
$\mathbf{0} < x_j\,,\, y_j,\, z_j < 1.$



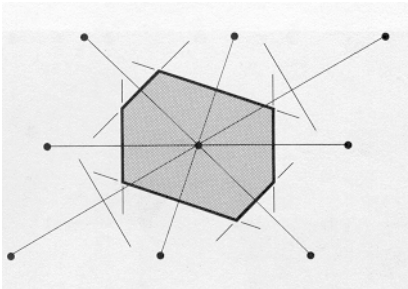
Celda Primitiva: paralepípedo definido por los vectores $\mathbf{a_1}\ \mathbf{a_2}\ \mathbf{a_3}$.

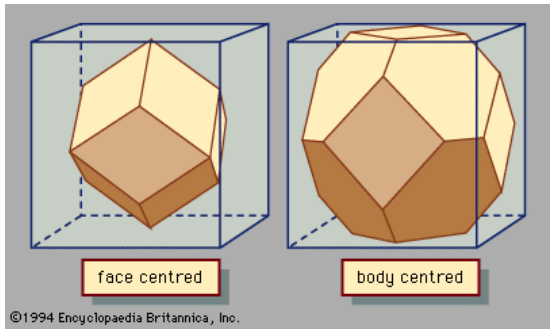
Hay un punto de la red por celda primitiva.

Vol= $|\, \mathbf{a_1}\, (\mathbf{a_2} \times \mathbf{a_3}) \,|$

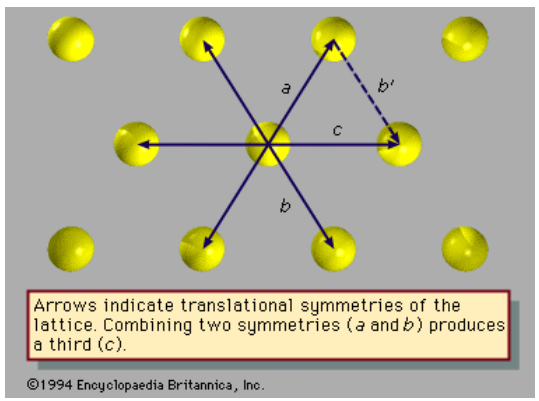


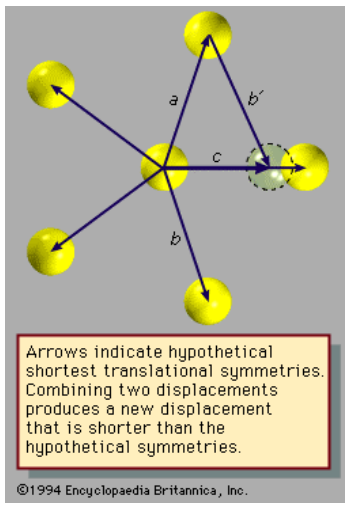
Construcción de Wigner-Seitz

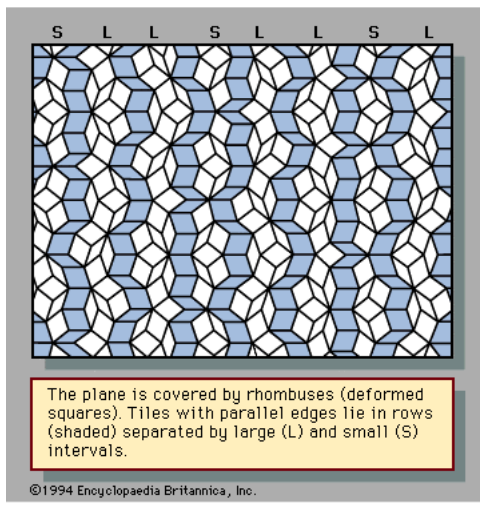




Tipos de Redes: Compatibilidad de rotaciones + traslaciones.
Sólo las rotaciones $2\pi/n$, n=1,2,3,4 y 6 están permitidas.



