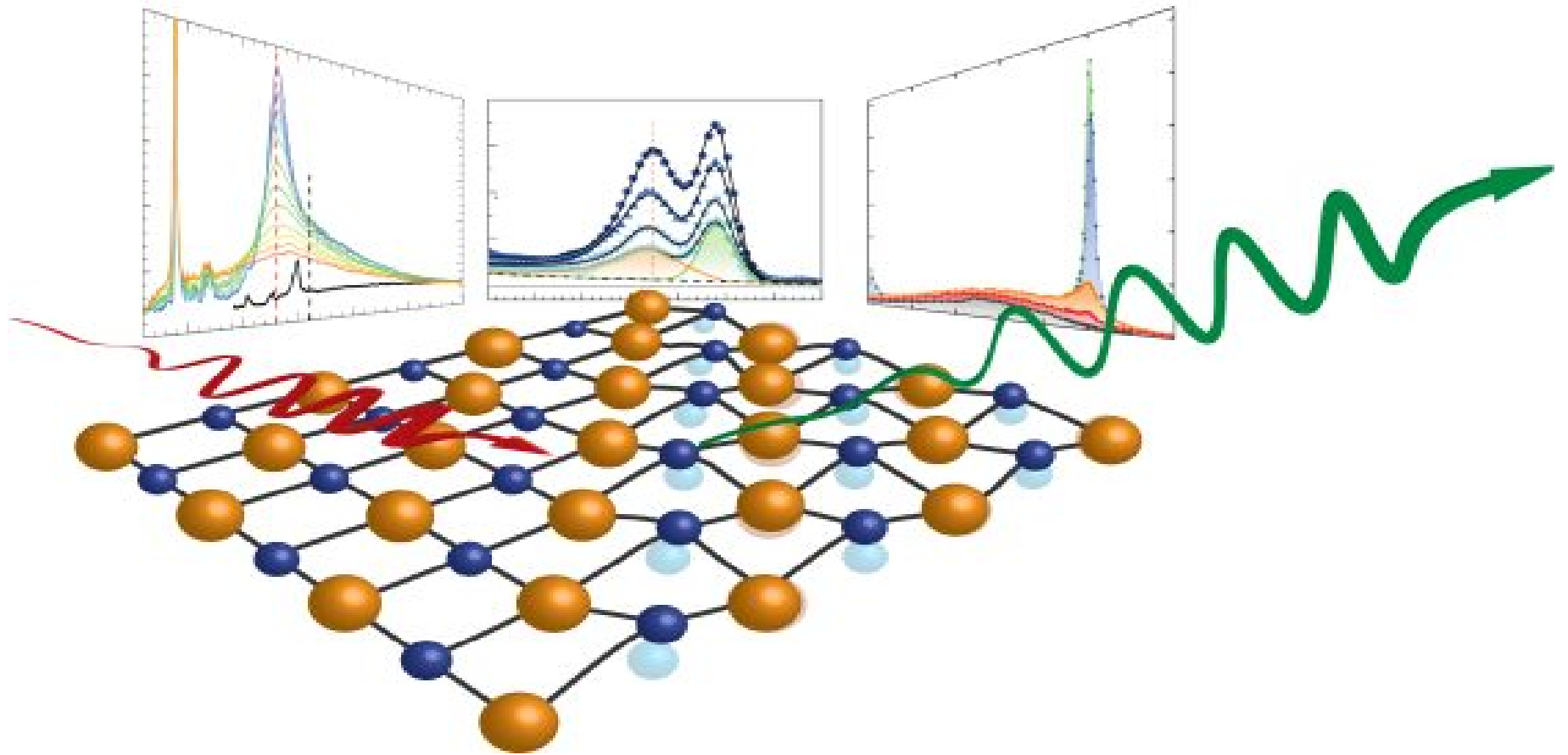


Bienvenidos a Materia Condensada



Licenciatura en Física (FCEIA- UNR)

<http://www.fceia.unr.edu.ar/~matcon/>

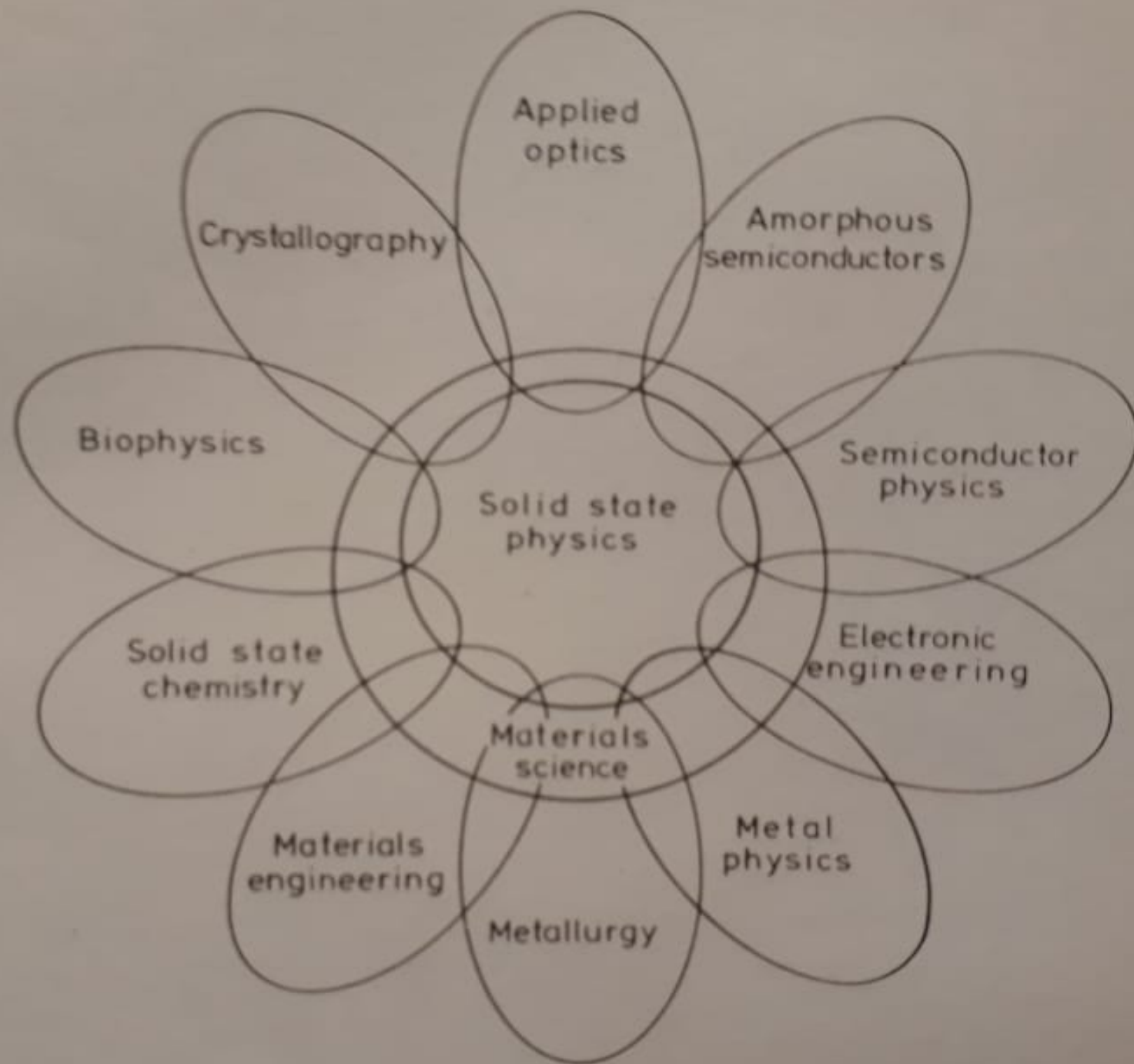
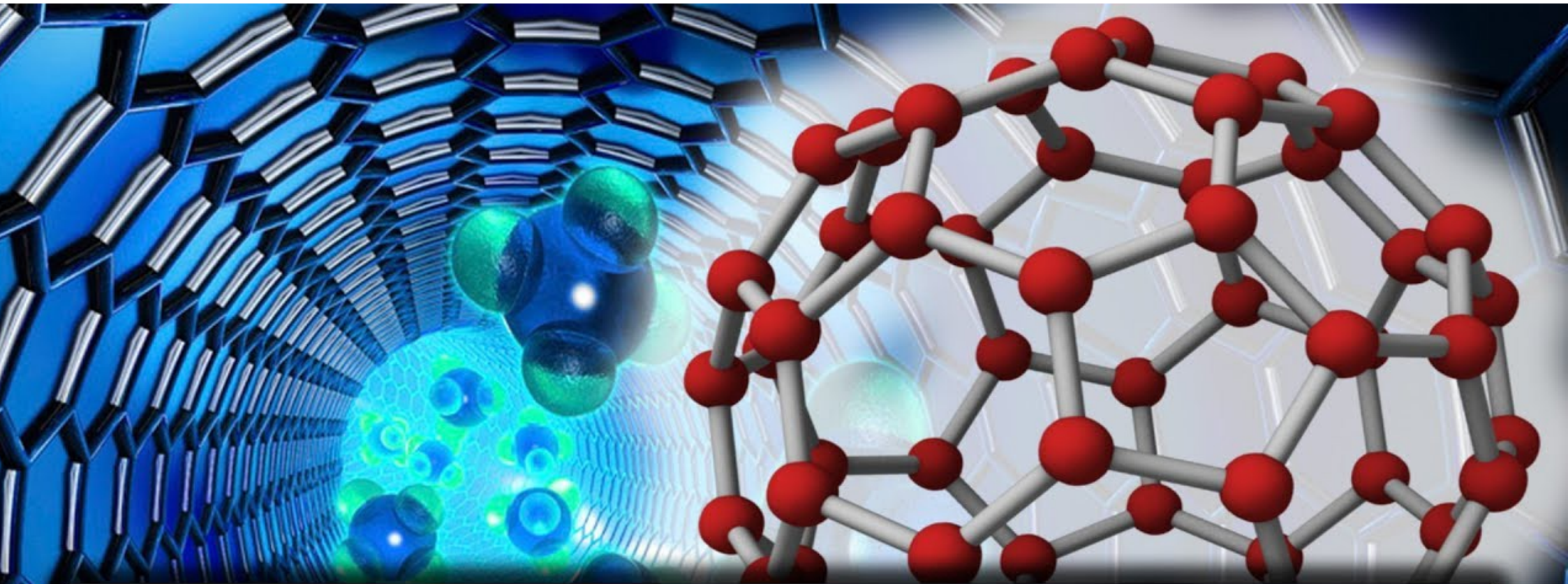


Figure 1 Some of the major overlapping research fields within Solid State Science. Solid State Physics is at the core of nearly all fields, while



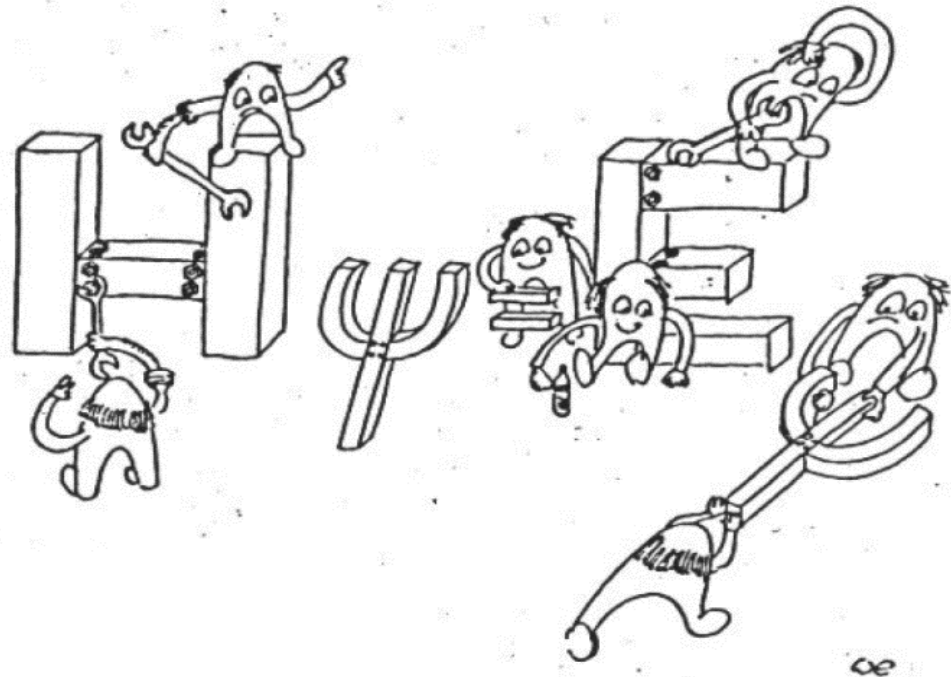
NANOTECHNOLOGY

Programa de la asignatura

OBJETIVOS: Conceptos básicos de estructura cristalina, técnica de difracción de rayos X, tipos de uniones en elementos y compuestos, dinámica de la red, modelo del gas de electrones para metales, estructura electrónica y transporte, semiconductores.

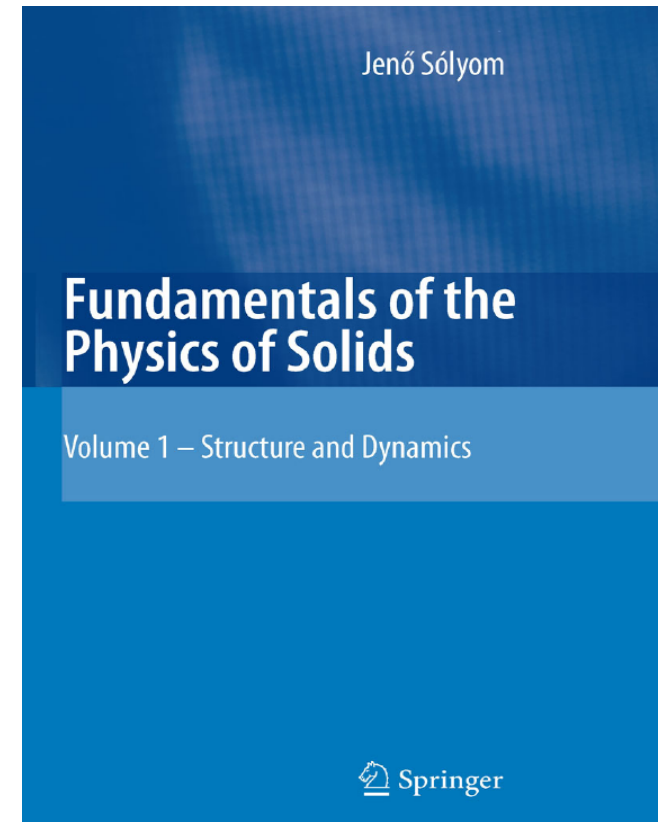
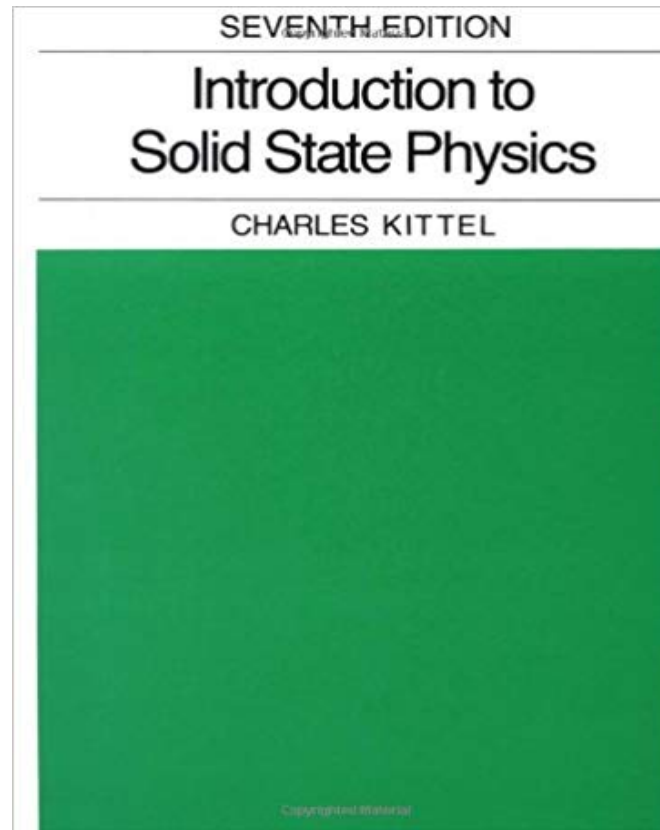
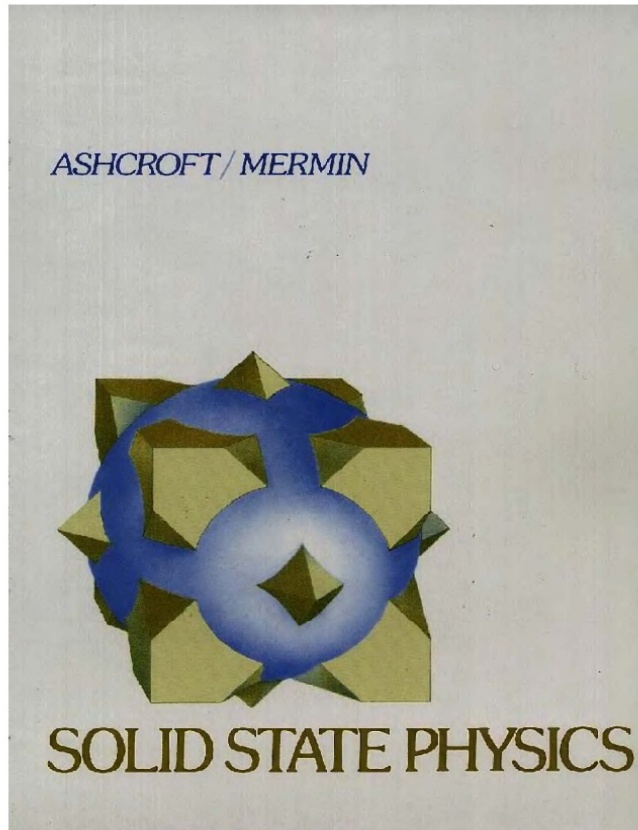
CARACTERÍSTICAS GENERALES: Se imparten los conocimientos teóricos básicos que permiten comprender el comportamiento de la materia en estado sólido, en particular cristalino, frente a diversas experiencias también descritas en el curso. Abarca un área muy amplia de la Física que involucra la mayor parte de sus aplicaciones tecnológicas. **Requiere conocimientos obtenidos en prácticamente toda la carrera**, pero en mayor grado de las materias a continuación mencionadas: Mecánica, Electromagnetismo, Mecánica del Continuo, Mecánica Cuántica, Mecánica Estadística.

Mecánica Cuántica y Estadística en acción



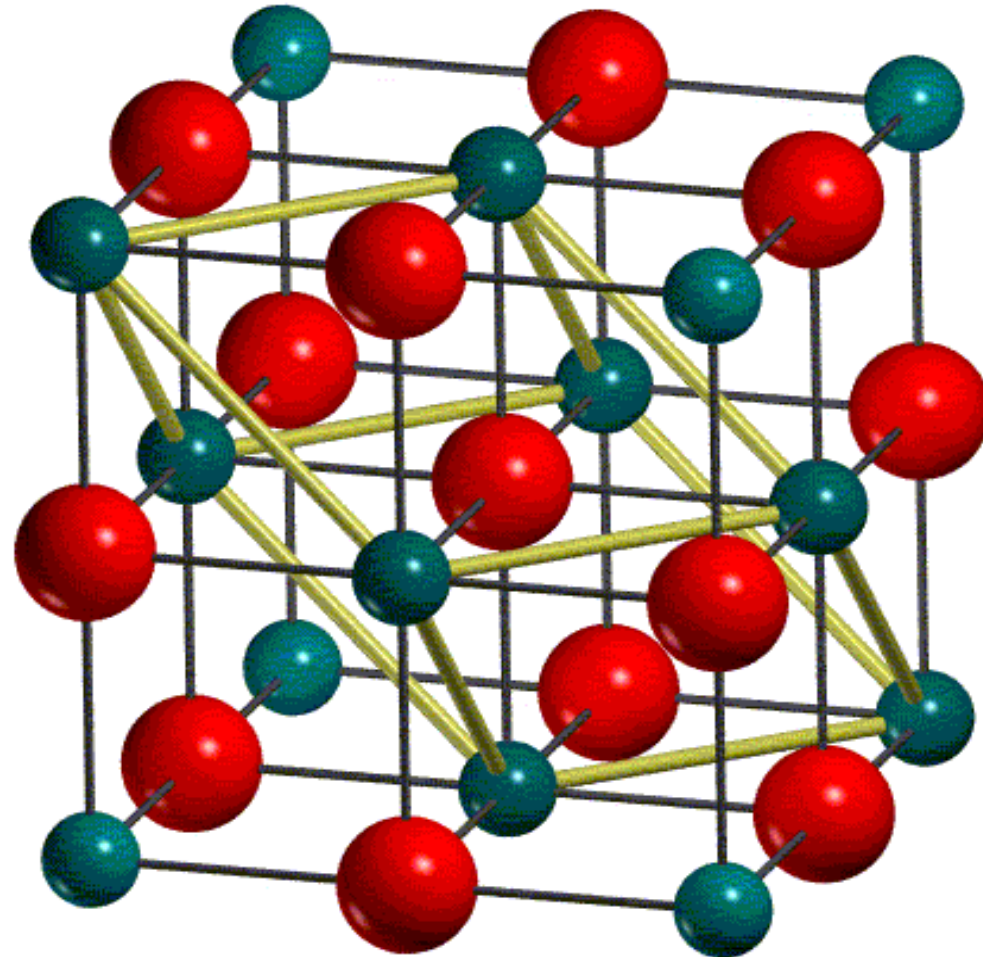
Bibliografía

- Solid State Physics, N.W. Ashcroft and N.D. Mermin (Saunders College, 1976)
- Introduction to Solid State Physics, C. Kittel (J. Wiley, 7a Edición, 1996)
- Fundamentals of the Physics of Solids (Volume I&II), J.Sólyom (Springer,2007)



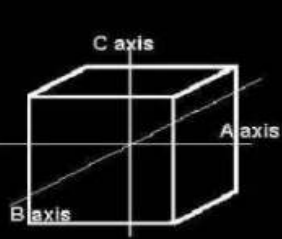
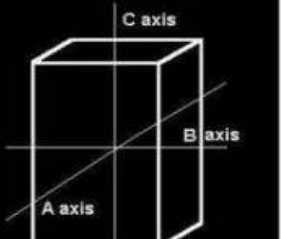
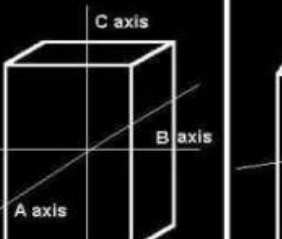
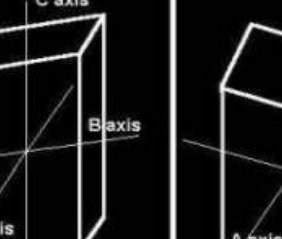
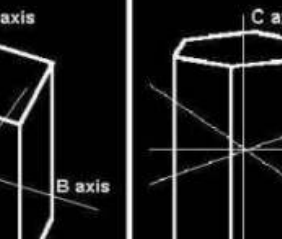
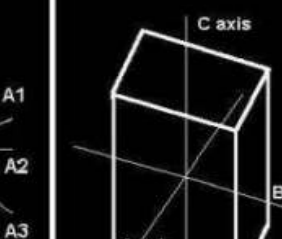





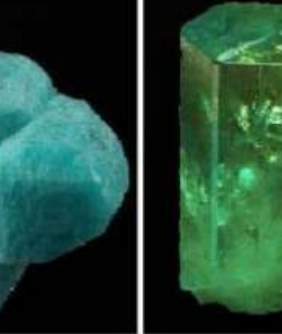


- Material adicional: Software Solid State Simulation Proyect

Capítulo 1: Estructuras Cristalinas



Como están ubicados los átomos en los sólidos?