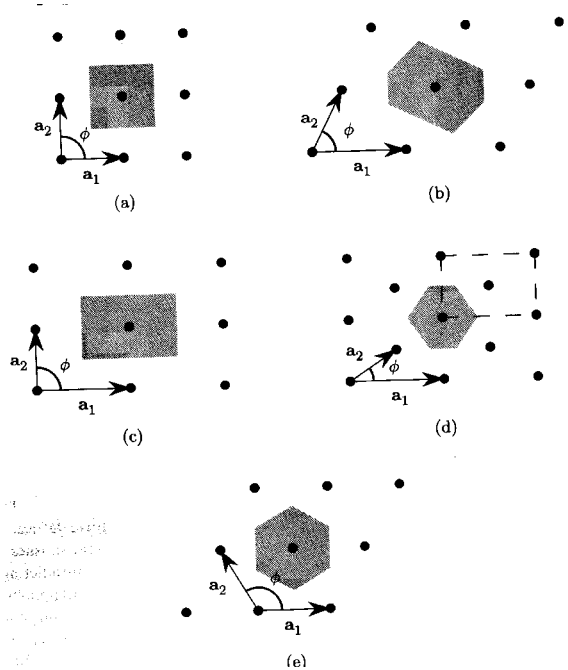




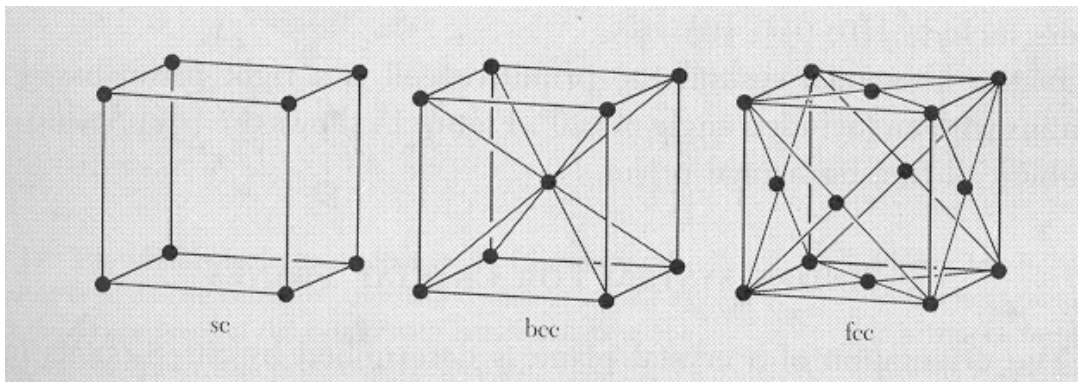
Redes en dos dimensiones:

5 redes de Bravais

Oblicua, Cuadrada, Hexagonal, Rectangular, Rectangular centrada.



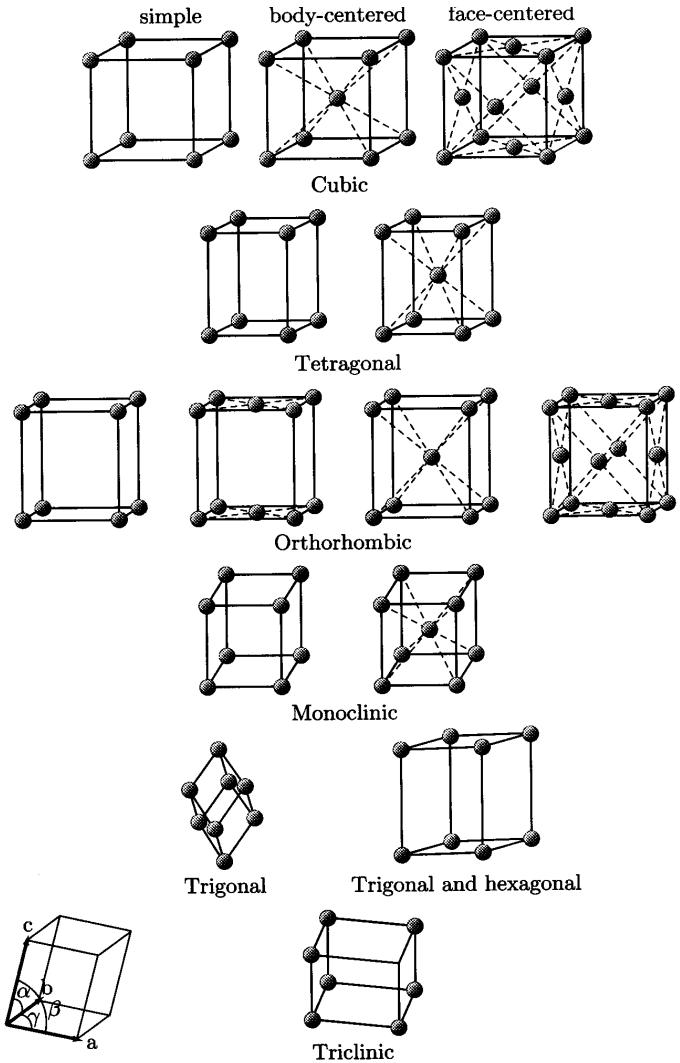
Redes en tres dimensiones: 14 redes de Bravais. Cúbica,....



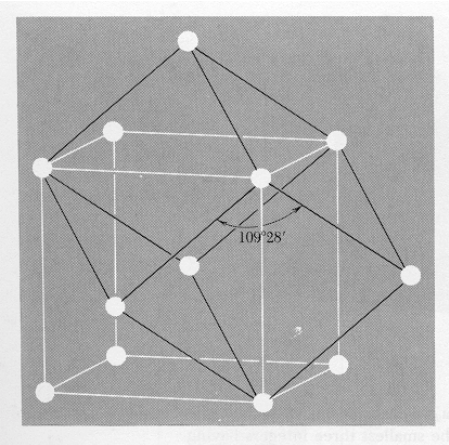
Las 14 redes de Bravais en 3 dimensiones