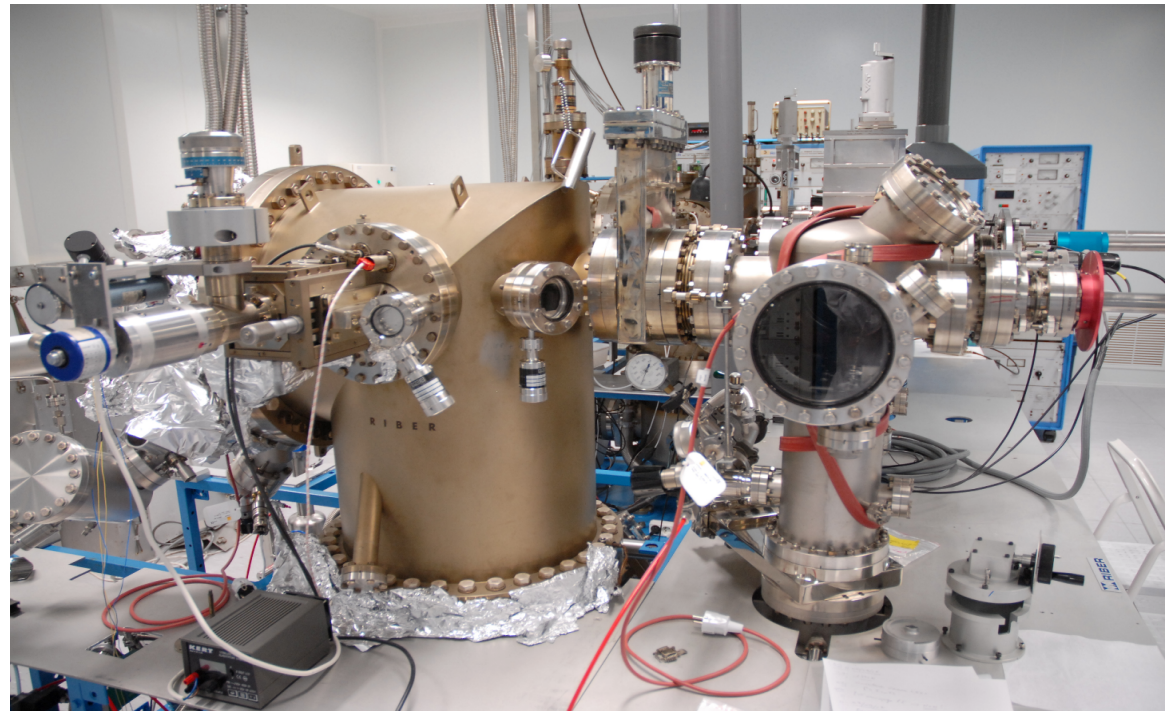
En algunos minerales la estructura macroscópica lo denota

Crystal Systems						
Isometric	Tetragonal	Orthorhombic	Monoclinic	Triclinic	Hexagonal	Trigonal
						
						
Fluorite	Wulfenite	Tanzanite	Azurite	Amazonite	Emerald	Rhodochrosite

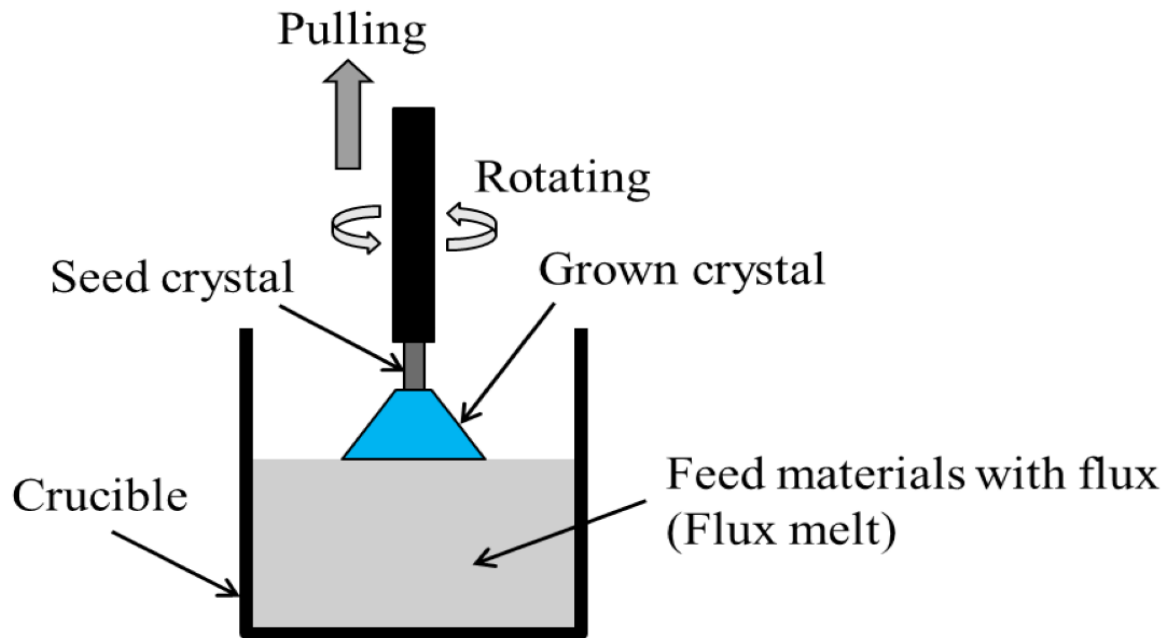
CUEVA DE CRISTALES (Mina de Maica, Mexico)



Cristales naturales de Selenita
($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$)



(MBE - Molecular Beam Epitaxy)



Cristal de KDP

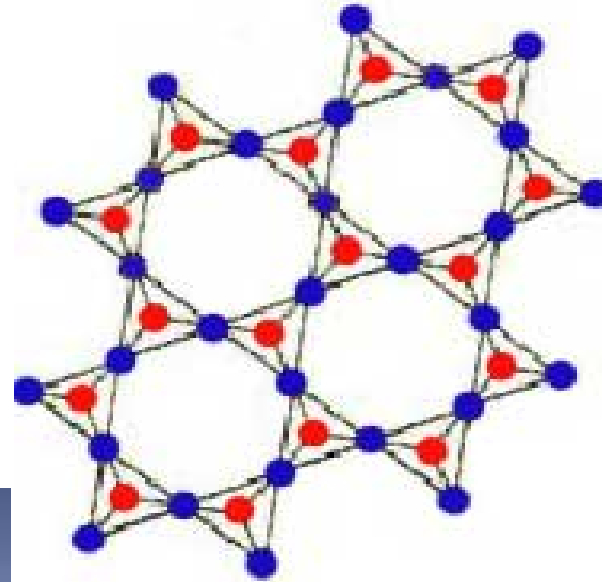


Estructuras Cristalinas

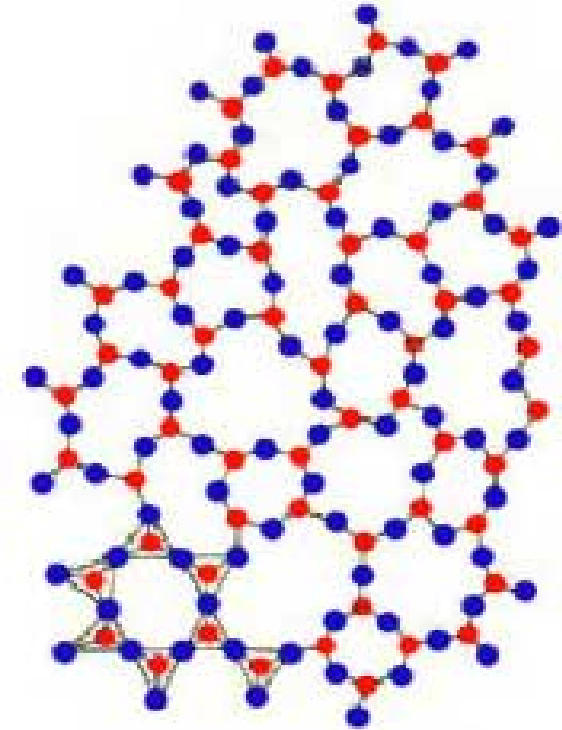


Cuarzo (SiO_2)

Crystalline SiO_2
(Quartz)



Amorphous SiO_2
(Glass)



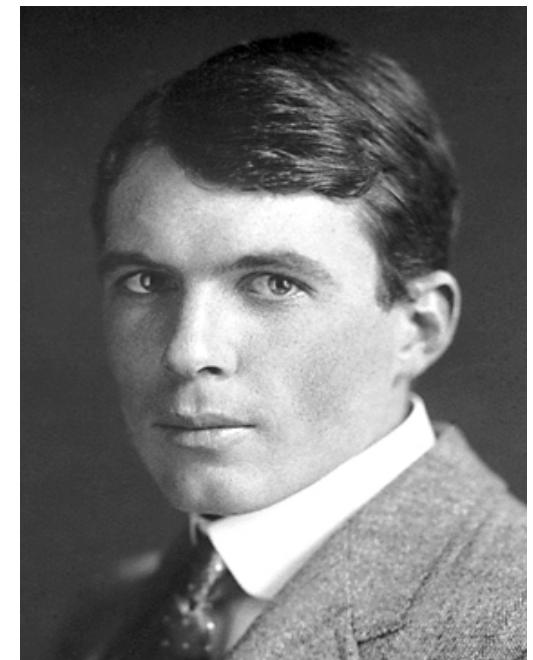
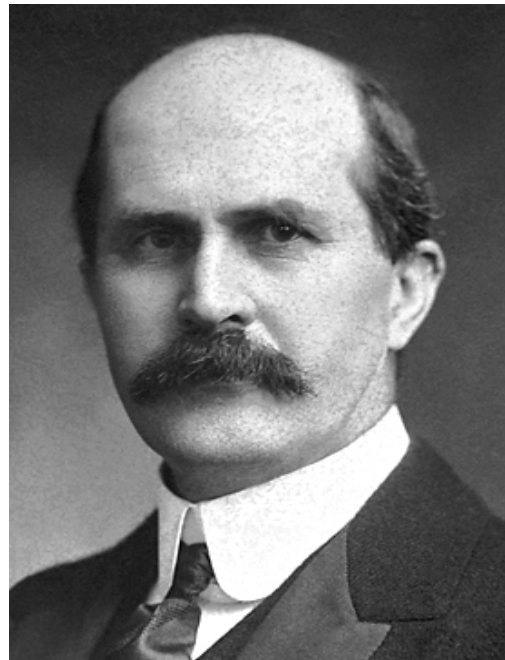
● Si ● O



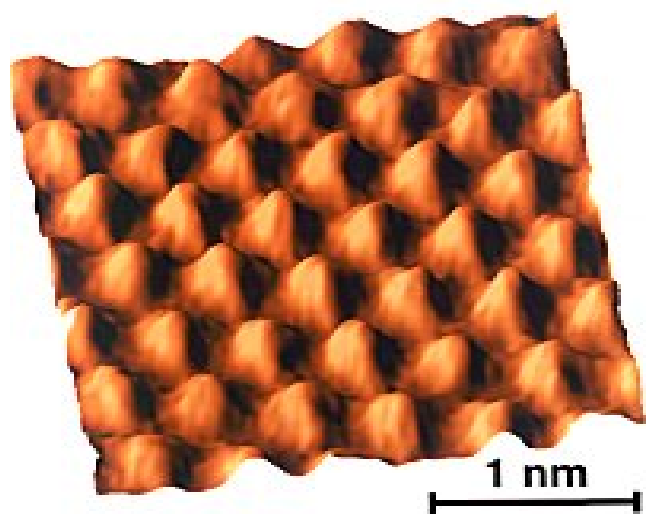
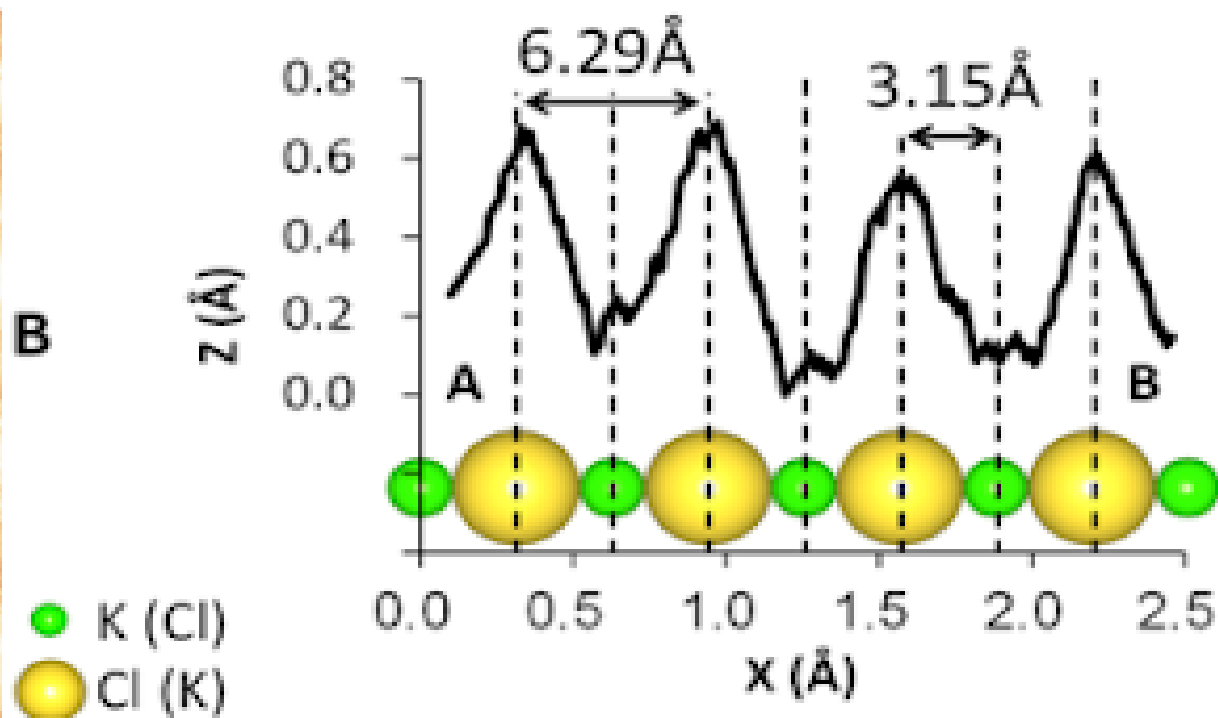
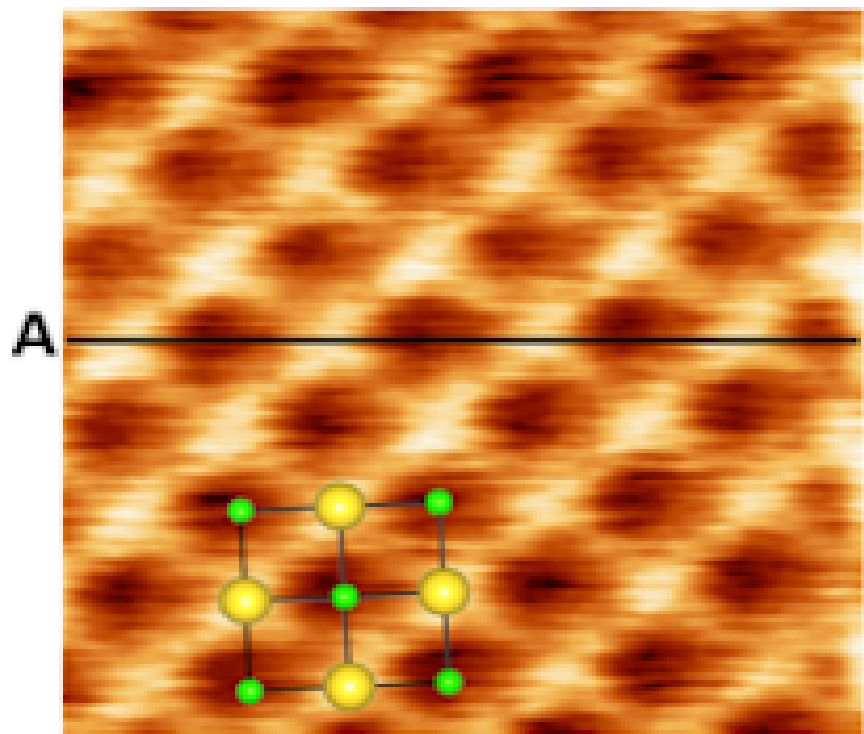
El ordenamiento atómico fue una hipótesis ad-hoc hasta que recibió confirmación experimental en 1913 mediante la técnica de **difracción de Rayos X (XRD)**



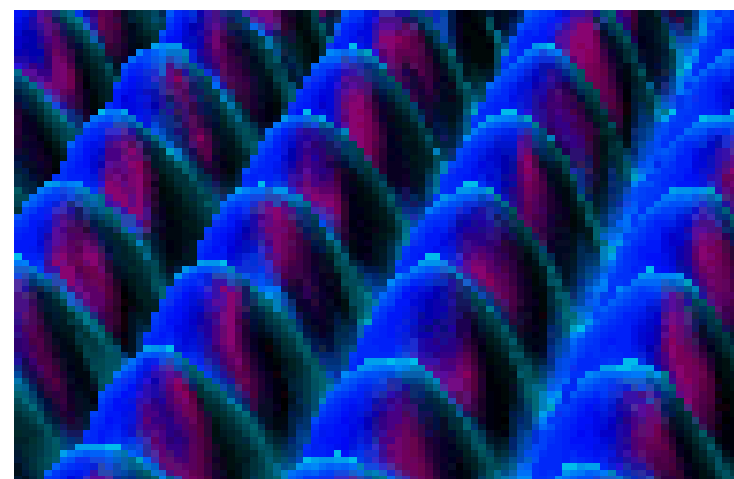
**Max von Laue
(Nobel 1914)**



**Los Bragg
(Nobel 1915)**

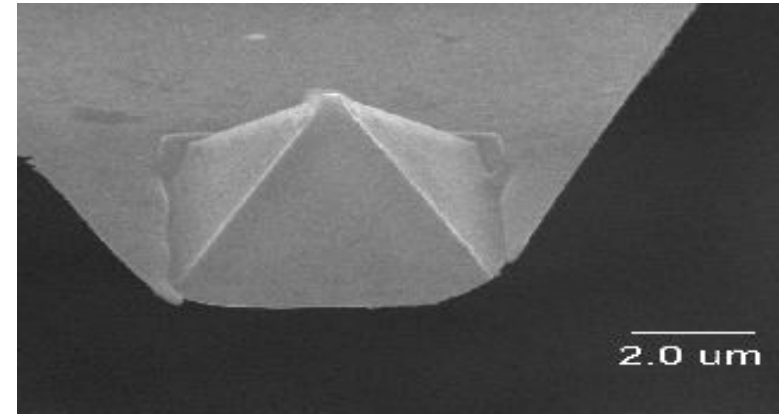
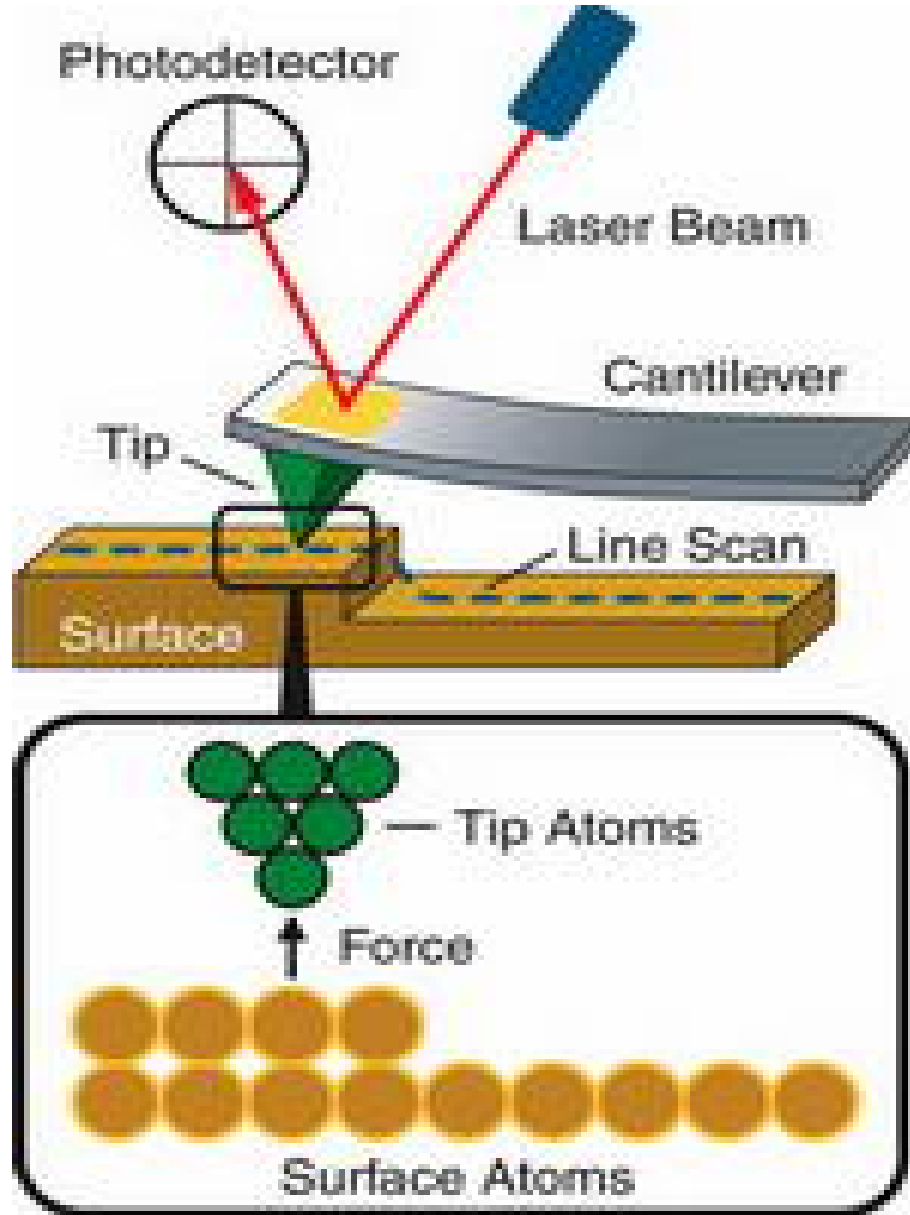