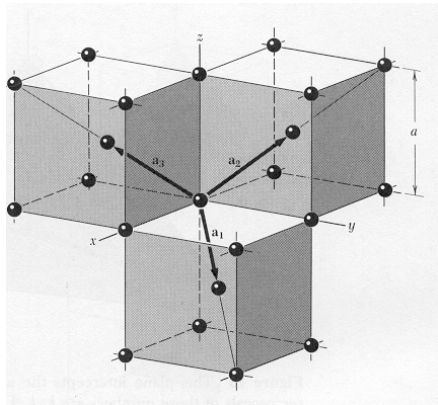
Table 2.6.1. *The 14 Bravais lattices in three dimensions.*

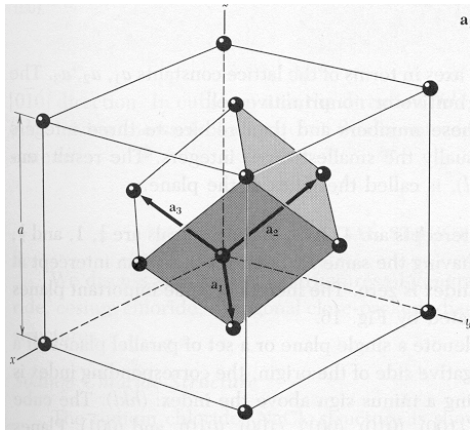
System	Number of lattices in system	Lattice symbols	Restrictions on conventional cell axes and angles
Triclinic	1	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	P,C	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	P,C,I,F	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	P,I	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
Cubic	3	P or SC I or BCC F of FCC	$a = b = c$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	R	$a = b = c$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	P	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$



Redes Cúbicas:



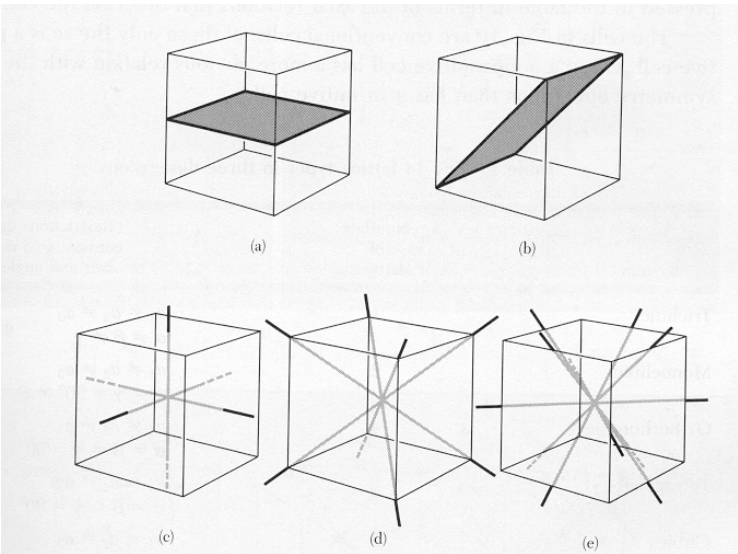




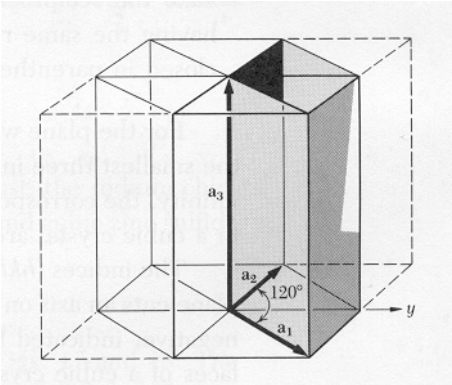
Celda primitivas BCC

FCC

Simetrías en la red cúbica

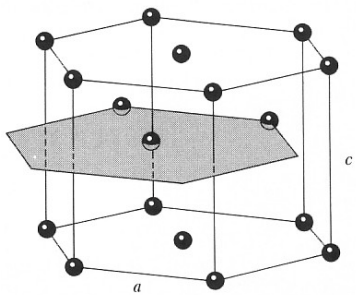


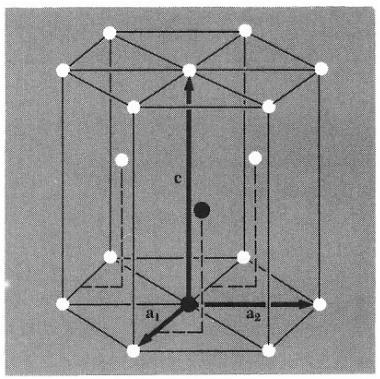
Red Hexagonal:

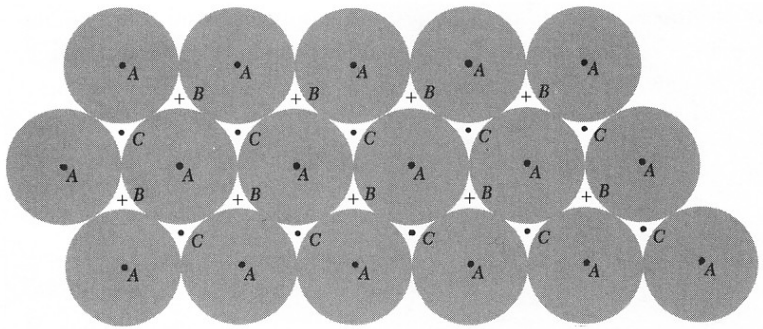


Hexagonal Compacta: HCP. Red hexagonal con base de dos átomos (0,0,0) y (2/3,1/3,½)

Máximo empaquetamiento (junto con la FCC) 0.74 si c/a = 1.633

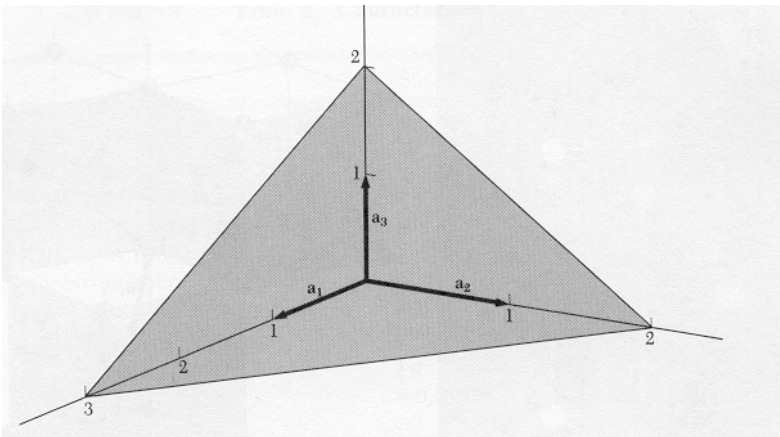






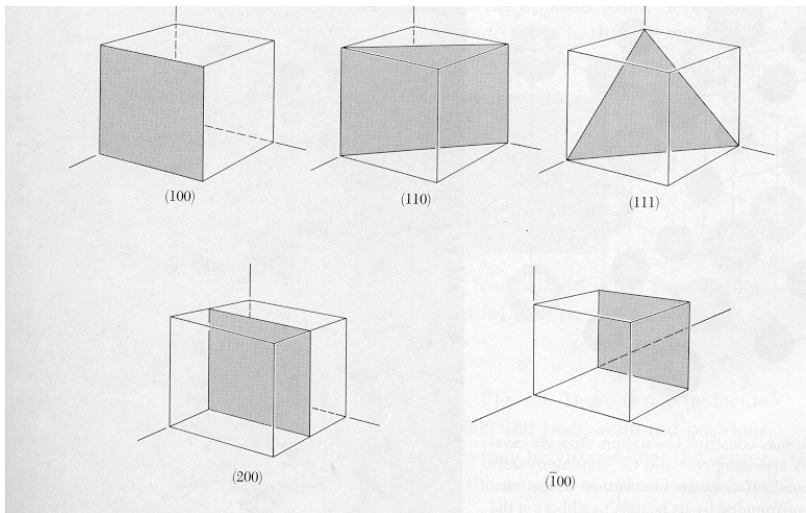
Sistema de Indices (Miller): Un plano está determinado por tres puntos. El plano se especifica por su corte con con los ejes de la celda.

Reglas para los índices:
Planos
-Encontrar los cortes con los ejes de la red.
-Tomar sus inversas y reducir a los enteros que tienen la misma proporción (p.e. Dividiendo por el más pequeño). El resultado son los índices del plano (hkl).
-Si el corte es por la parte negativa se pone una barra al índice.
-El conjunto de planos relacionados por simetría Se representan por {hkl}.



Direcciones:
-Los enteros más pequeños que tienen la misma proporción que las componentes del vector en la base de la celda. Se representan por [hkl].

En el sistema cúbico son perpendiculares planos y direcciones con los mismos índices. (Demuéstralo)