Superficie de Xenon



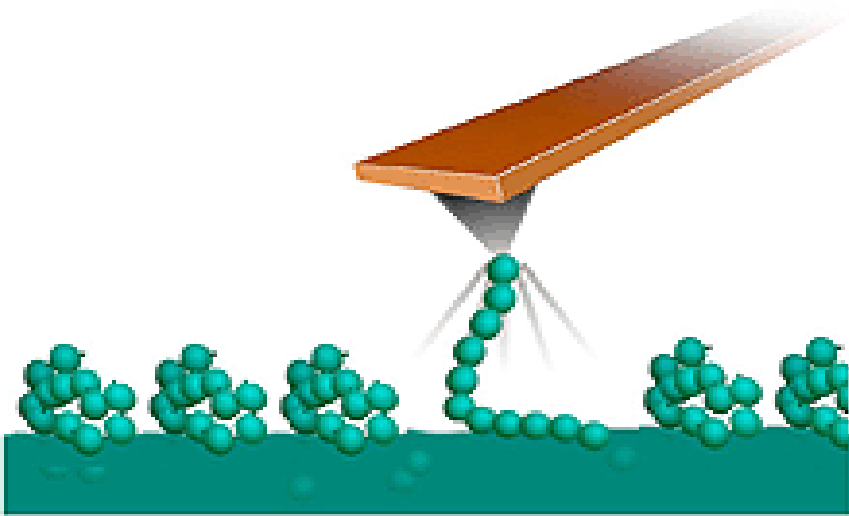
Superficie de Niquel

Microscopio de fuerza atómica (AFM)

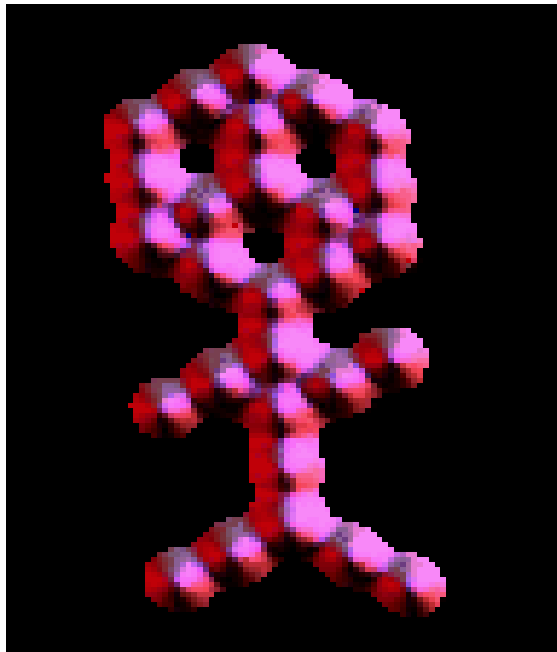
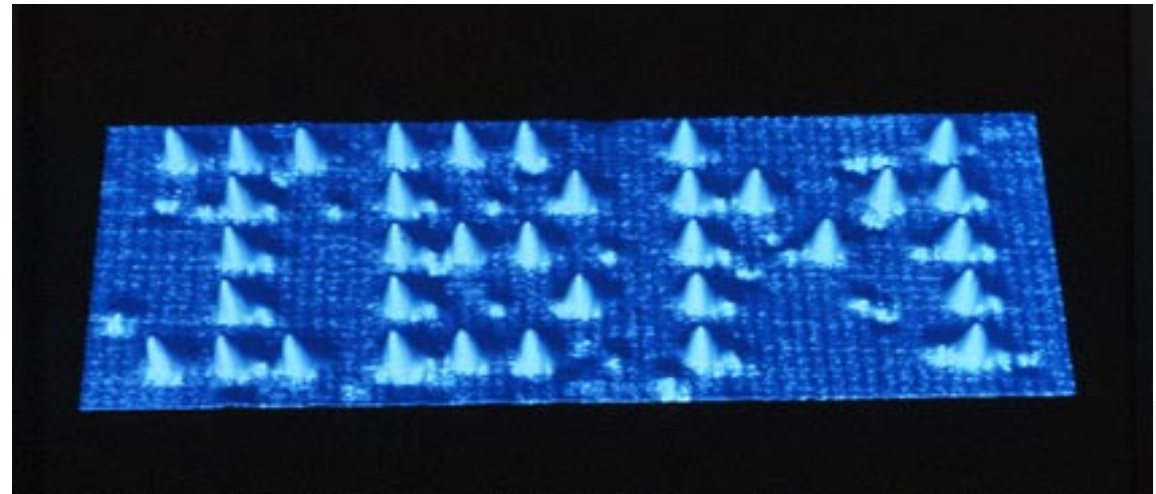


**Rohrer & Binnig
(Nobel 1986)**

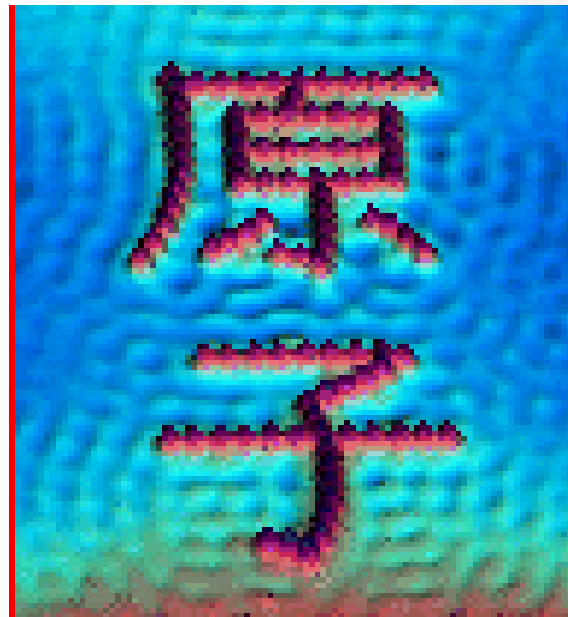
IBM (1990) *Xe sobre Ni (110)*



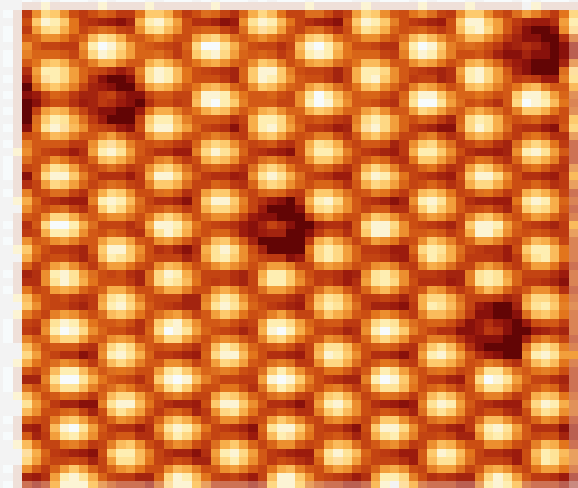
(Figure 9) Force Pulling illustration



CO sobre Pt (111)

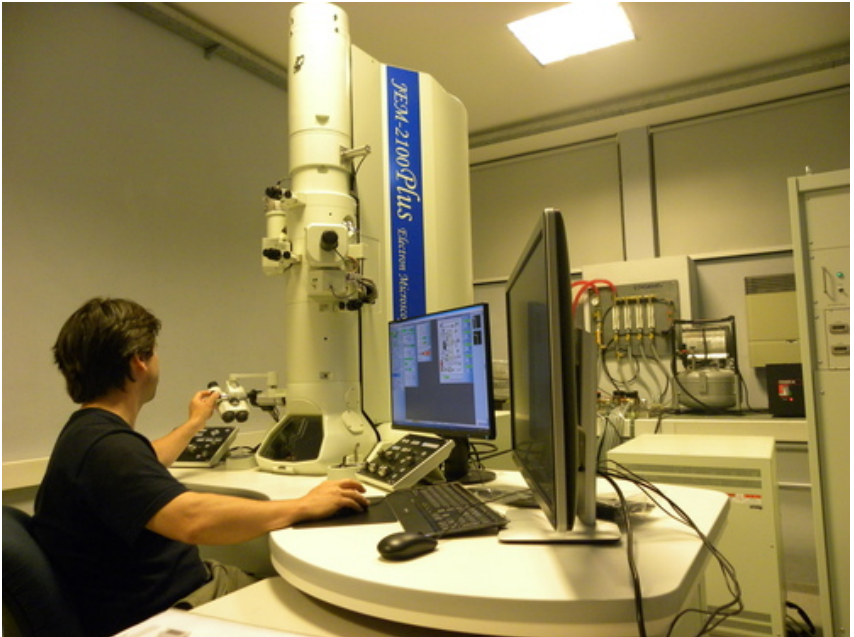
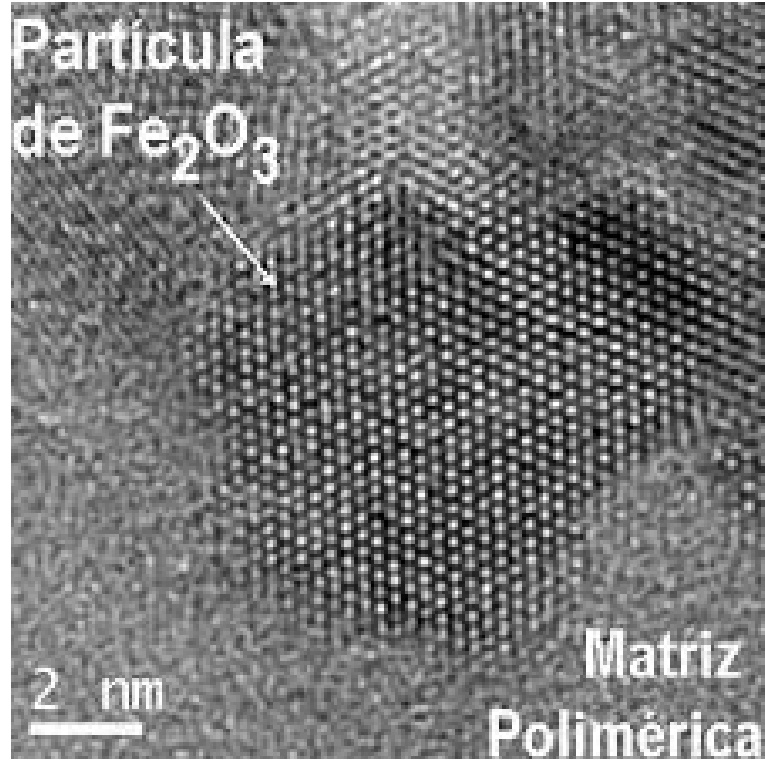


Fe sobre Cu (111)

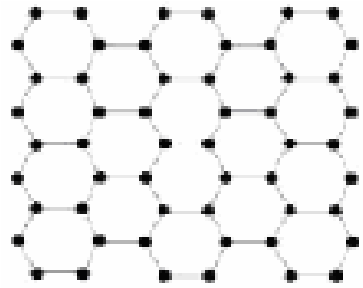


Sn por Si (2008)

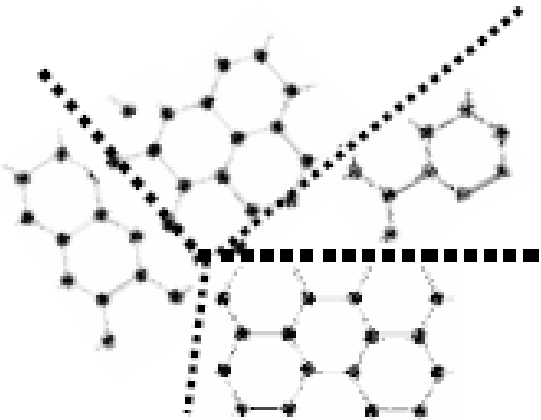
Microscopio electrónico de transmisión (TEM)



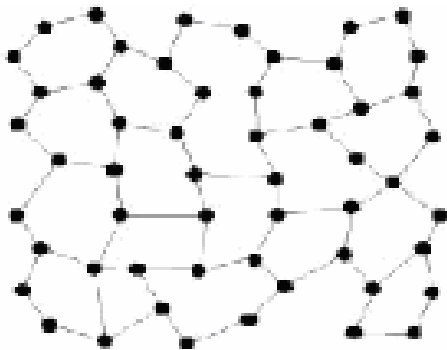
Policristales



MONOCRISTAL
Anisotropía



POLICRISTAL
Isotropía
Estadística



AMORFO

Muchos de los materiales de origen tanto natural como sintético (minerales, metales, cerámicas etc.) son **policristalinos**.

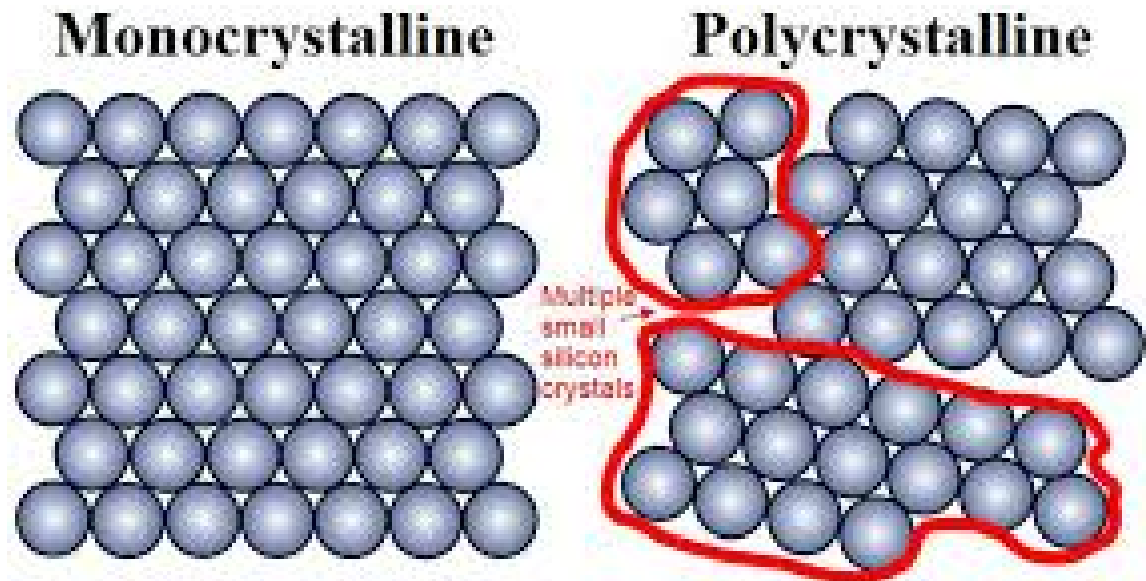
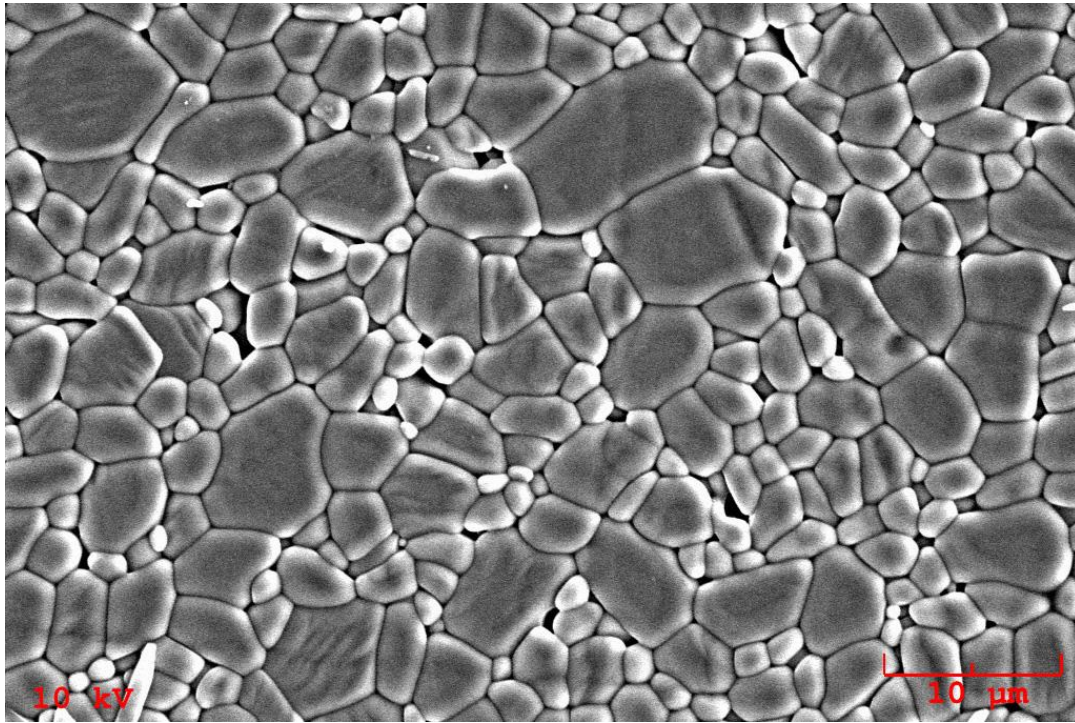
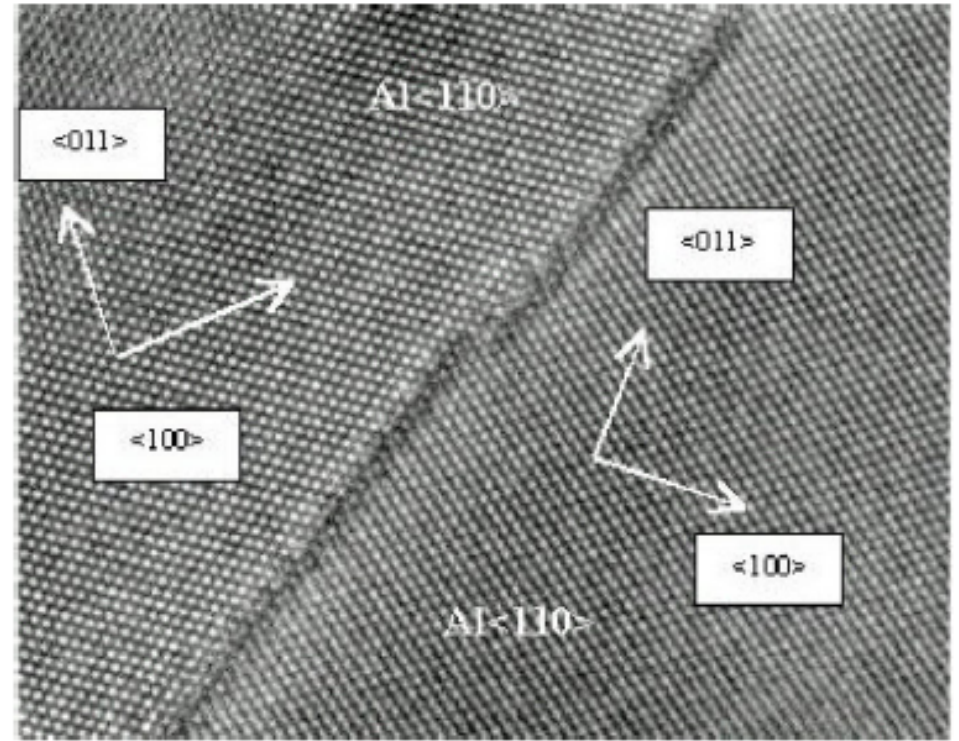
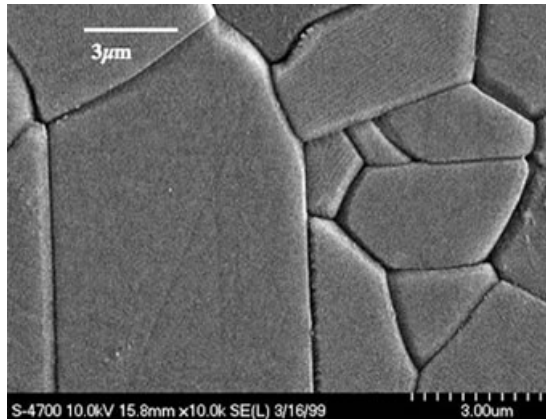


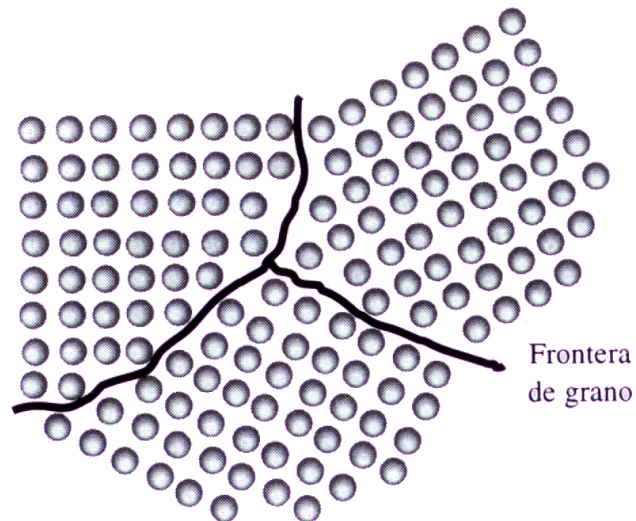
Fig. 2. Monocrystalline Structure (No Gaps - Rigid) vs Polycrystalline Structure (Presents Gaps - Flexible)



Cerámica



Metal



Estructuras Cristalinas: Red de Bravais

Estudiamos la geometría de arreglos regulares de puntos para aplicarlo a la estructura cristalina en sólidos

Definición de Red de Bravais:

1. Arreglo infinito de puntos cuyas posiciones $\bar{\mathbf{R}}$ están dadas por

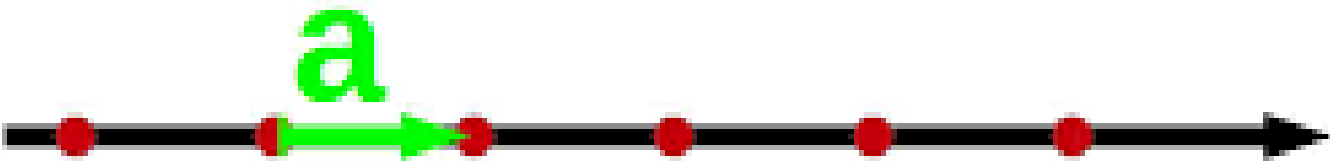
$$\bar{\mathbf{R}} = l_1 \bar{\mathbf{a}}_1 + l_2 \bar{\mathbf{a}}_2 + l_3 \bar{\mathbf{a}}_3 \quad \text{donde}$$

$\bar{\mathbf{a}}_1$, $\bar{\mathbf{a}}_2$ y $\bar{\mathbf{a}}_3$: vectores LI (*vectores bases o primitivos*)

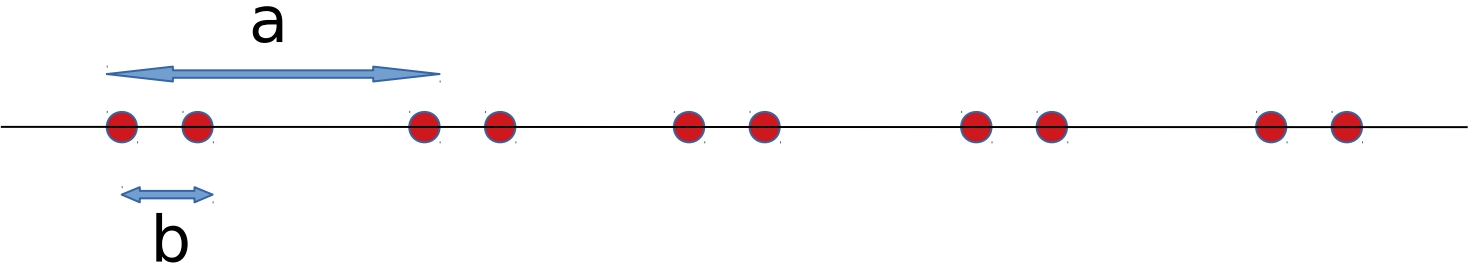
l_1 , l_2 y l_3 : números enteros

2. Arreglo infinito de puntos que se ve igual desde cualquiera de ellos.

Redes de Bravais en 1D

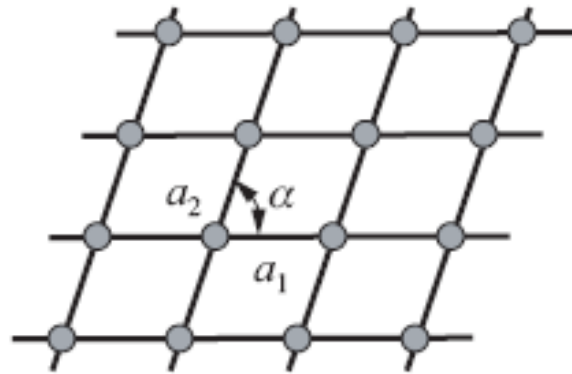


$$\bar{\mathbf{R}} = n \bar{\mathbf{a}}$$

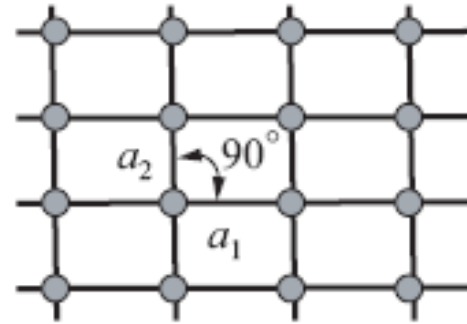


Red de Bravais?