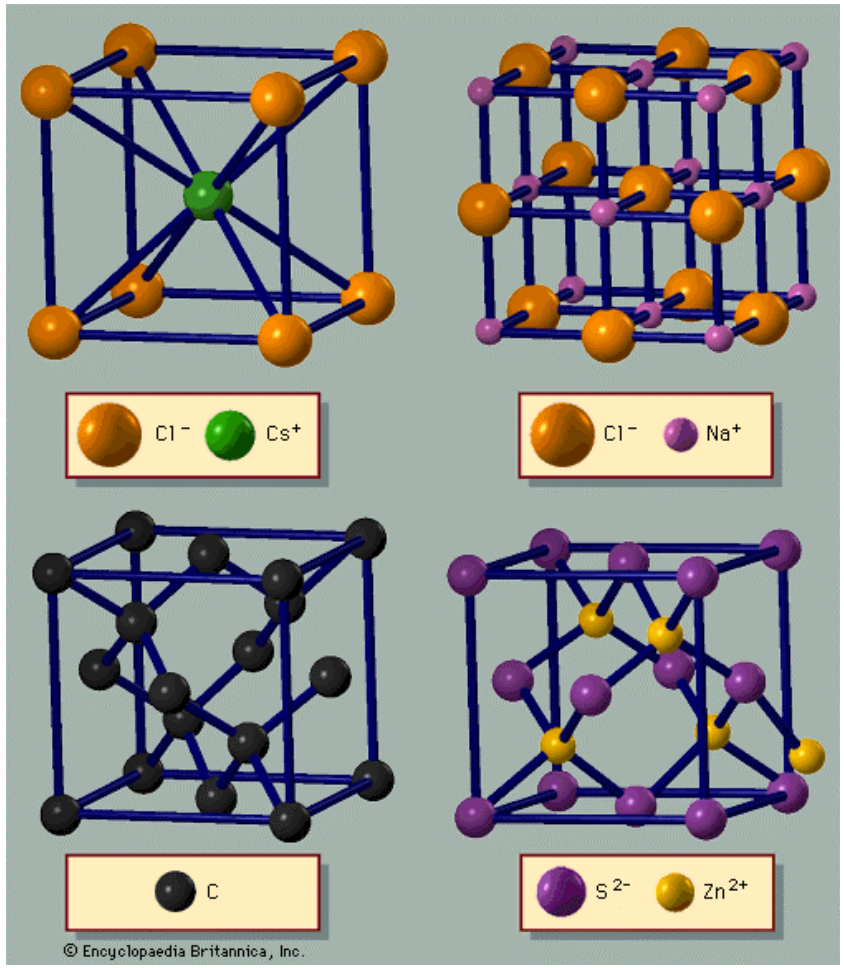
Algunas estructuras sencillas:

NaCl: FCC con base 2 átomos
4 moléculas por celda unidad.
Cl: 000; ½, ½,0; ½,0,½ ; 0, ½, ½
Na: ½, ½, ½; 0,0, ½; 0, ½,0; ½,0,0

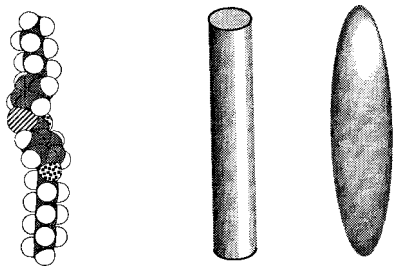
ClCs: SC con base de 2 átomos
1 molécula por celda unidad.
Cl: 000 Cs: ½,½,½

Diamante: FCC con base de 2 átomos
8 átomos por cubo unidad
C: 0,0,0 ; ¼ , ¼, ¼;

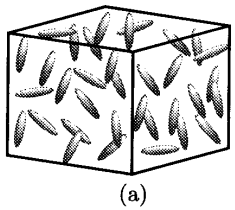
SZn: FCC con base de 2 átomos.
4 moléculas por celda unidad
S: 000; ½, ½,0; ½,0,½ ; 0, ½, ½
Zn; ¼, ¼, ¼; ¼, ¾, ¾; ¾, ¼, ¾; ¾, ¾, ¼;



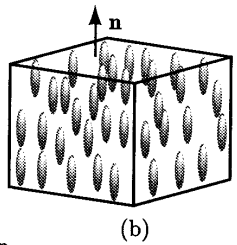
Otros ordenamientos: Cristales Líquidos.