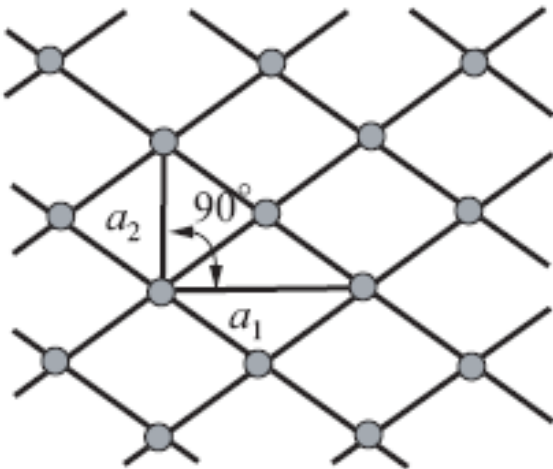
Redes de Bravais en 2D



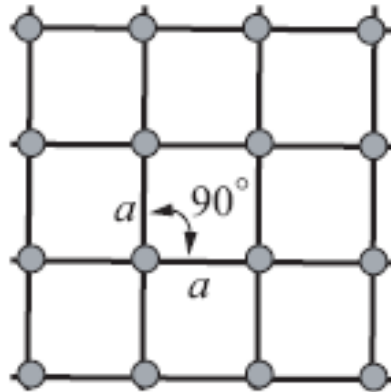
(a)



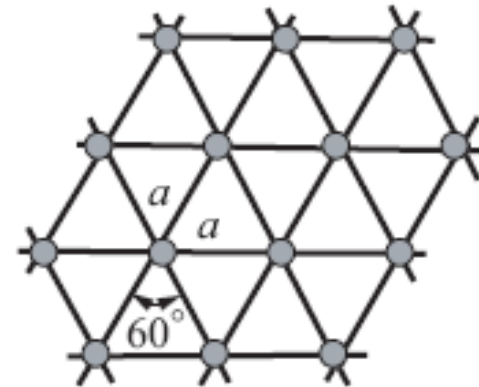
(b)



(c)



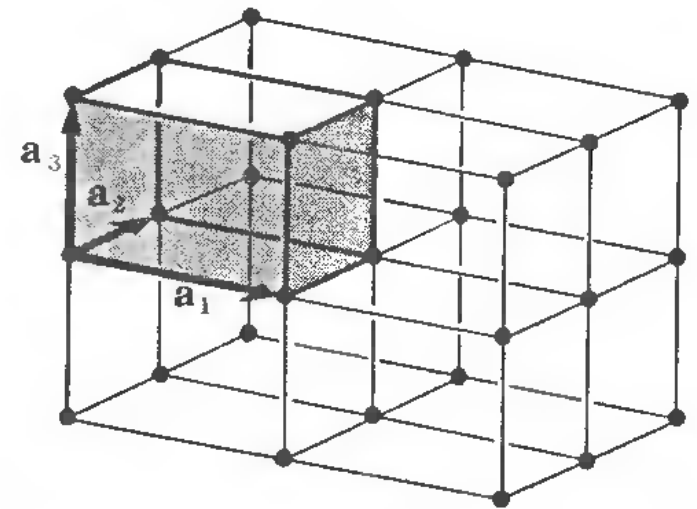
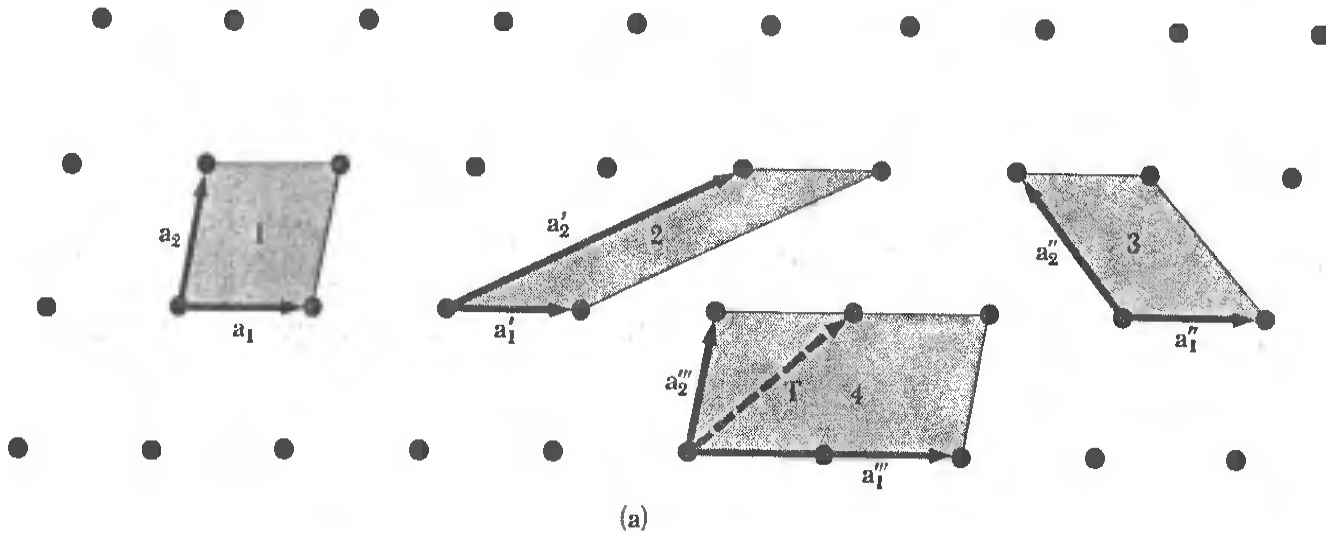
(d)



(e)

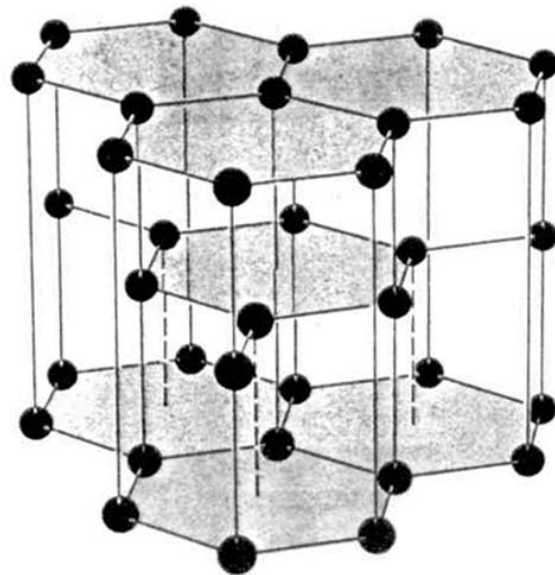
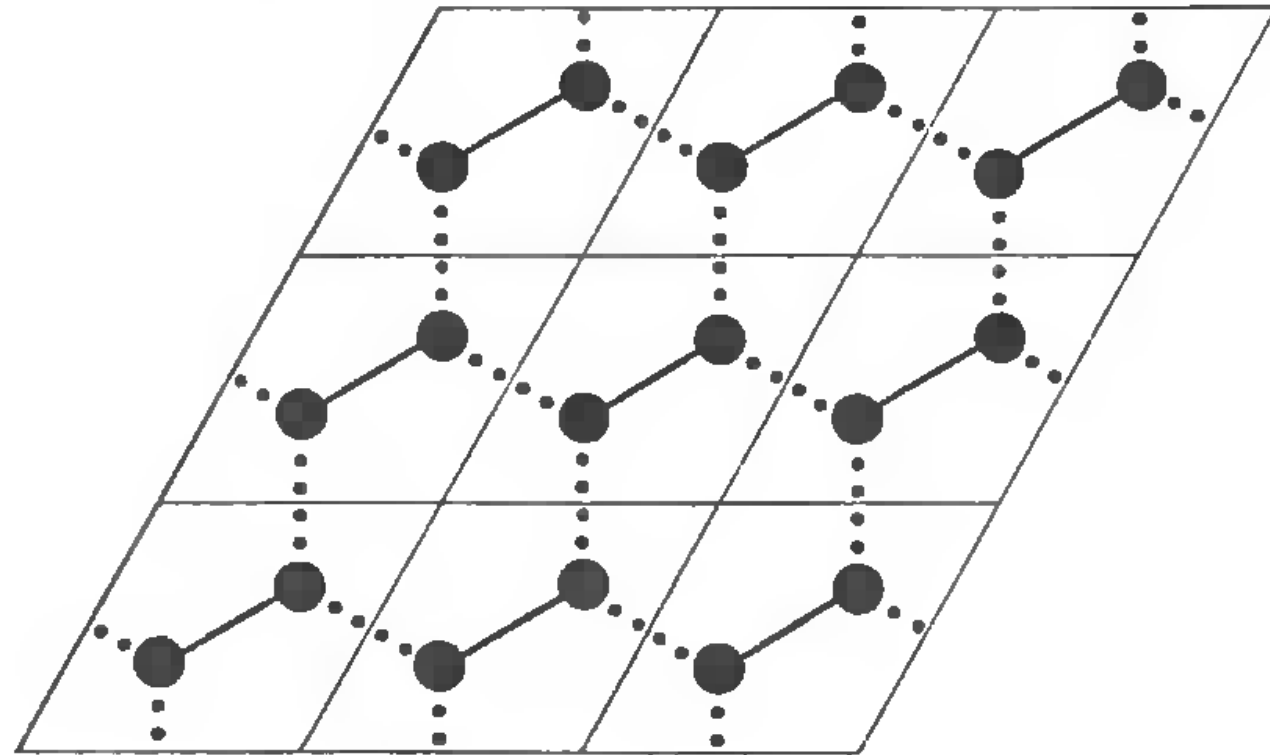
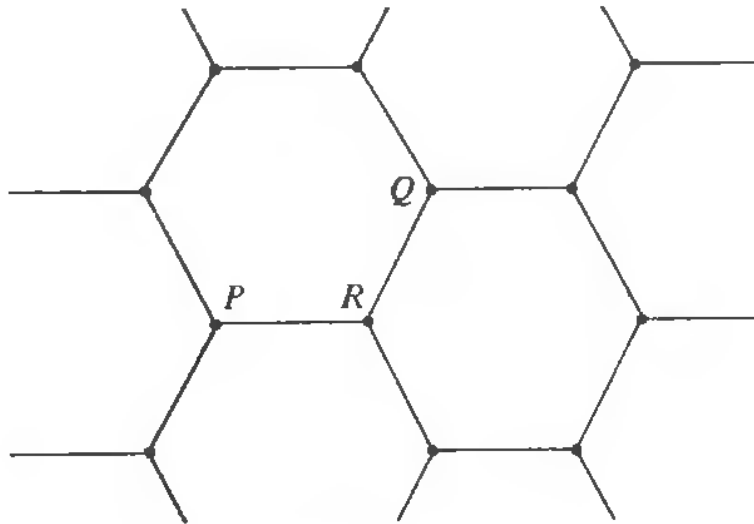
The 2D Bravais lattices: (a) Oblique; (b) rectangular; (c) rhombic; (d) square; (e) hexagonal.

Los vectores primitivos no son únicos:



Pero una vez elegidos los vectores primitivos todos los puntos tienen que poder alcanzarse por combinaciones enteras ($l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3$).

No todo arreglo periódico de puntos es una red de Bravais

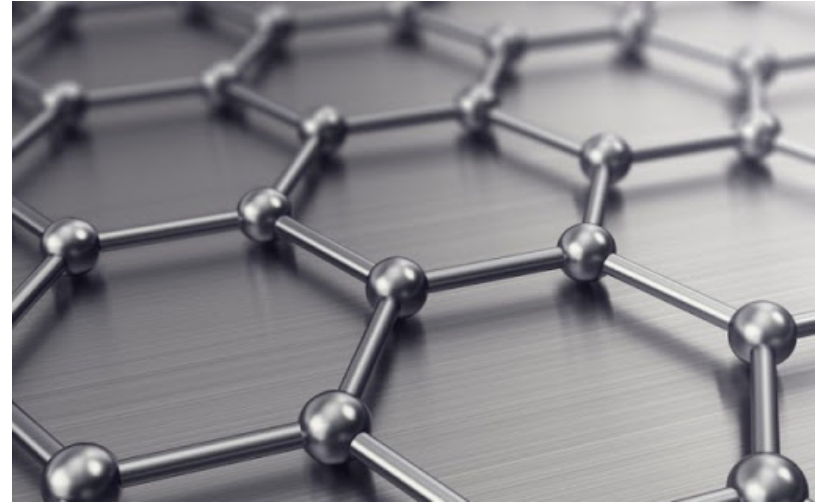


Grafito

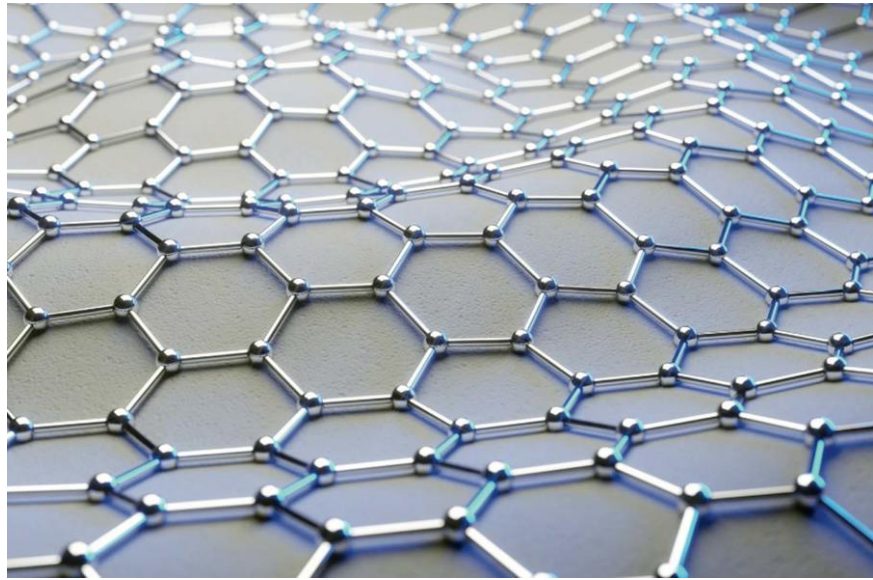
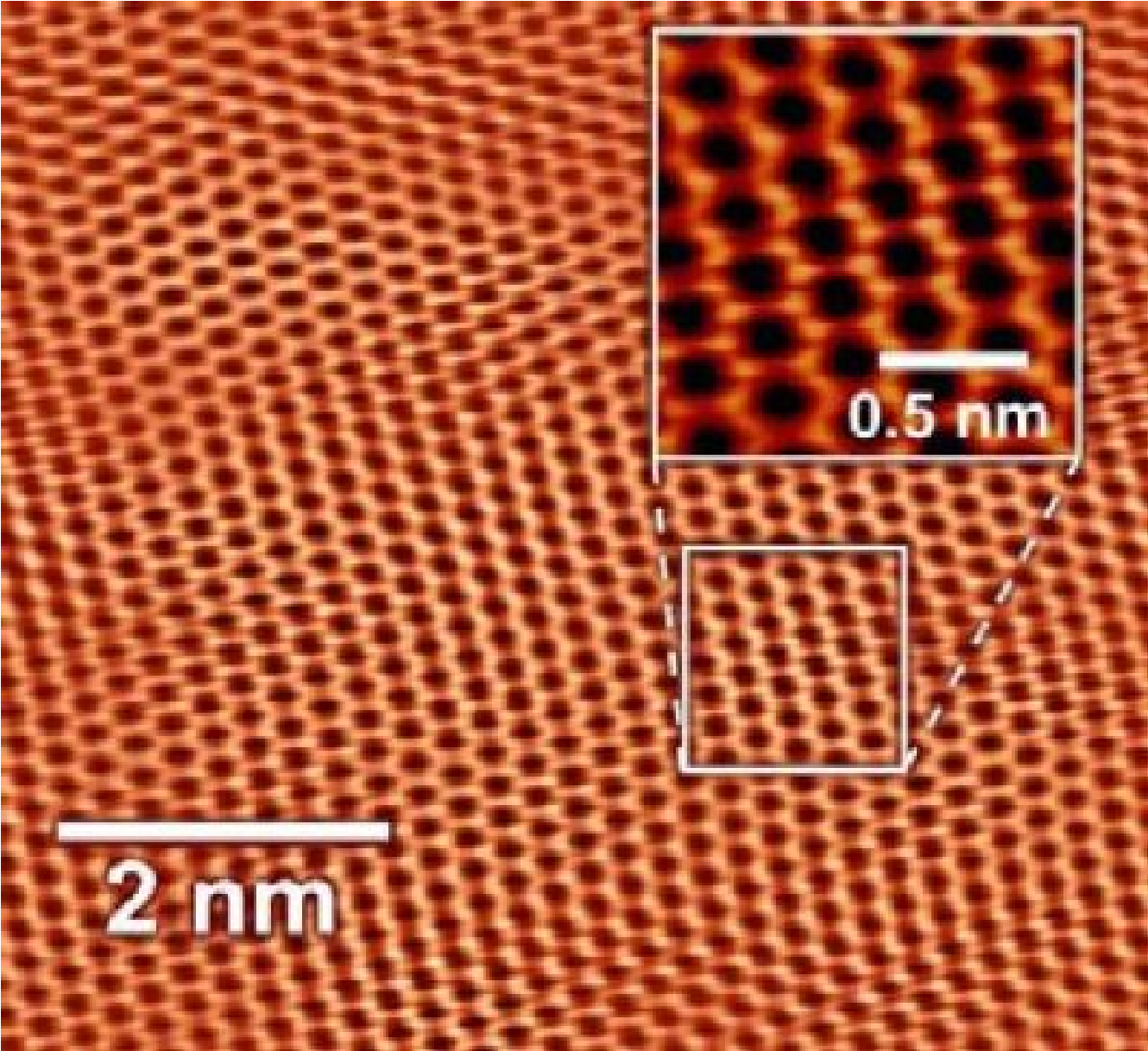
Gueim y Novosiolov pudieron aislar un plano: GRAFENO



Nobel 2010

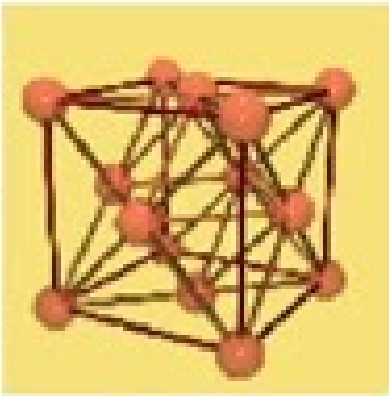


Técnica: "Scotch-tape"