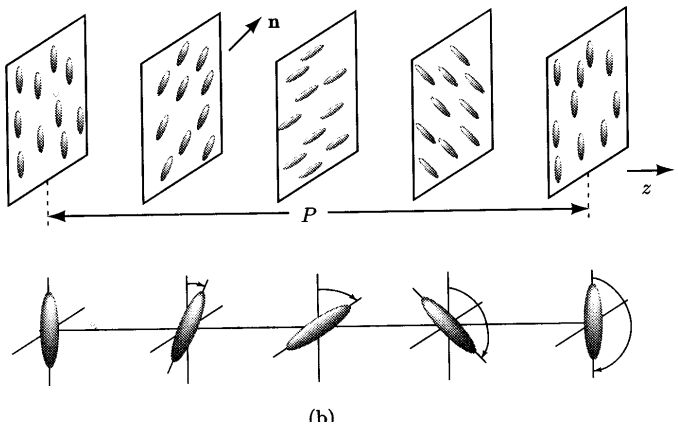


Isótropo

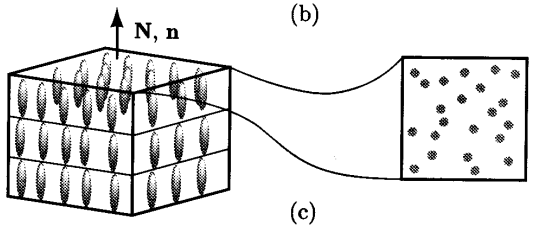


Nemático

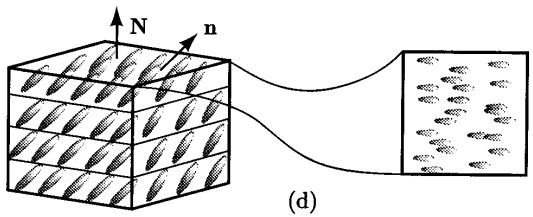




Esméctico A

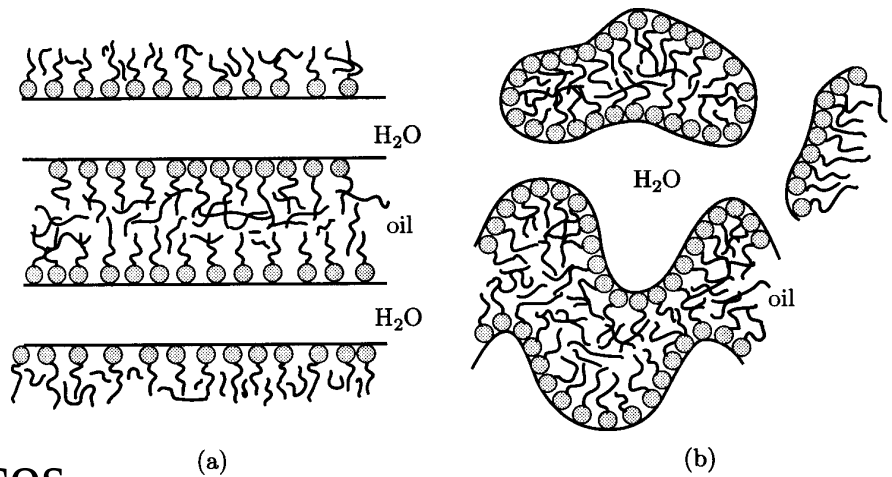


Esméctico C

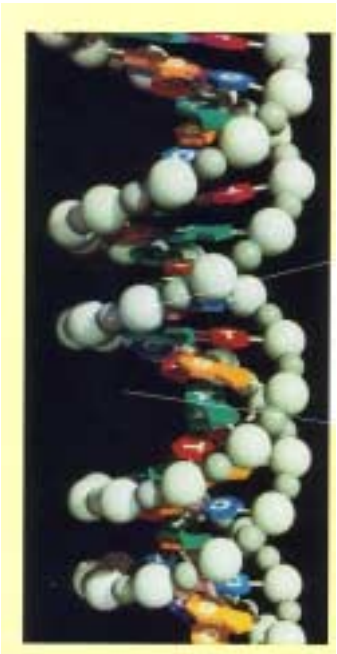


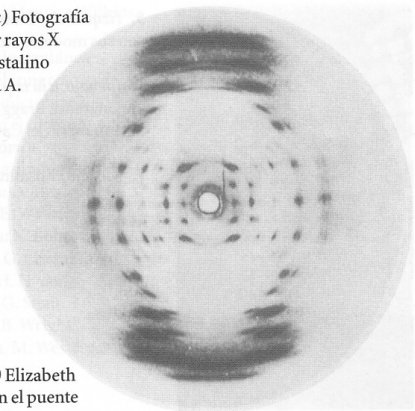
Colestérico

Estructuras Biológicas: membranas.



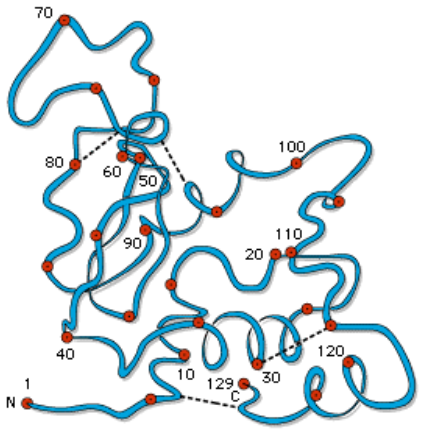
Proteínas y acidos nucleícos





8. *(derecha)* Fotografía tomada por rayos X de ADN cristalino en su forma A.

9. *(debajo)* Elizabeth Watson, con el puente



The simplified structure of lysozyme from hen's egg white has a single peptide chain of 129 amino acids. The amino acid residues are numbered from the terminal α amino group (N) to the terminal carboxyl group (C). Circles indicate every fifth residue; every tenth residue is numbered. Broken lines indicate the four disulfide bridges. Alpha-helices are visible in the ranges 25 to 35, 90 to 100, and 120 to 125.

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Estructuras conmensuradas e inconmensuradas: Películas adsorbidas en grafito.

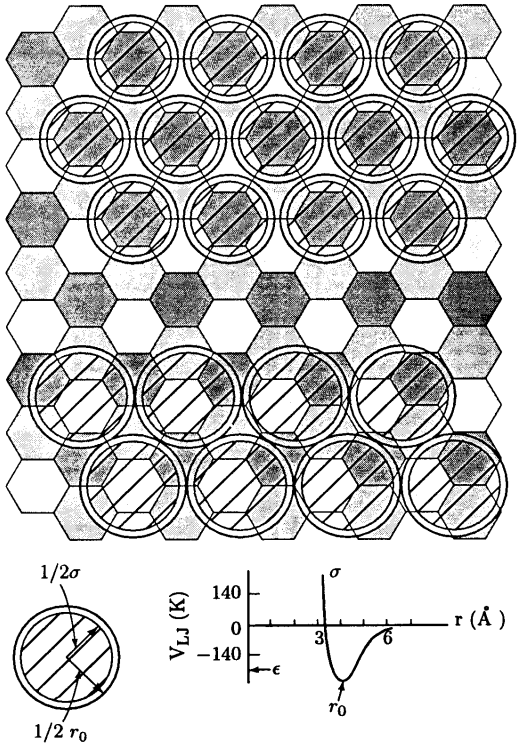
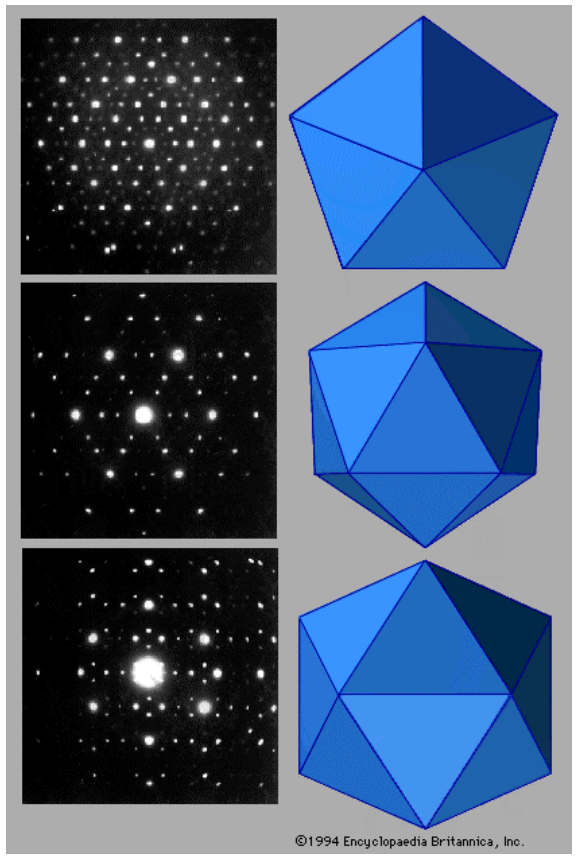


Fig. 2.9.1. Krypton (top) and xenon (bottom) on a graphite lattice. The size of krypton is such that it can occupy every third hexagon of the graphite lattice to produce a $\sqrt{3} \times \sqrt{3}R30°$ commensurate lattice. Xe is larger than Kr, and the Kr commensurate structure is prohibited. An incommensurate phase is often preferred. [R.J. Birgeneau and P. M. Horn, *Science* **232**, 329 (1986).]

Cuasicristales



Ordenamiento magnético:

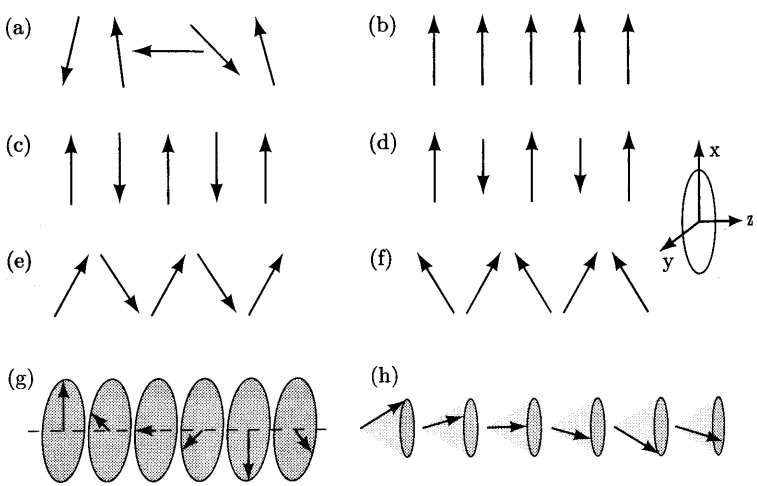


Fig. 2.11.1. Schematic representation of spins in (a) a paramagnetic, (b) a ferromagnetic, (c) an antiferromagnetic, (d) a ferrimagnetic, (e) a canted, (f) a fan, and (g) and (h) two helical phases. With the pitch axis parallel to the z-axis, the spins in the helical phases can be represented as $\mathbf{S}(\mathbf{x}) = (S_\perp \cos k_0 z, S_\perp \sin k_0 z, S_z)$ where k_0 is the twist wave vector. In (g) there is no spin component S_z along the pitch axis, whereas in (h) there is.