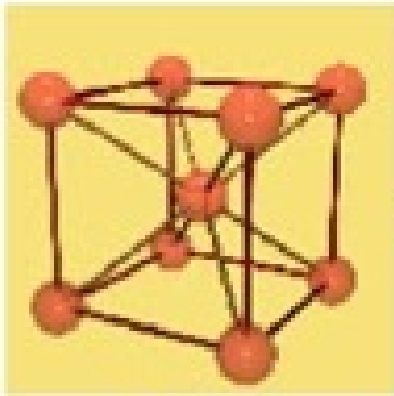


Grafeno

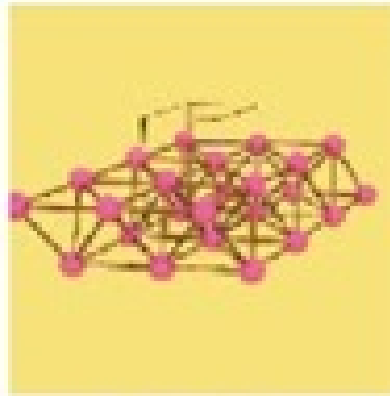
Estructuras cristalinas en 3D



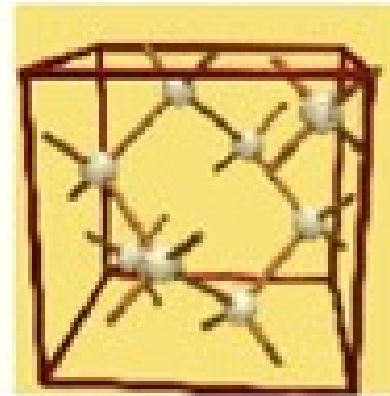
A1: Cu



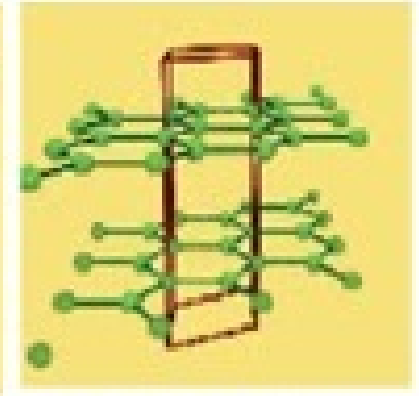
A2: Li



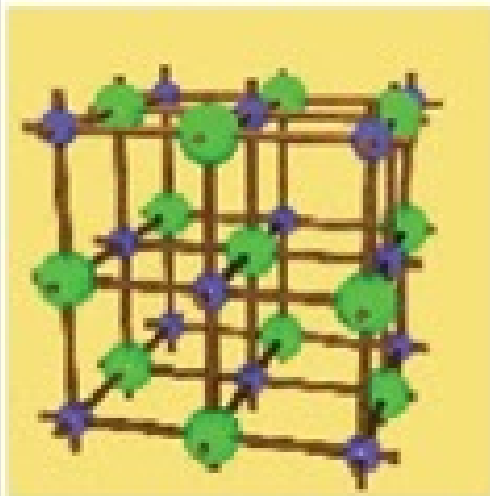
A3: Be



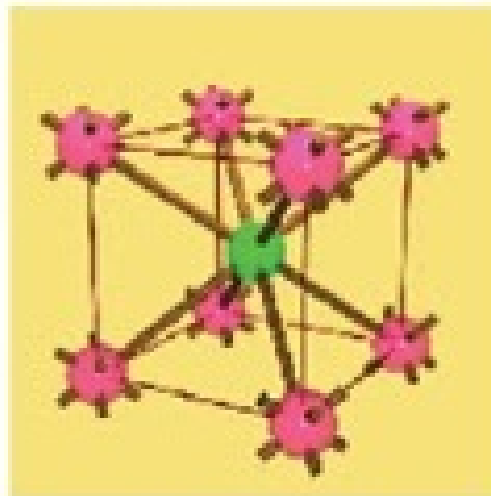
A4: diamante



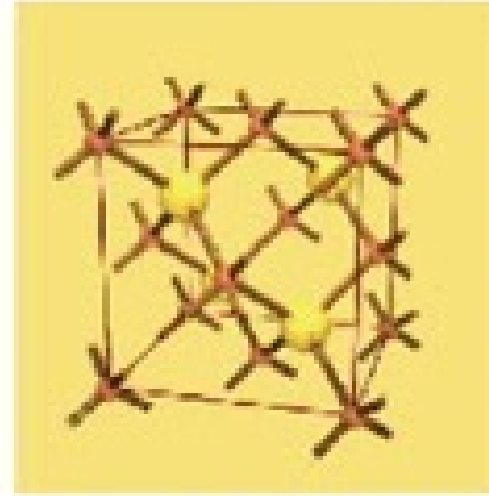
A9: grafito



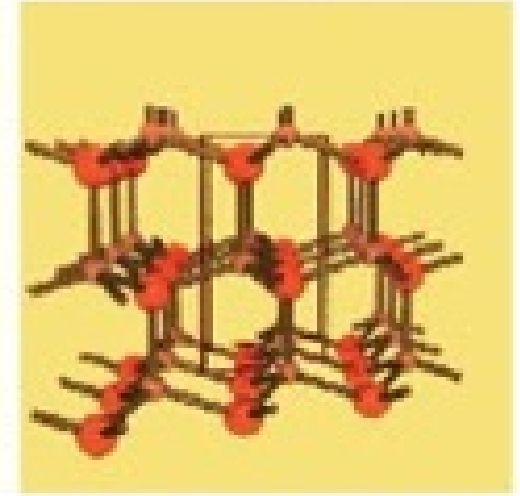
B1: NaCl



B2: CsCl



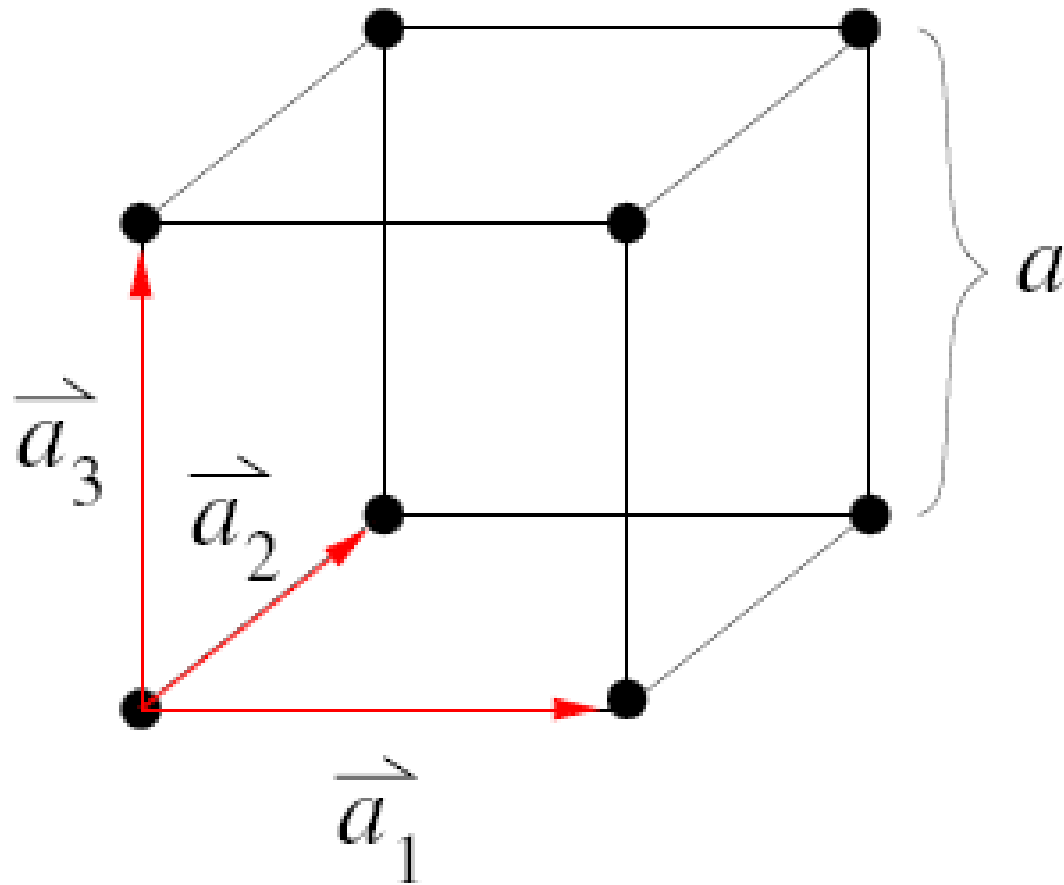
B3: ZnS (blenda)



B4: ZnO (wurtzita)

Red de Bravais en 3D

Cúbica simple (SC)

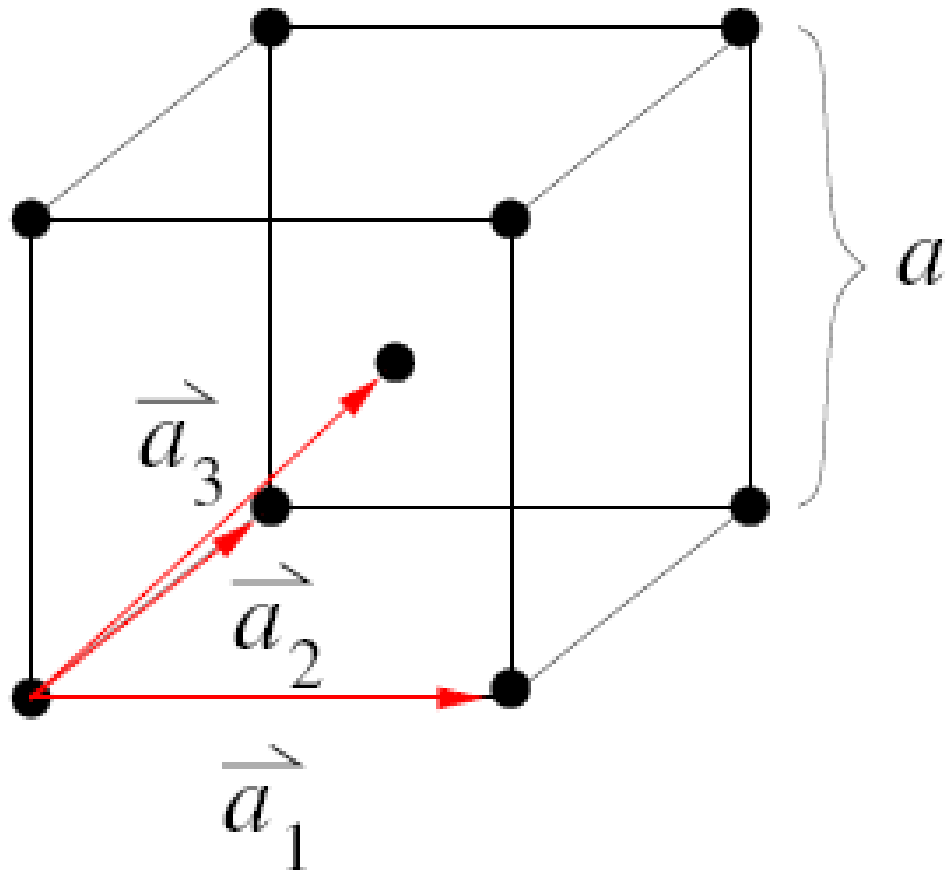


$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

$$\vec{a}_3 = a\hat{z}$$

Cúbica centrada en el cuerpo (bcc)

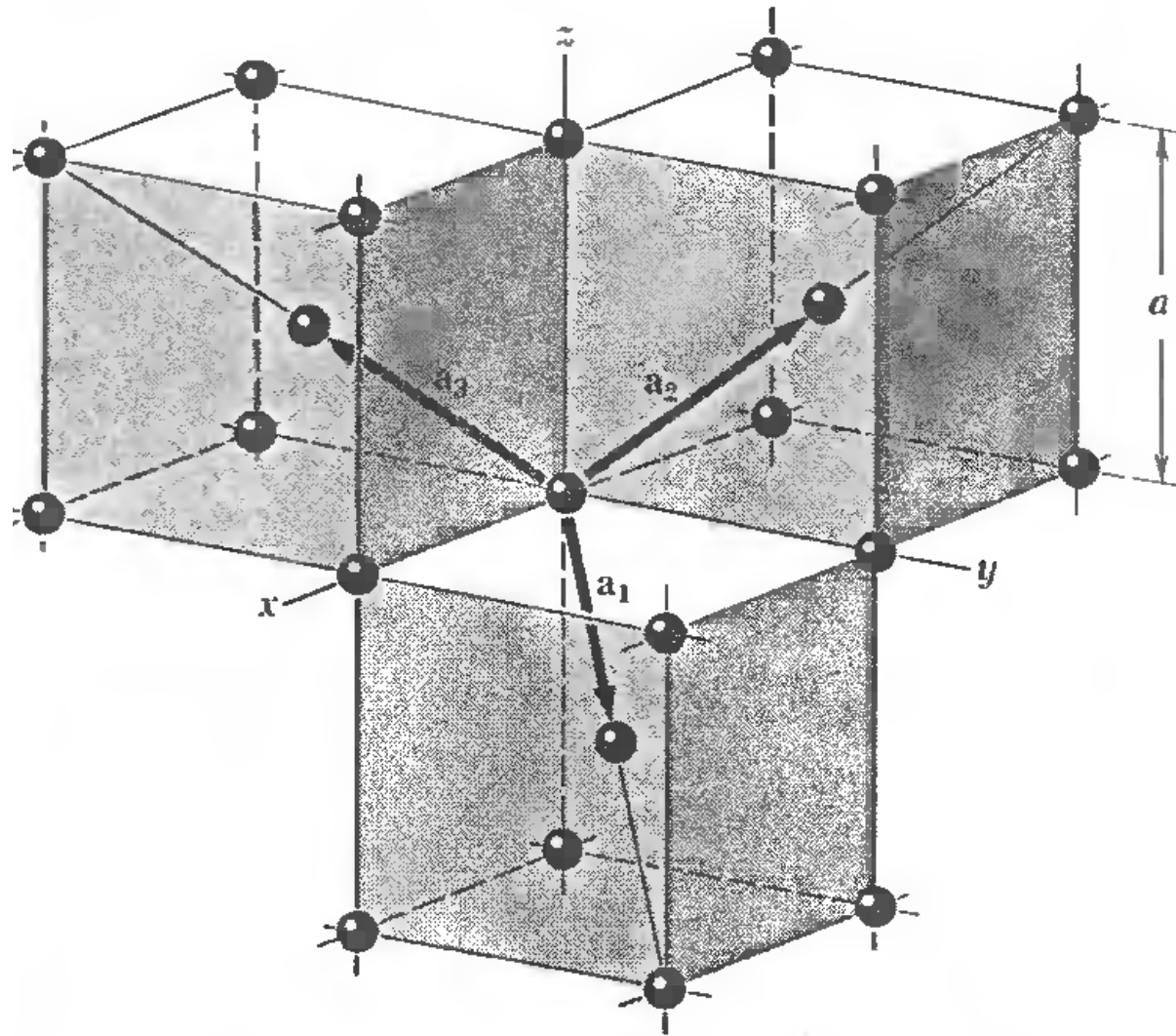


$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

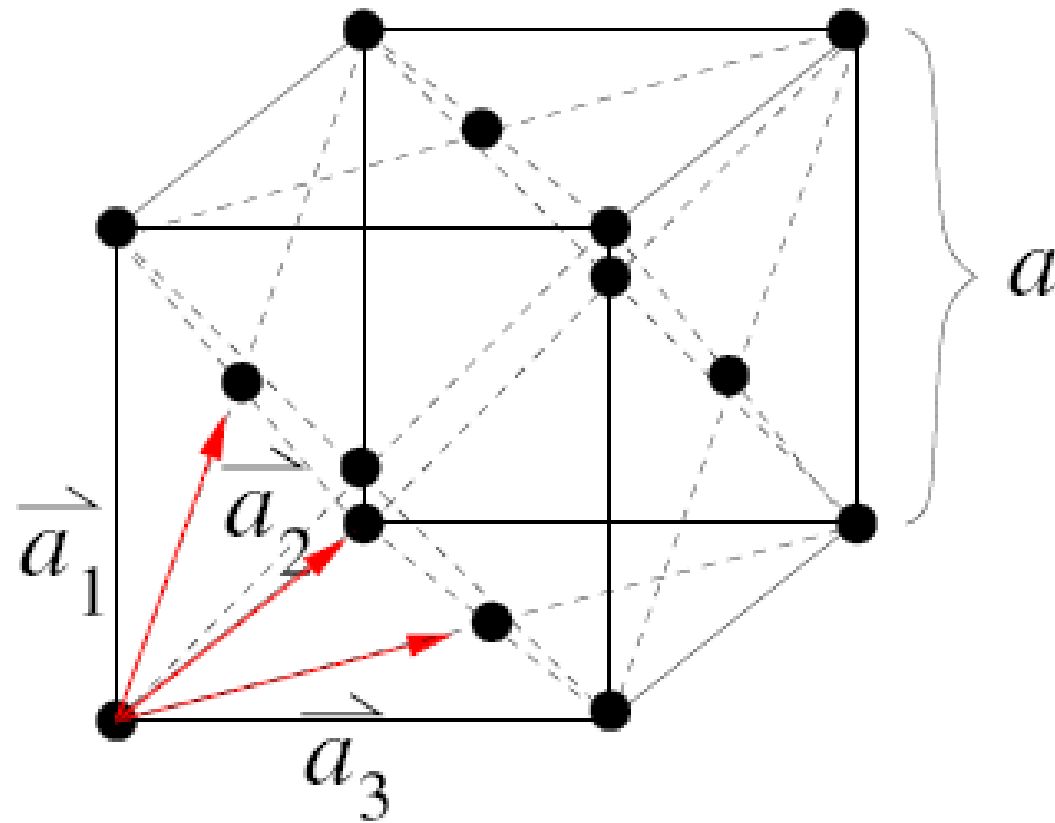
$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$$

bcc



$$\vec{a}'_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$
$$\vec{a}'_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$
$$\vec{a}'_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

Cúbica centrada en las caras (FCC)



$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$
$$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$

Red hexagonal simple

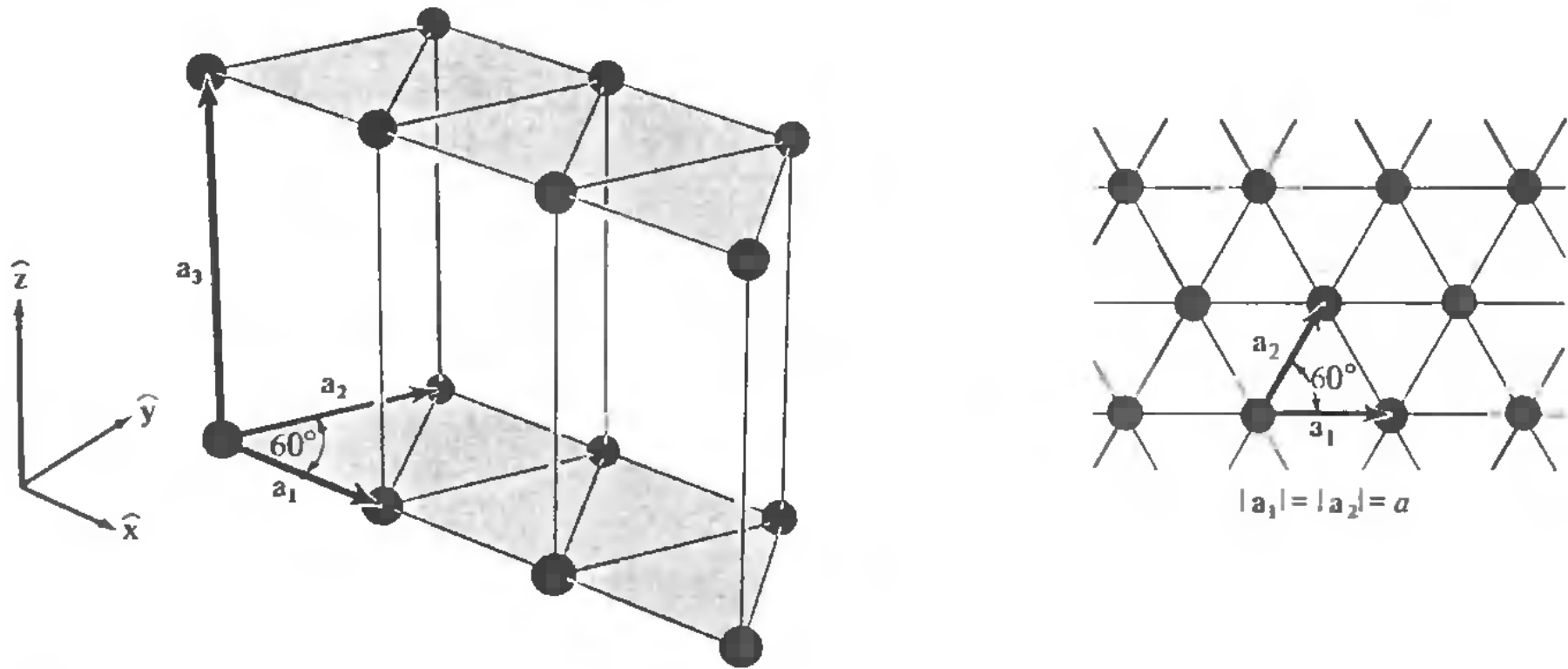


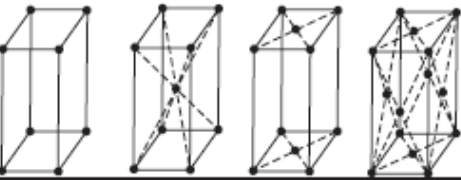
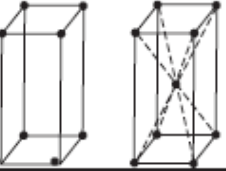
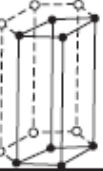
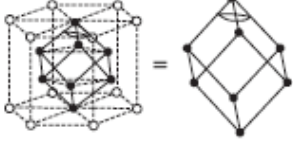
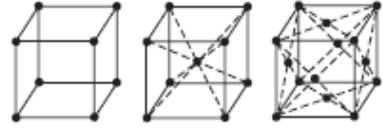


Figure 4.19

The simple hexagonal Bravais lattice. Two-dimensional triangular nets (shown in inset) are stacked directly above one another, a distance c apart.

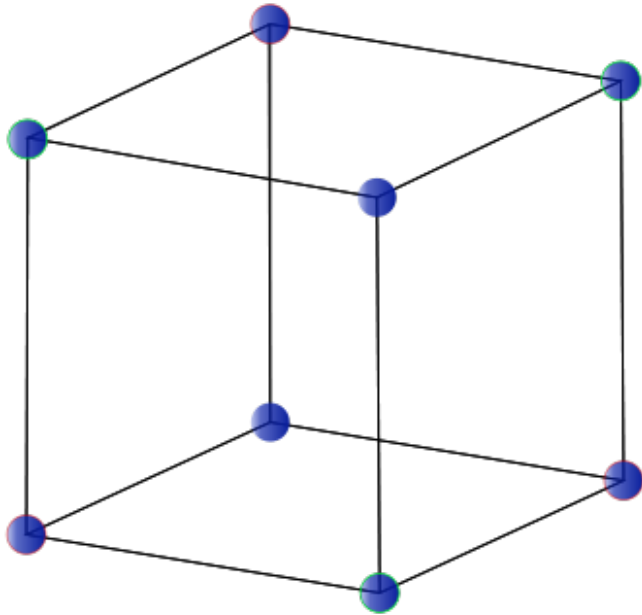
Bravais 3D

14 sistemas cristalinos

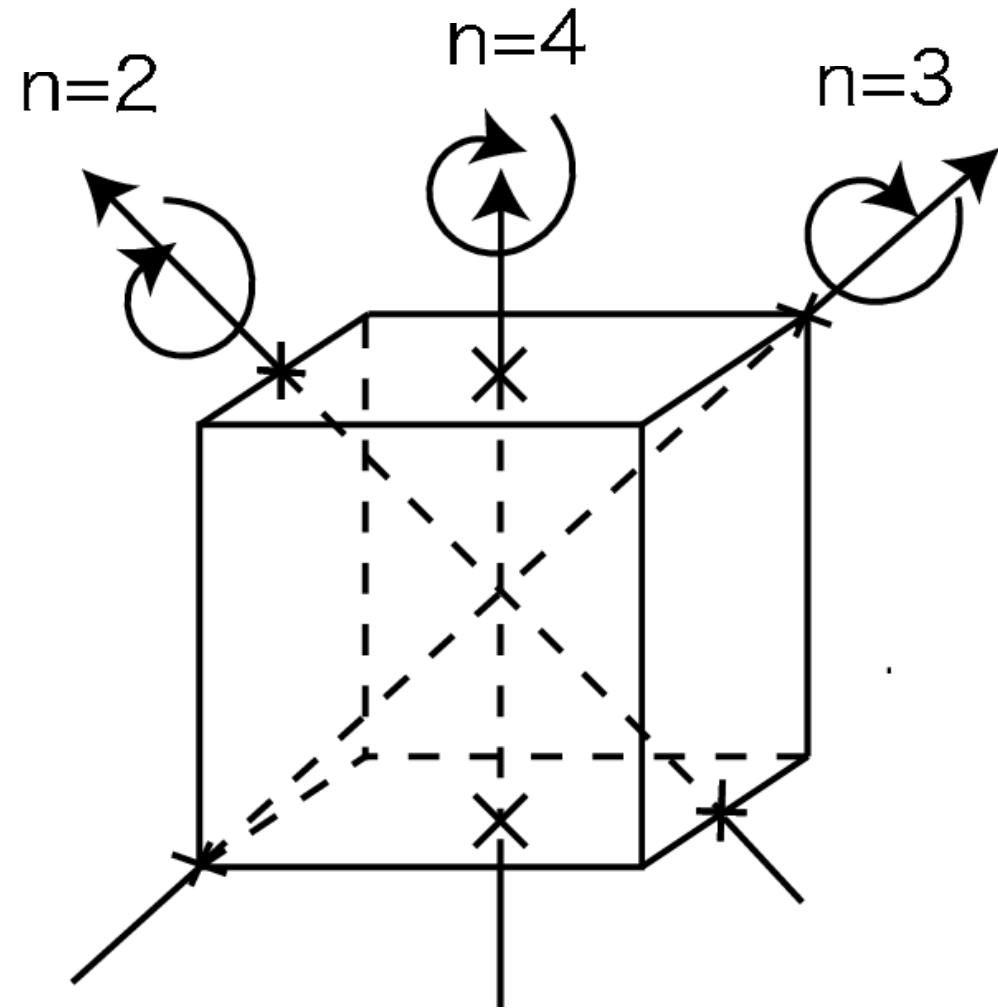
Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90$						$1, \bar{1}$
Monoclinic $a \neq b \neq c$ $\alpha = \gamma = 90$ $\beta \neq 90$						$2, m, \frac{2}{m}$
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90$						$222, 2mm, \frac{2}{m} \frac{2}{m} \frac{2}{m} (mmm)$
Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90$						$4, \bar{4}, \frac{4}{m}, 422, 4mm, \bar{4} 2m, \frac{4}{m} \frac{2}{m} \frac{2}{m} (4/mmm)$
Hexagonal $a = b \neq c$ $\alpha = \beta = 90$ $\gamma = 120$						$6, \frac{3}{m}, \frac{6}{m}, 622, 6mm, \bar{6} 2m, \frac{6}{m} \frac{2}{m} \frac{2}{m} (6/mmm)$
Rhombohedral $a = b = c$ $\alpha = \beta = \gamma \neq 90$						$3, \bar{3}, 32, 3m, \bar{3} \frac{2}{m} (\bar{3}m)$
Cubic $a = b = c$ $\alpha = \beta = \gamma = 90$						$23, \frac{2}{m} \bar{3} (\bar{3}m), 432, \bar{4} 3m, \frac{4}{m} \bar{3} \frac{2}{m} (m\bar{3}m)$

P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombohedron)

Simetrías ?



- plano reflexión $(xyz) \rightarrow (xy-z)$
- centro de inversión $(xyz) \rightarrow (-x-y-z)$
- eje de rotación $(xyz) \rightarrow (y-xz)$
- plano de deslizamiento
- eje helicoidal

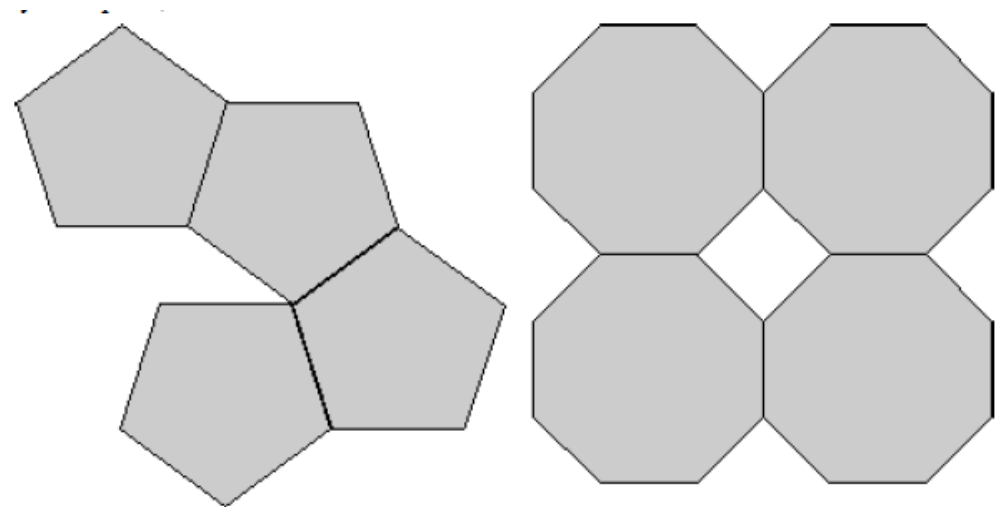
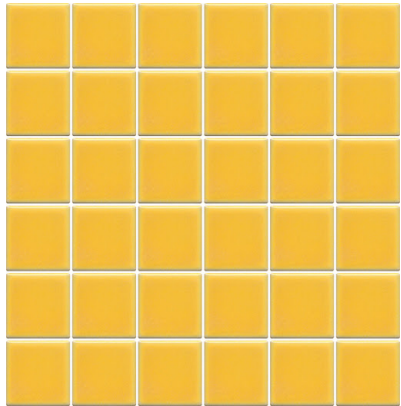


Eje de rotación de orden n ($\varphi = 2\pi/n$)

En cristales $n=2,3,4,6$

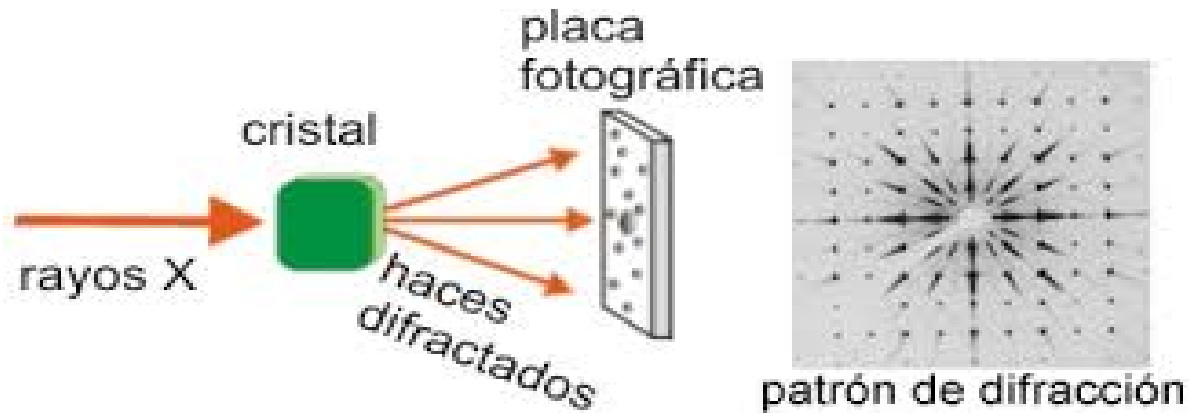
Nombre	Ejes de orden 2 binarios	Ejes de orden 3 ternarios	Ejes de orden 4 cuaternarios	Ejes de orden 6 sexenarios
Vista en planta y símbolos				
Vista en alzado y símbolos				
Actuación de los ejes	Repite elementos idénticos cada 180°	Repite elementos idénticos cada 120°	Repite elementos idénticos cada 90°	Repite elementos idénticos cada 60°

2 Dimensiones



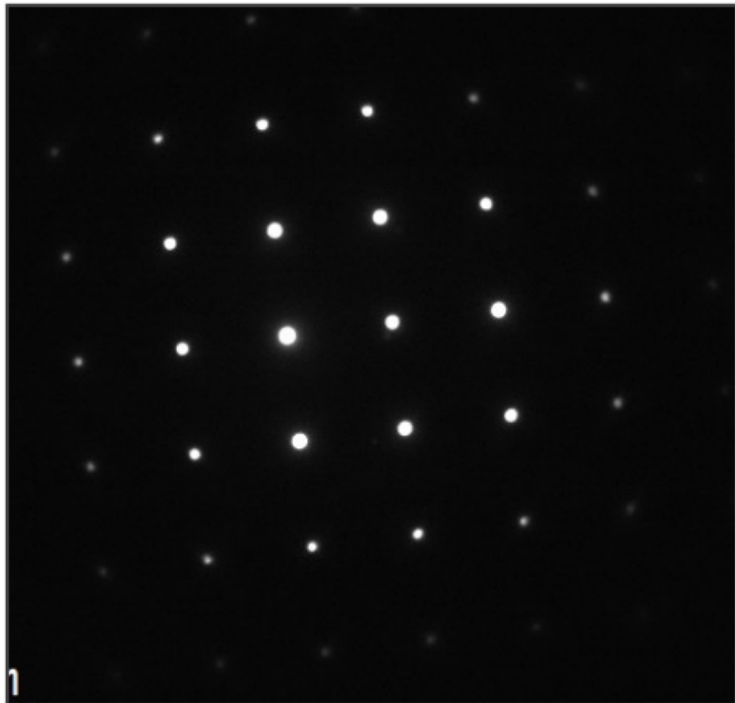
No puede haber ejes de orden $n=5, 7$

No se puede llenar el espacio con pentágonos o heptágonos

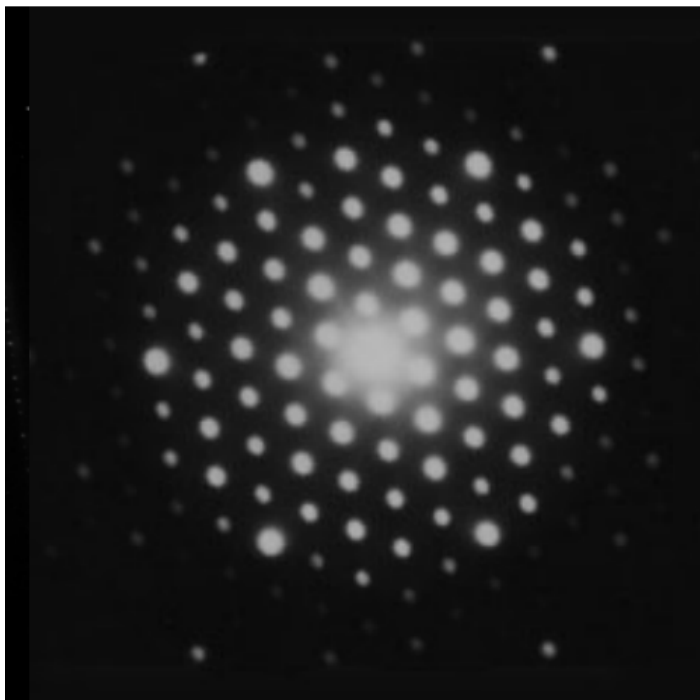


El patrón refleja la simetría del cristal

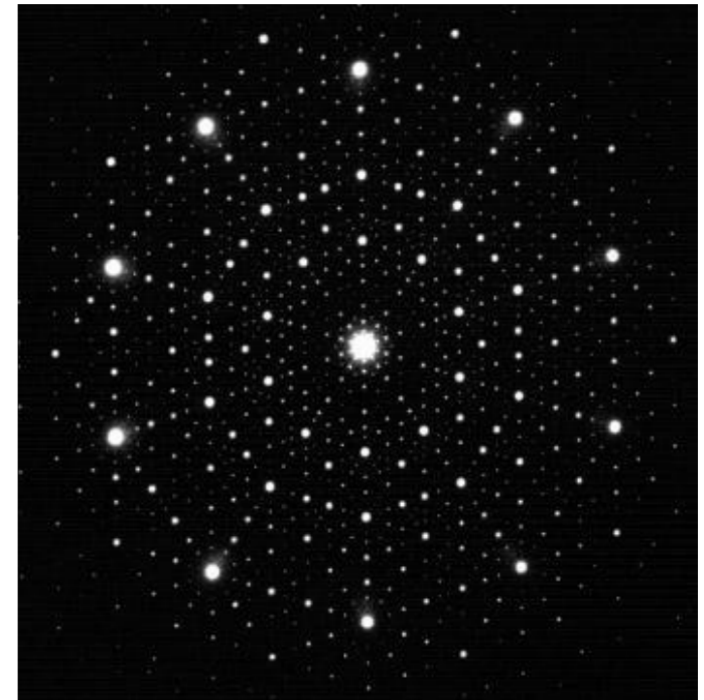
Aleación de Al-Mg (1984)



cubica

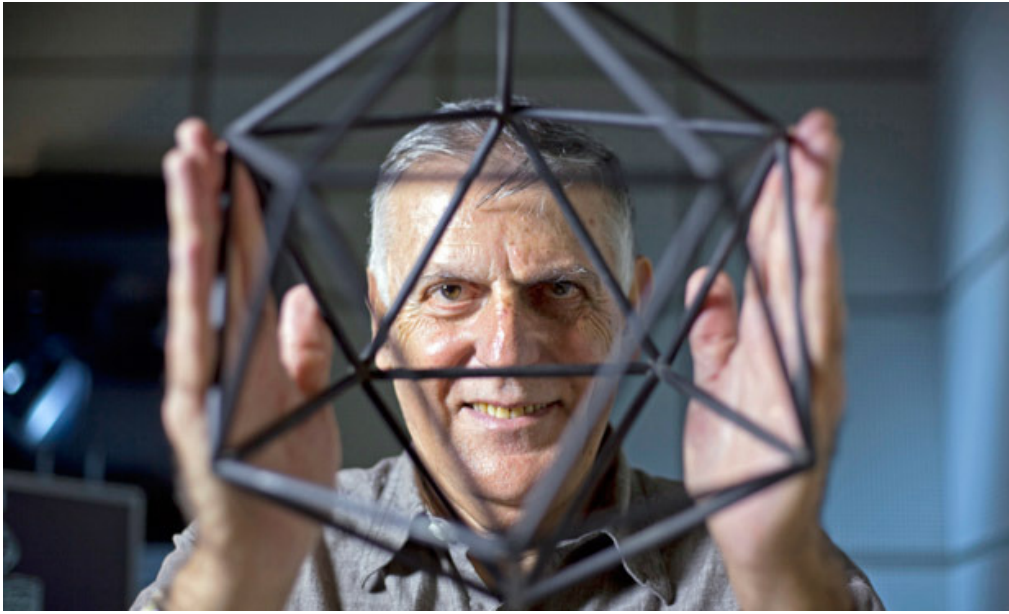


hexagonal

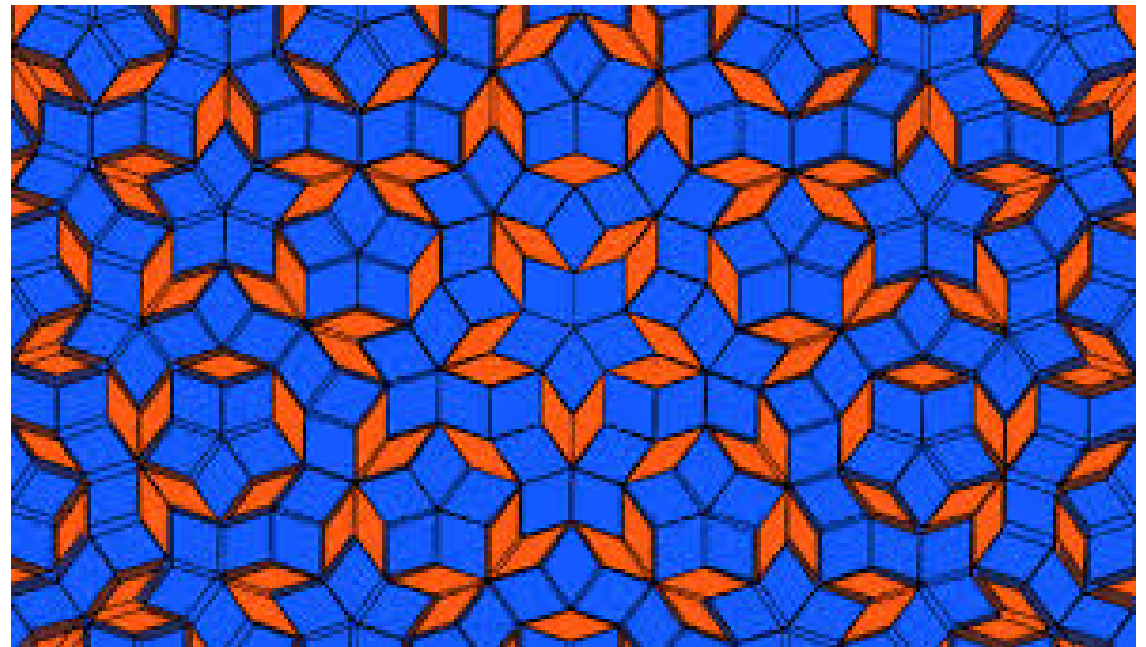
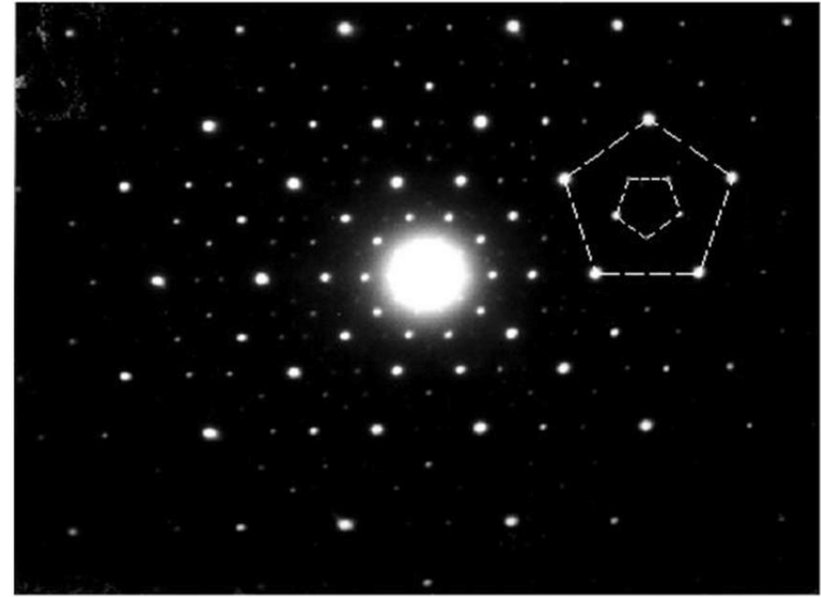


n=5 !!!!

Cuasicristales !!!

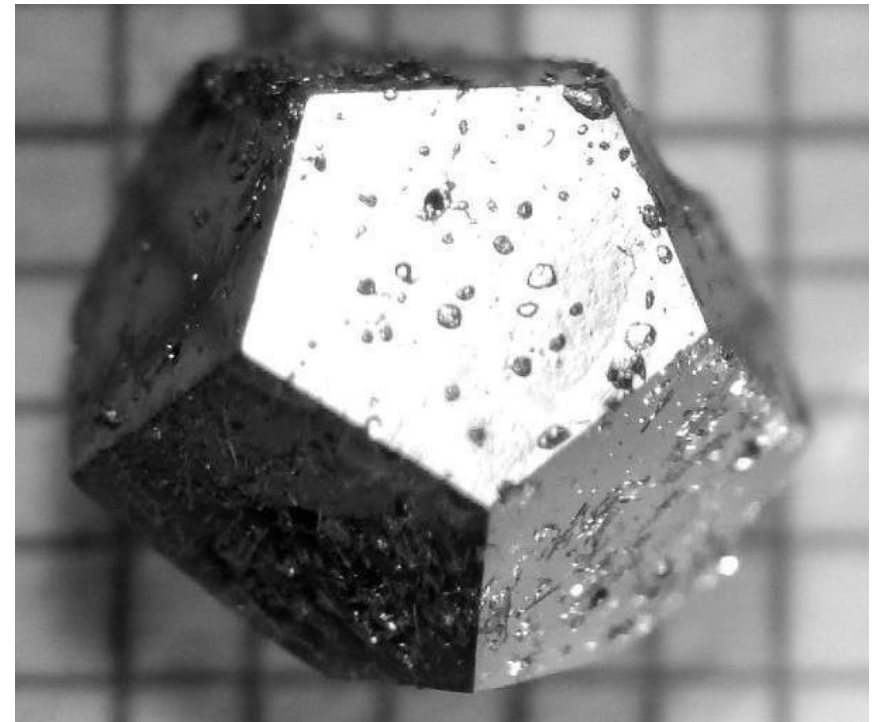
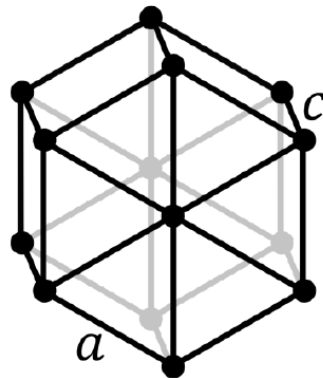
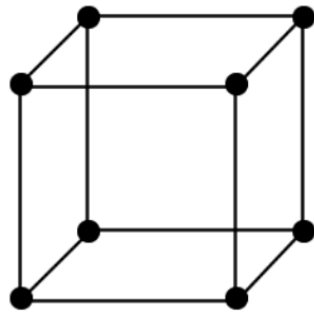
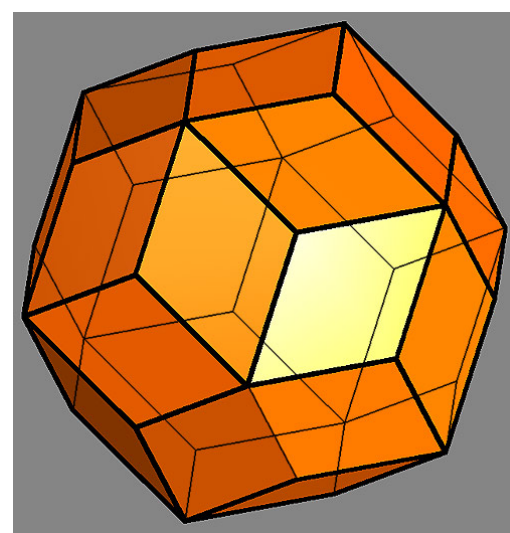


**Dan Shechtman
(Nobel Química 2011)**



**Modelos se basaron en “tiling”
de Penrose
(embaldozado o teselado)**

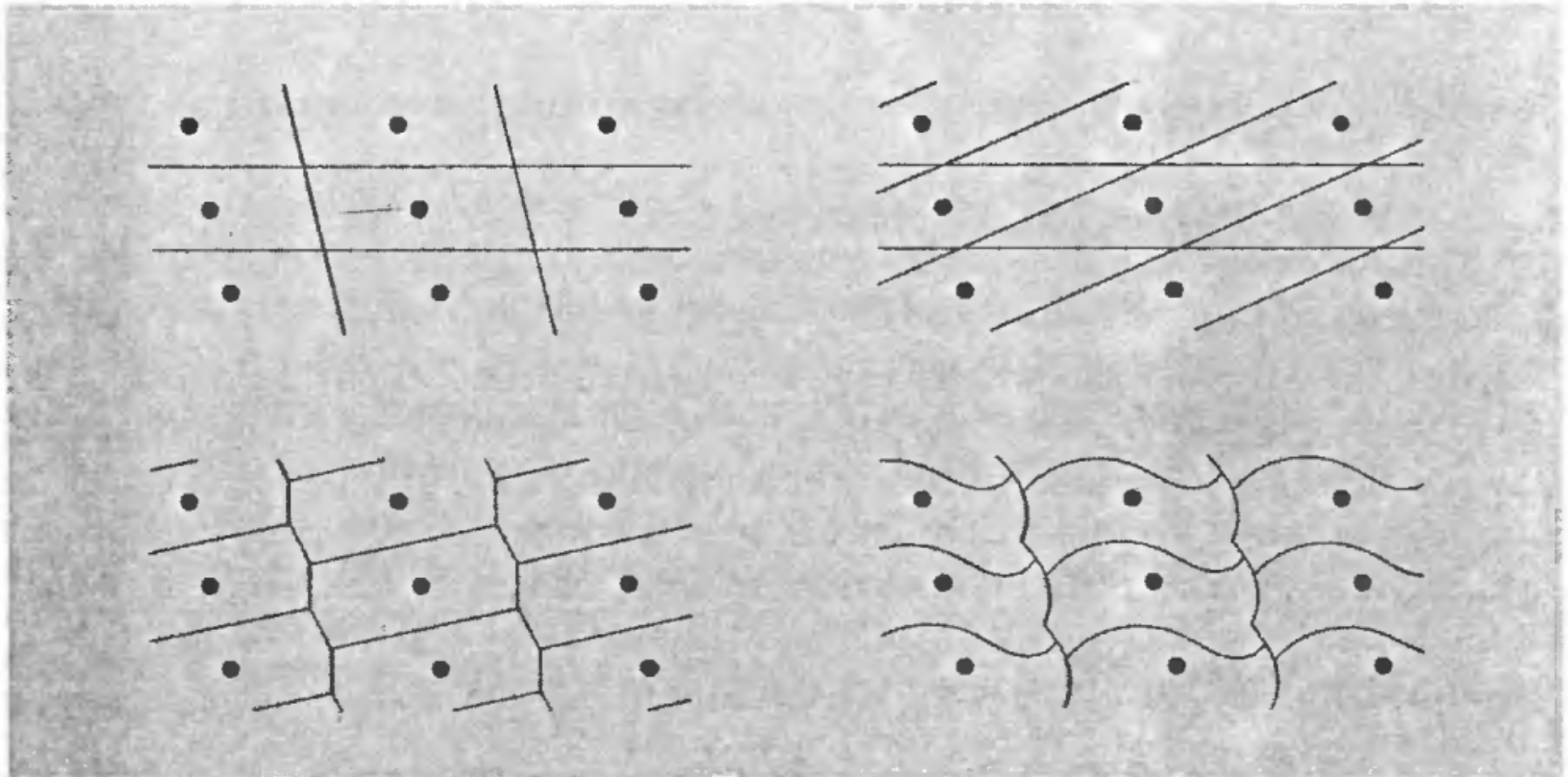
**Teselaciones en 3D:
octaedros, tetraedros y otras
figuras**



Cuasicristal

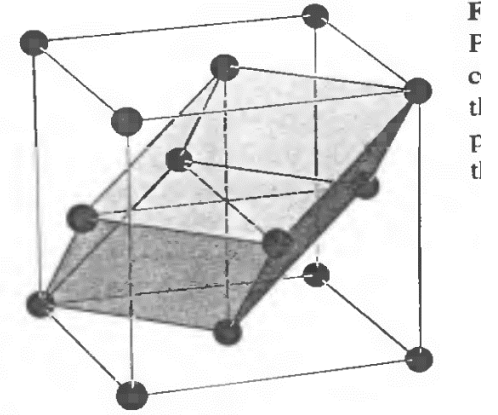
Celda primitiva

Una celda primitiva es un volumen del espacio que cuando se lo traslada aplicandole **todos** los vectores de la RB, llena completamente el espacio sin superposición.