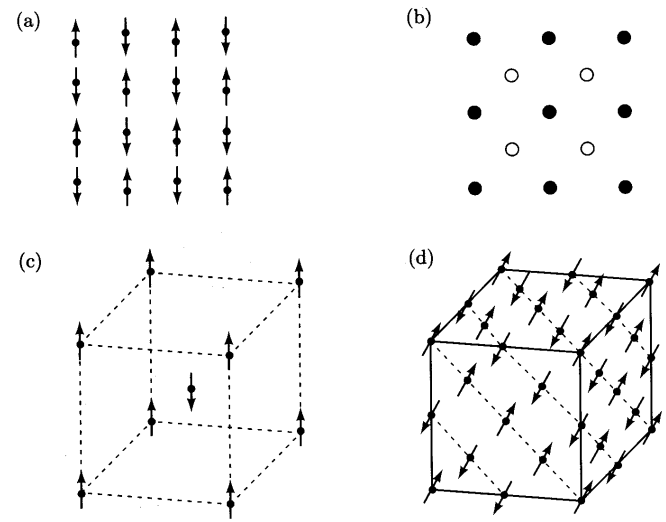
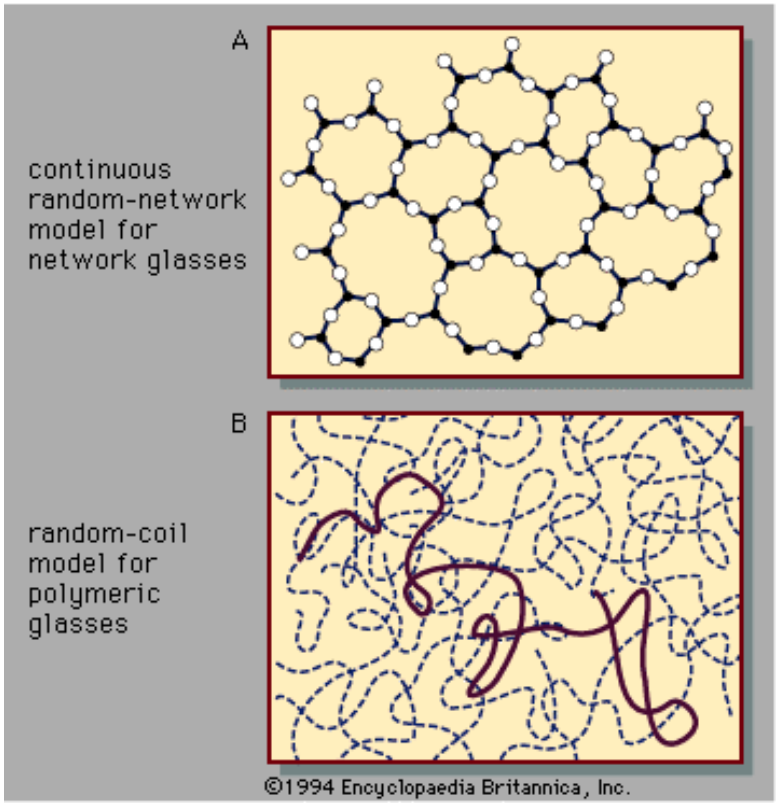


Fig. 2.11.2. (a) Antiferromagnetic order on a square lattice showing the doubling of the unit cell size. (b) Bragg peaks for antiferromagnetic order on a square lattice. The solid circles indicate Bragg peaks from the chemical unit cell. The open circles indicate magnetic superlattice peaks. (c) Antiferromagnetic order on a BCC lattice. (d) Antiferromagnetic order on an FCC lattice. The atoms shown correspond to the Mn^{2+} ions in MnO.

Estructuras no-periódicas: amorfos, vidrios y fractales.



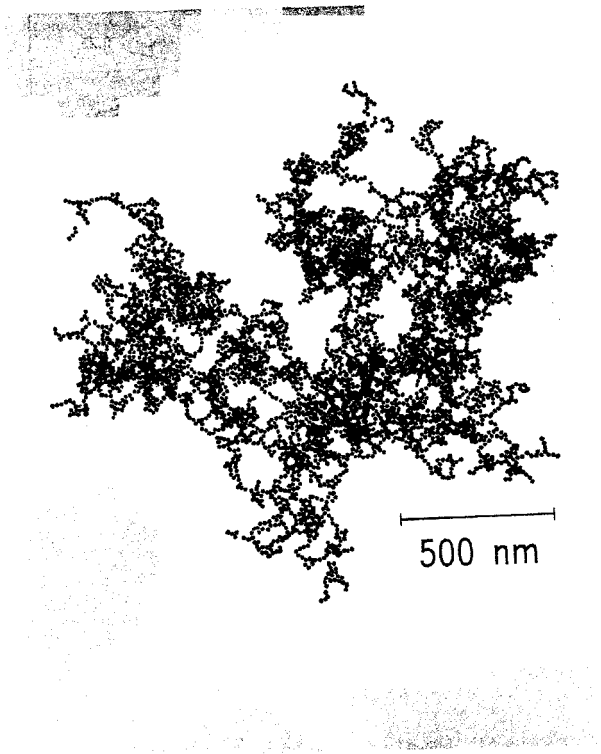


Fig. 2.12.4. A fractal aggregate of gold particles. [Courtesy of D. A. Weitz.]