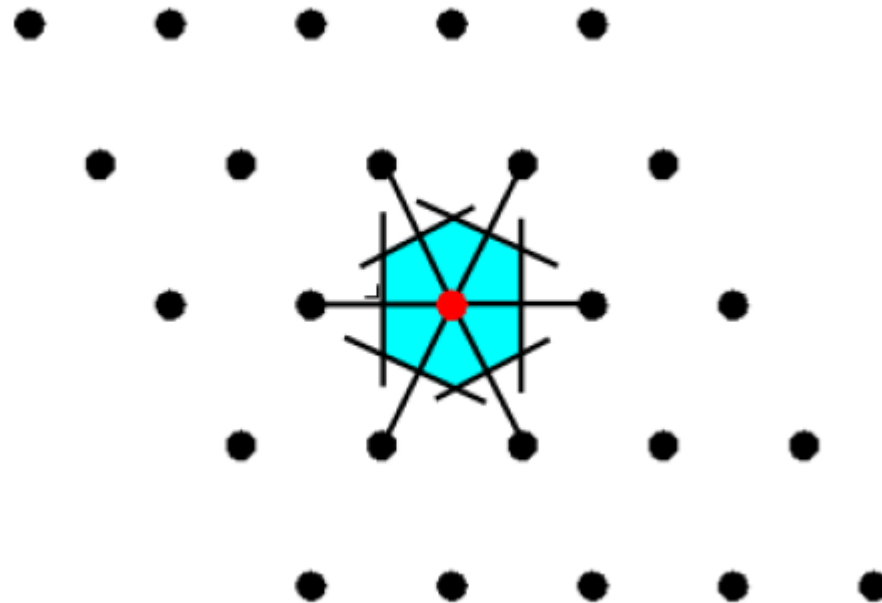


Una celda primitiva posible es el paralelepipedo de lados \mathbf{a}_i

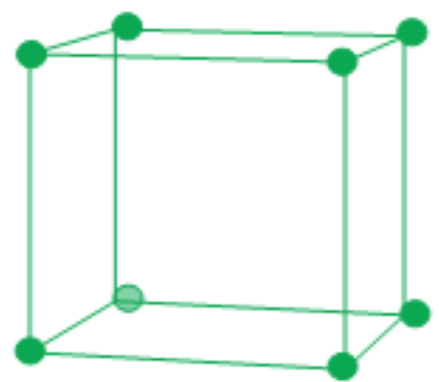
$$\mathbf{r} = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_3 \mathbf{a}_3 \quad 0 \leq x_i \leq 1$$



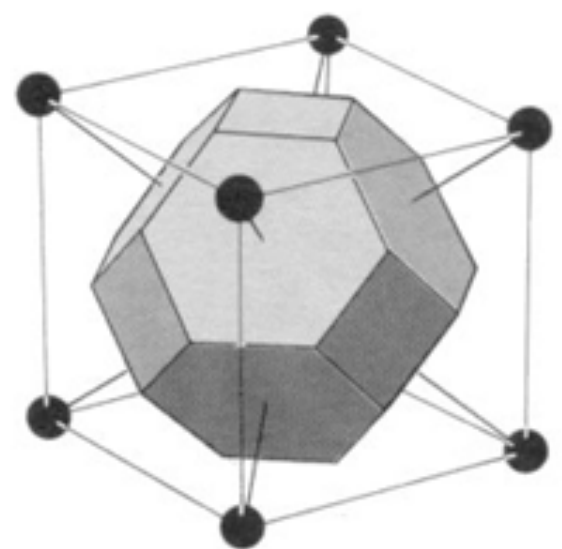
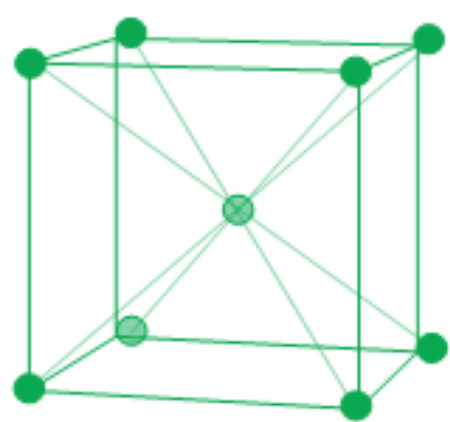
Otra elección que respeta las simetrias de la red es la de la celda de **Wigner-Seitz** -> Es el conjunto de puntos que está más cercano a uno dado de la red que a todos los otros.



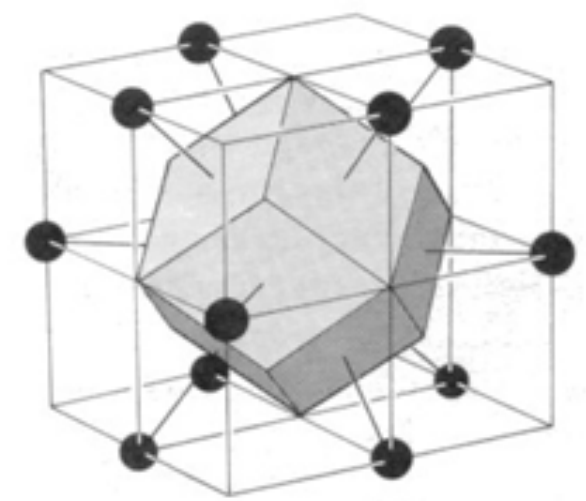
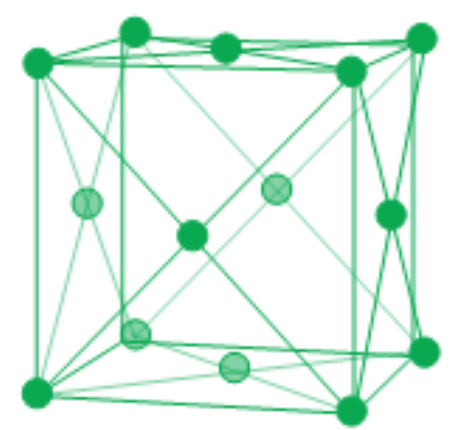
- Ejemplos de celdas de Wigner-Seitz



Cubo ↙



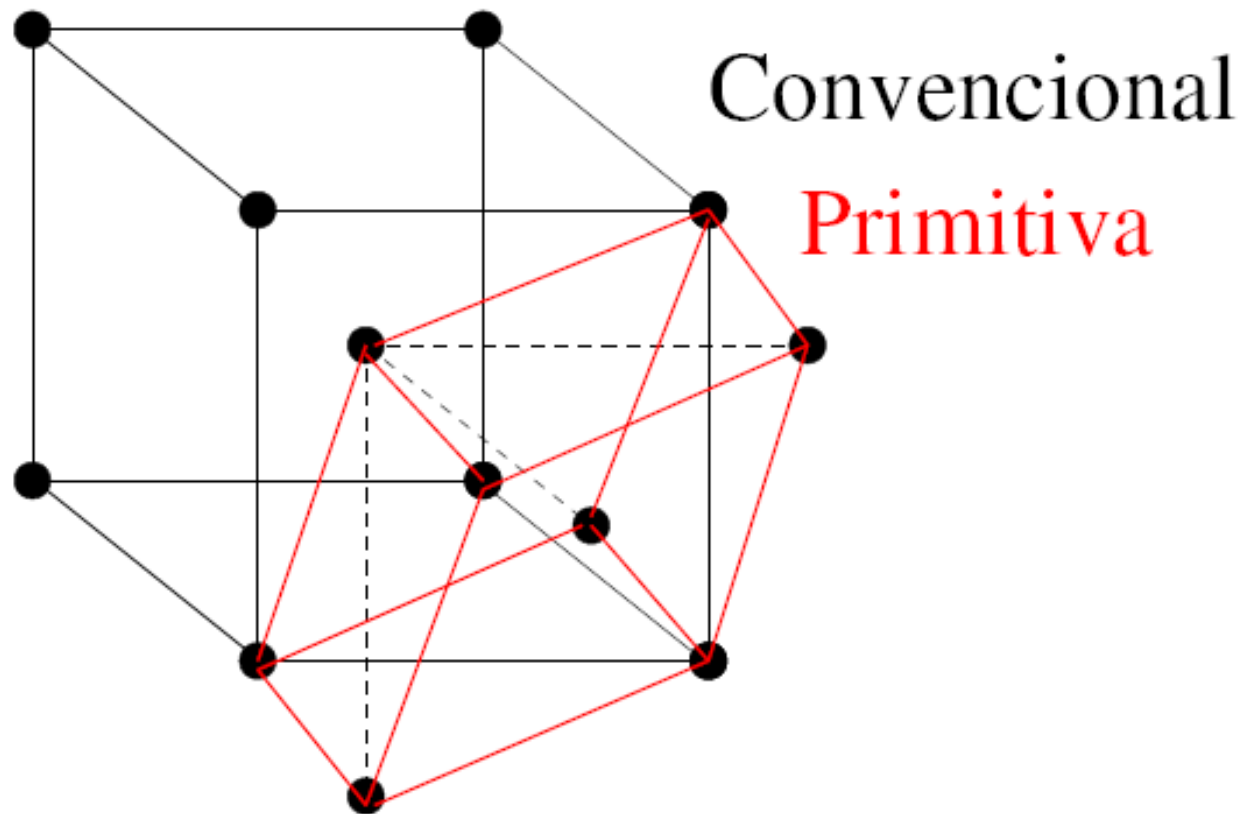
Octaedro truncado ↙



Dodecaedro rómbico

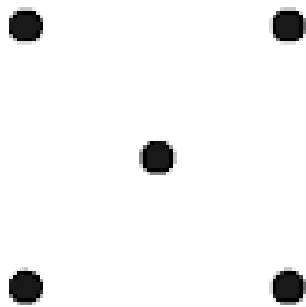
Celda convencional

Es un volumen tal que que llena todo el espacio sin traslaparse al ser trasladado a través de algún subconjunto de vectores de la red de Bravais. En general, la celda convencional es elegida de mayor tamaño que la celda primitiva y poseyendo las simetrías de la estructura.

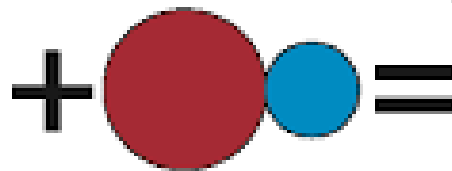


Estructuras cristalinas

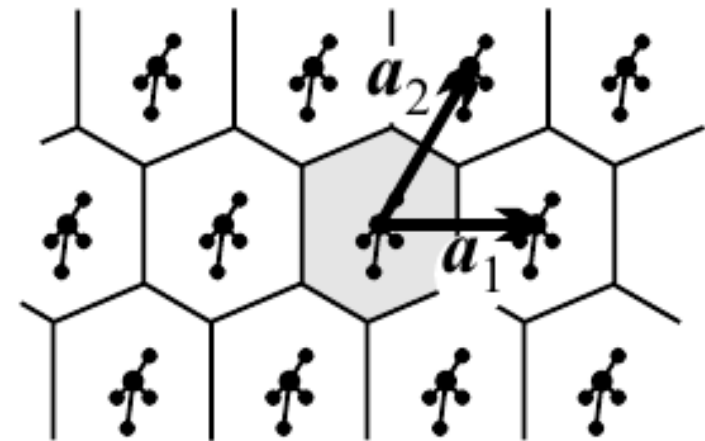
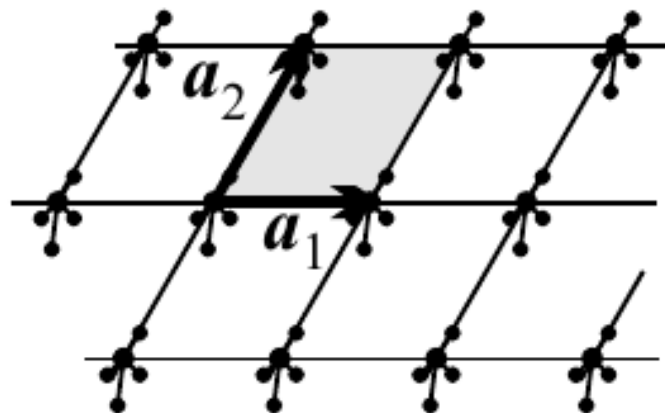
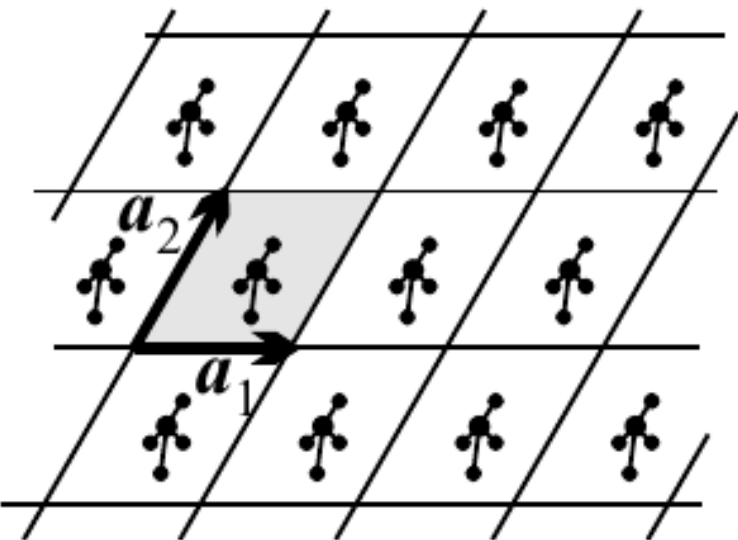
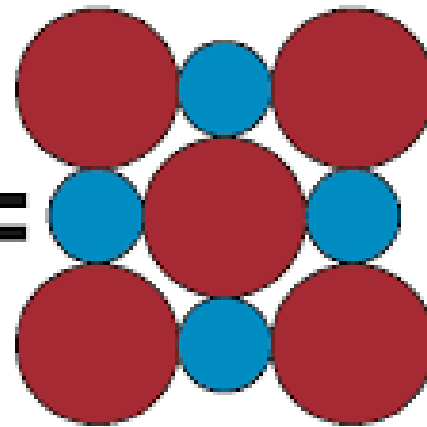
Bravais
lattice



basis



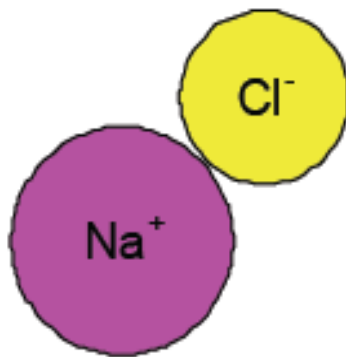
crystal



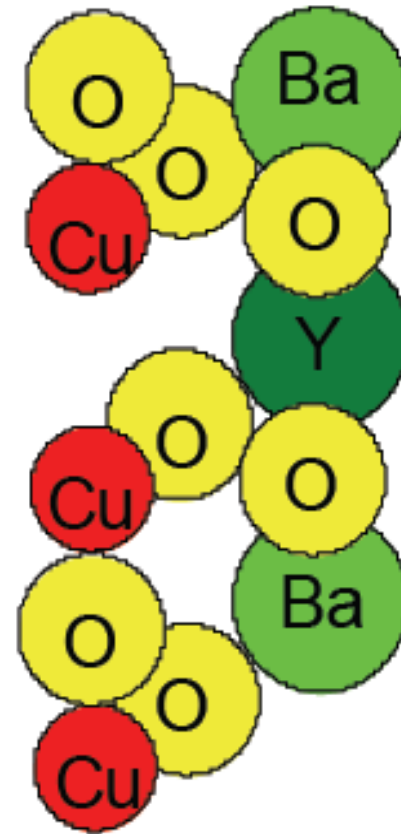
Algunos ejemplos de bases reales



átomo
(de cobre)



molécula (sal)



otras cosas más complicadas

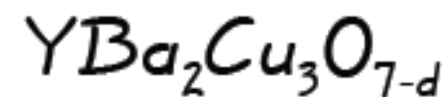


Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED
CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ -Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β -Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

Table 4.2
ELEMENTS WITH THE MONATOMIC BODY-CENTERED
CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

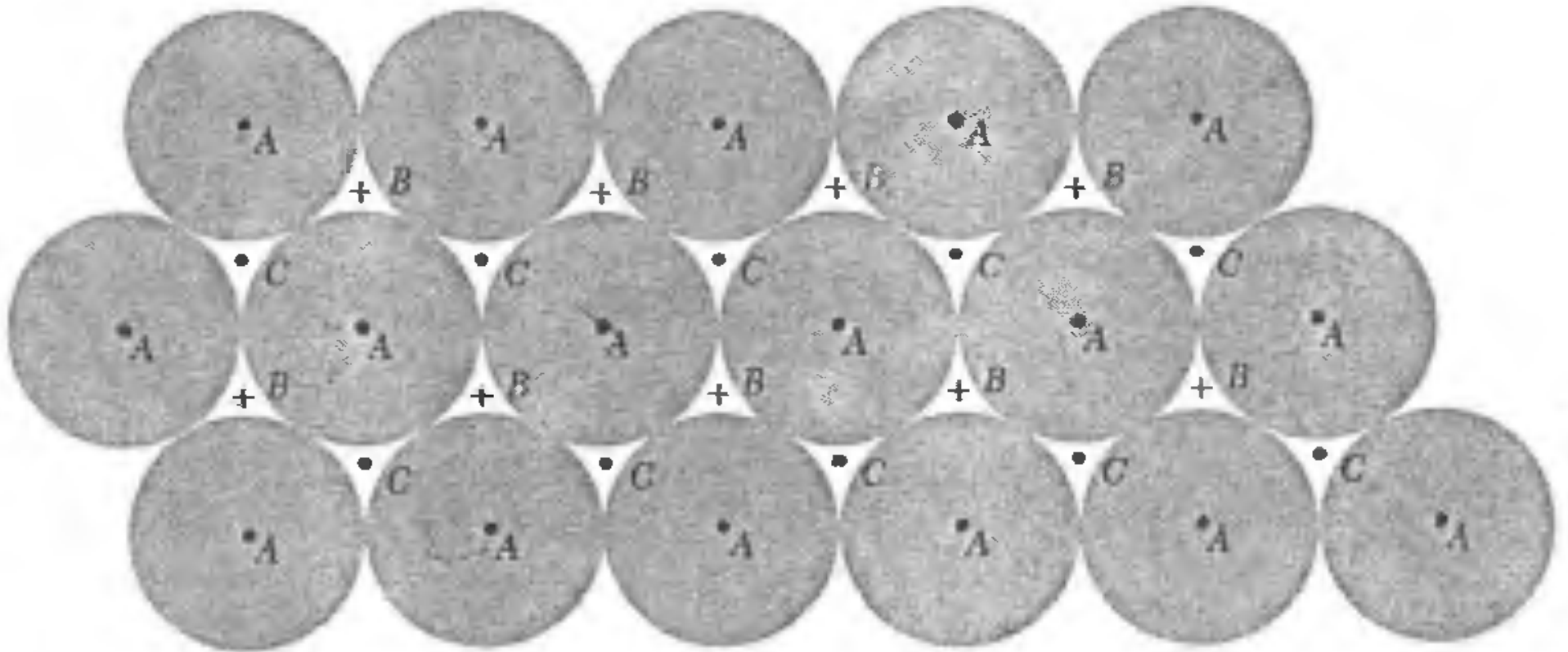
Table 3 Crystal structures of the elements

The data given are at room temperature for the most common form, or at the stated temperature in deg K. For further descriptions of the elements see Wyckoff, Vol. 1, Chap. 2. Structures labeled complex are described there.

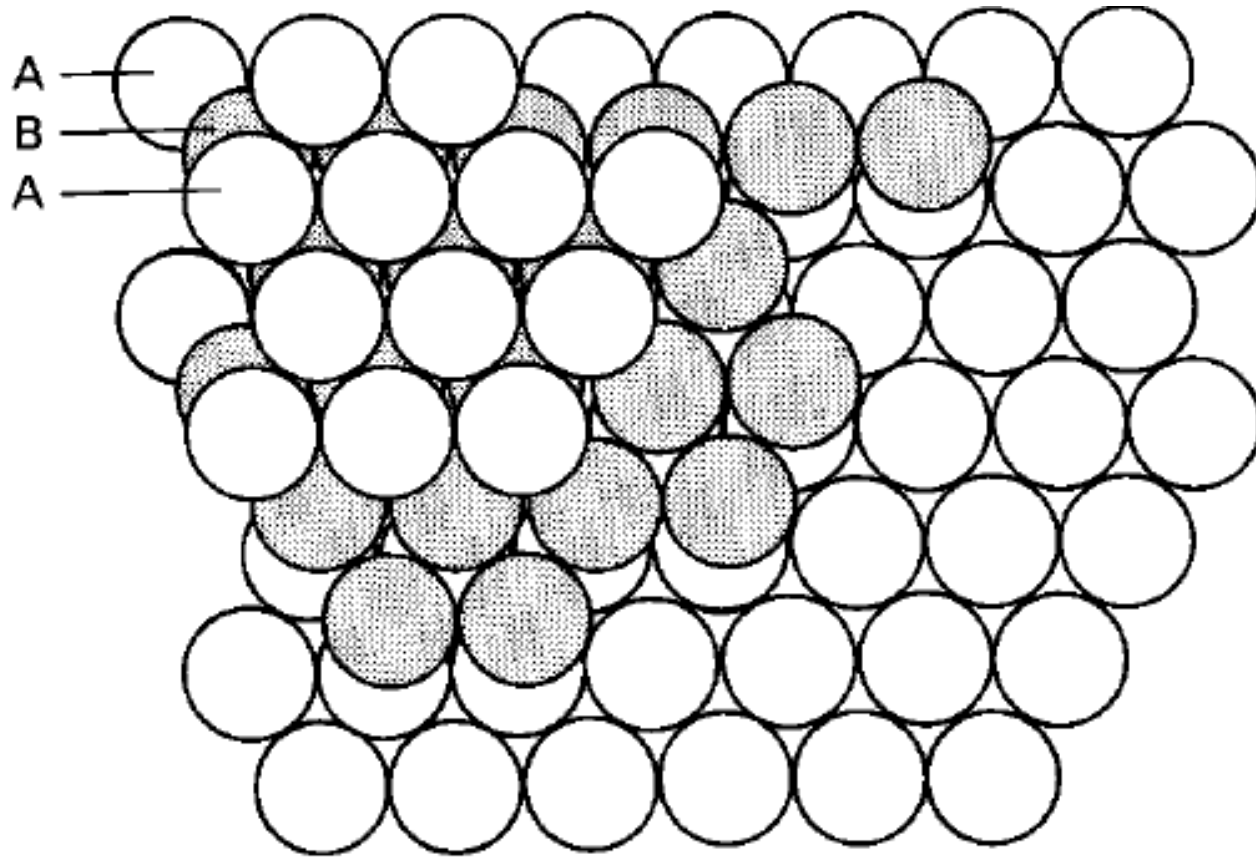
H¹ 4K hcp 3.75 6.12												He⁴ 2K hcp 3.57 5.83																																	
Li 78K bcc 3.491	Be hcp 2.27 3.59											B rhomb.	C diamond 3.567	N 20K cubic 5.66 (N ₂)	O complex (O ₂)	F	Ne 4K fcc 4.46																												
Na 5K bcc 4.225	Mg hcp 3.21 5.21	←———— Crystal structure. —————→ ←———— a lattice parameter, in Å —————→ ←———— c lattice parameter, in Å —————→										Al fcc 4.05	Si diamond 5.430	P complex	S complex	Cl complex (Cl ₂)	Ar 4K fcc 5.31																												
K 5K bcc 5.225	Ca fcc 5.58	Sc hcp 3.31 5.27	Ti hcp 2.95 4.68	V bcc 3.03	Cr bcc 2.88	Mn cubic complex	Fe bcc 2.87	Co hcp 2.51 4.07	Ni fcc 3.52	Cu fcc 3.61	Zn hcp 2.66 4.95	Ga complex	Ge diamond 5.658	As rhomb.	Se hex. chains	Br complex (Br ₂)	Kr 4K fcc 5.64																												
Rb 5K bcc 5.585	Sr fcc 6.08	Y hcp 3.65 5.73	Zr hcp 3.23 5.15	Nb bcc 3.30	Mo bcc 3.15	Tc hcp 2.74 4.40	Ru hcp 2.71 4.28	Rh fcc 3.80	Pd fcc 3.89	Ag fcc 4.09	Cd hcp 2.98 5.62	In tetr. 3.25 4.95	Sn (α) diamond 6.49	Sb rhomb.	Te hex. chains	I complex (I ₂)	Xe 4K fcc 6.13																												
Cs 5K bcc 6.045	Ba bcc 5.02	La hex. 3.77 ABAC	Hf hcp 3.19 5.05	Ta bcc 3.30	W bcc 3.16	Re hcp 2.76 4.46	Os hcp 2.74 4.32	Ir fcc 3.84	Pt fcc 3.92	Au fcc 4.08	Hg rhomb.	Tl hcp 3.46 5.52	Pb fcc 4.95	Bi rhomb.	Po sc 3.34	At —	Rn —																												
Fr —	Ra —	Ac fcc 5.31	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td>Ce fcc 5.16</td> <td>Pr hex. 3.67 ABAC</td> <td>Nd hex. 3.66</td> <td>Pm —</td> <td>Sm complex</td> <td>Eu bcc 4.58</td> <td>Gd hcp 3.63 5.78</td> <td>Tb hcp 3.60 5.70</td> <td>Dy hcp 3.59 5.65</td> <td>Ho hcp 3.58 5.62</td> <td>Er hcp 3.56 5.59</td> <td>Tm hcp 3.54 5.56</td> <td>Yb fcc 5.48</td> <td>Lu hcp 3.50 5.55</td> </tr> <tr> <td>Th fcc 5.08</td> <td>Pa tetr. 3.92 3.24</td> <td>U complex</td> <td>Np complex</td> <td>Pu complex</td> <td>Am hex. 3.64 ABAC</td> <td>Cm —</td> <td>Bk —</td> <td>Cf —</td> <td>Es —</td> <td>Fm —</td> <td>Md —</td> <td>No —</td> <td>Lr —</td> </tr> </table>															Ce fcc 5.16	Pr hex. 3.67 ABAC	Nd hex. 3.66	Pm —	Sm complex	Eu bcc 4.58	Gd hcp 3.63 5.78	Tb hcp 3.60 5.70	Dy hcp 3.59 5.65	Ho hcp 3.58 5.62	Er hcp 3.56 5.59	Tm hcp 3.54 5.56	Yb fcc 5.48	Lu hcp 3.50 5.55	Th fcc 5.08	Pa tetr. 3.92 3.24	U complex	Np complex	Pu complex	Am hex. 3.64 ABAC	Cm —	Bk —	Cf —	Es —	Fm —	Md —	No —	Lr —
Ce fcc 5.16	Pr hex. 3.67 ABAC	Nd hex. 3.66	Pm —	Sm complex	Eu bcc 4.58	Gd hcp 3.63 5.78	Tb hcp 3.60 5.70	Dy hcp 3.59 5.65	Ho hcp 3.58 5.62	Er hcp 3.56 5.59	Tm hcp 3.54 5.56	Yb fcc 5.48	Lu hcp 3.50 5.55																																
Th fcc 5.08	Pa tetr. 3.92 3.24	U complex	Np complex	Pu complex	Am hex. 3.64 ABAC	Cm —	Bk —	Cf —	Es —	Fm —	Md —	No —	Lr —																																

Estructuras cristalinas compactas

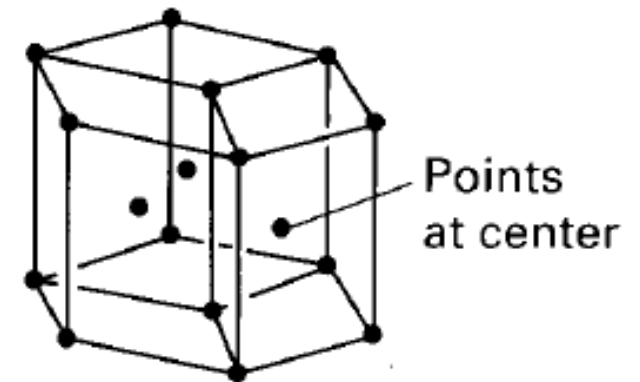
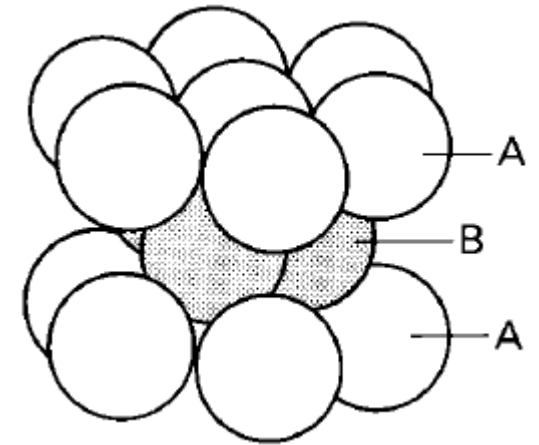
Dos formas de apilar esferas (fcc vs hcp):
el problema del verdulero.



hcp



$$c = \sqrt{\frac{8}{3}} a = 1.63299a.$$



Hexagonal Compacta (hcp)

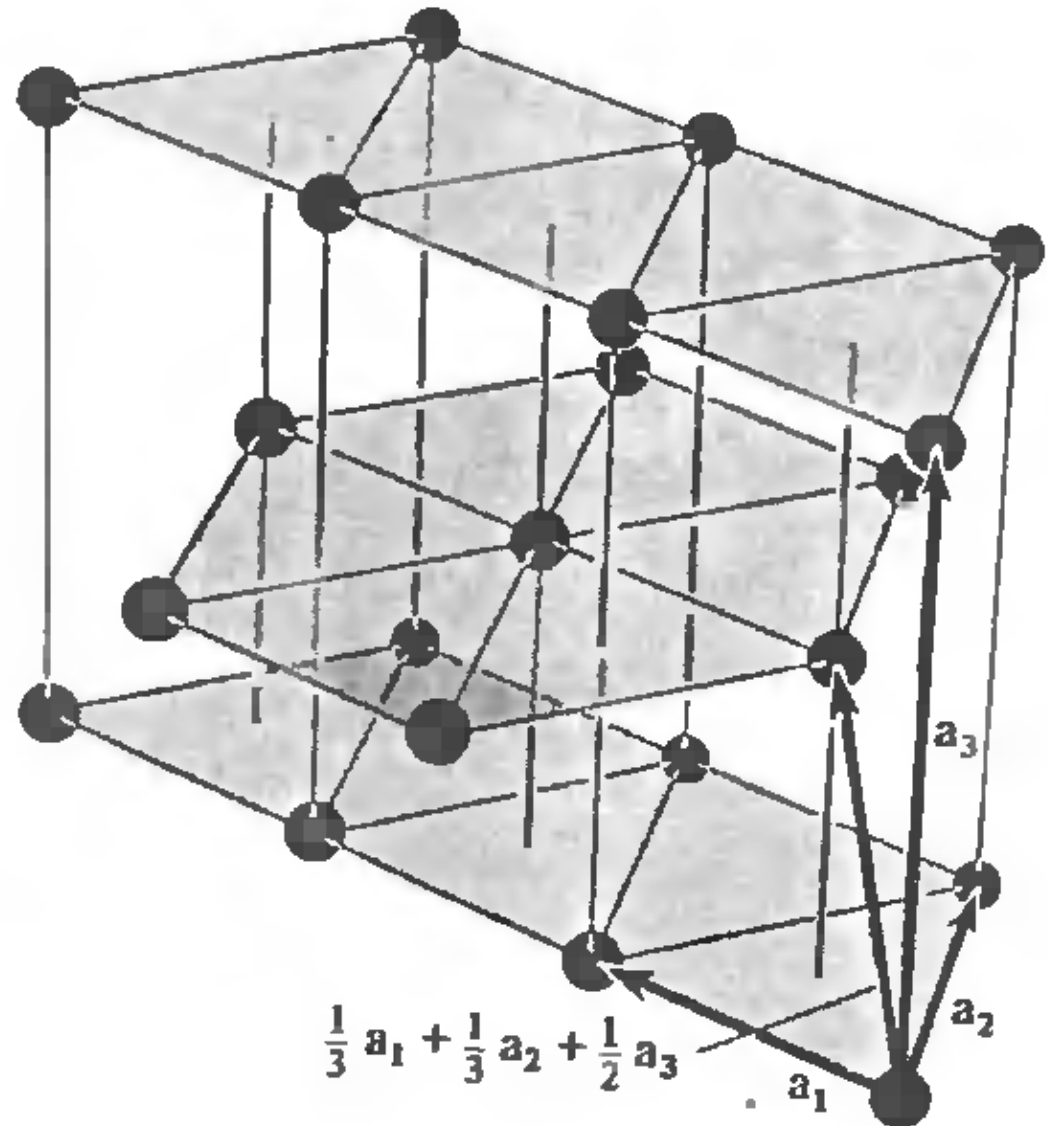
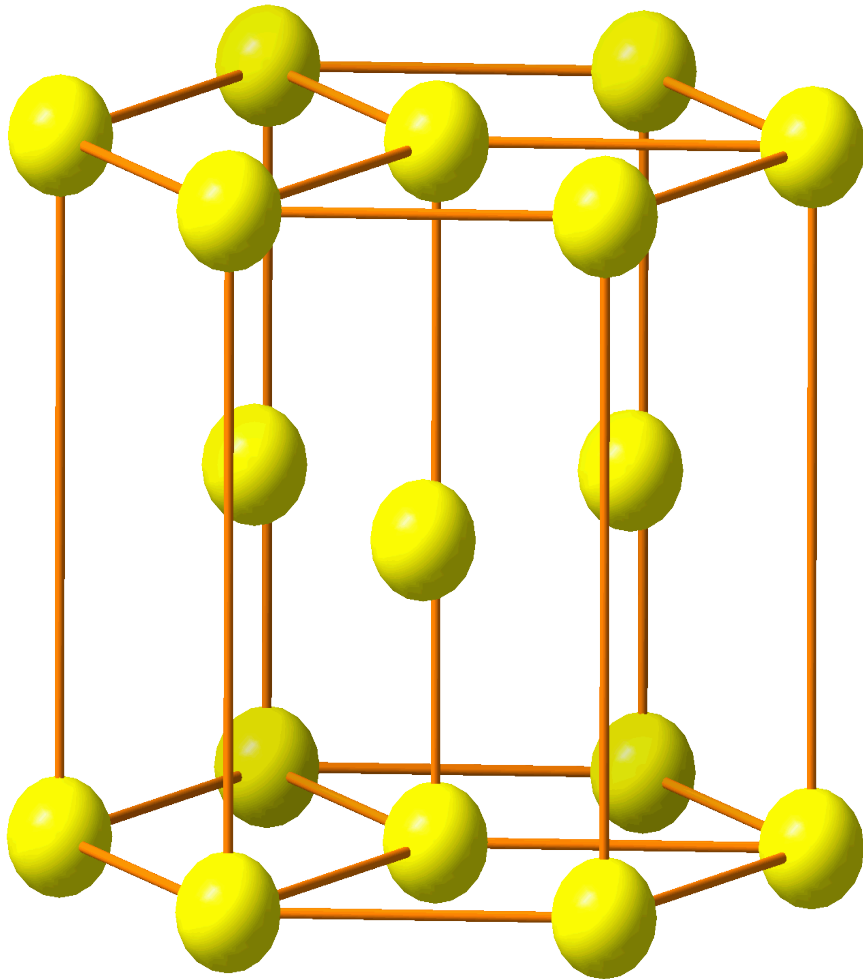
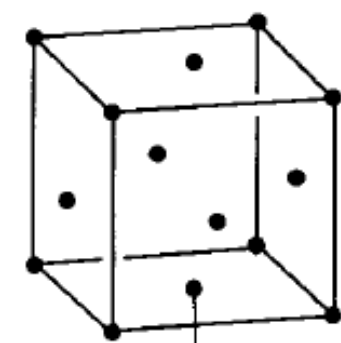
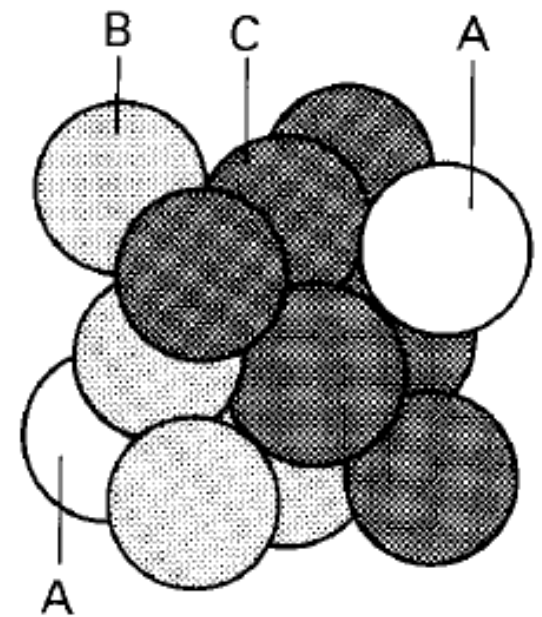
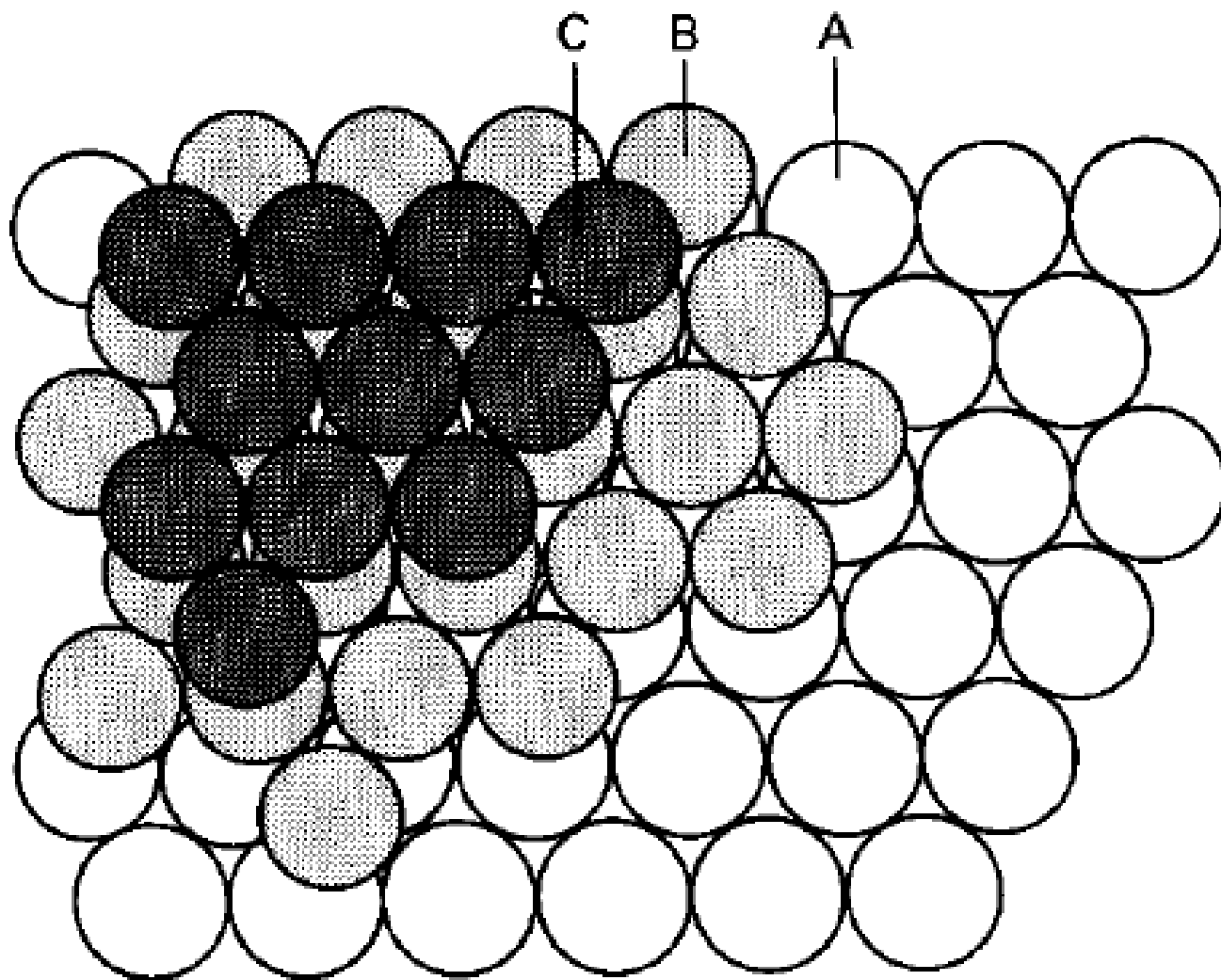


Table 4.4

**ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL
STRUCTURE**

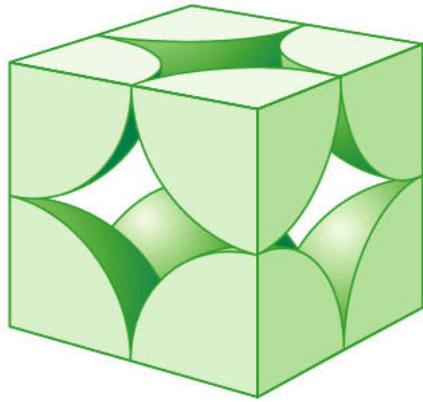
ELEMENT	a (Å)	c	c/a	ELEMENT	a (Å)	c	c/a
Be	2.29	3.58	1.56	Os	2.74	4.32	1.58
Cd	2.98	5.62	1.89	Pr	3.67	5.92	1.61
Ce	3.65	5.96	1.63	Re	2.76	4.46	1.62
α -Co	2.51	4.07	1.62	Ru	2.70	4.28	1.59
Dy	3.59	5.65	1.57	Sc	3.31	5.27	1.59
Er	3.56	5.59	1.57	Tb	3.60	5.69	1.58
Gd	3.64	5.78	1.59	Ti	2.95	4.69	1.59
He (2 K)	3.57	5.83	1.63	Tl	3.46	5.53	1.60
Hf	3.20	5.06	1.58	Tm	3.54	5.55	1.57
Ho	3.58	5.62	1.57	Y	3.65	5.73	1.57
La	3.75	6.07	1.62	Zn	2.66	4.95	1.86
Lu	3.50	5.55	1.59	Zr	3.23	5.15	1.59
Mg	3.21	5.21	1.62		—	—	
Nd	3.66	5.90	1.61	"Ideal"			1.63

fcc

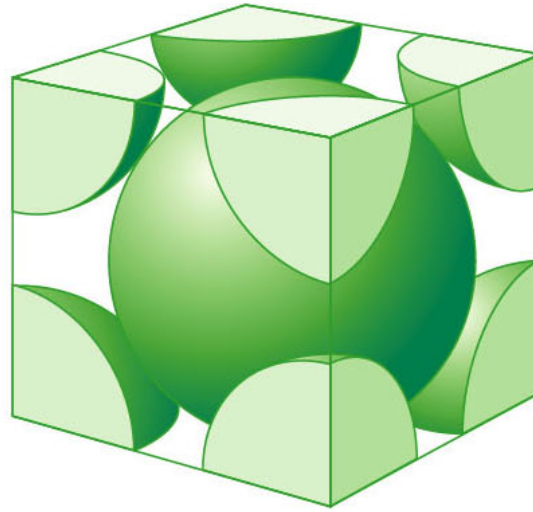


Points on faces

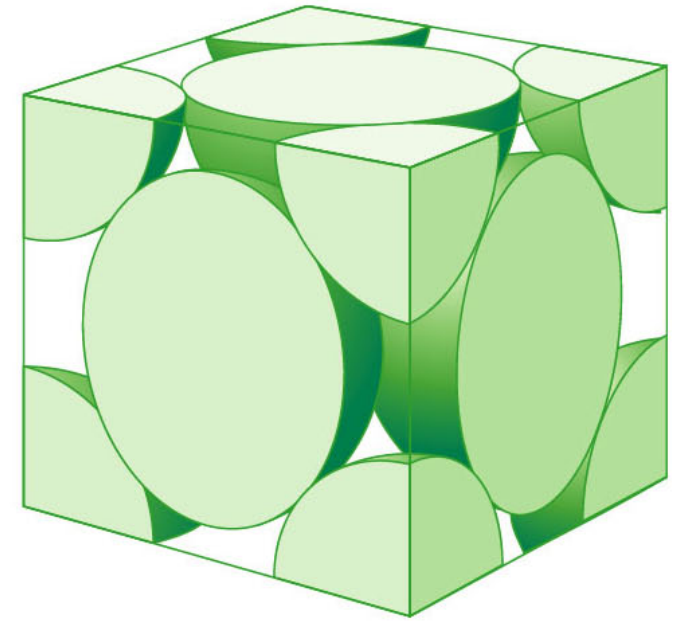
Cristales cúbicos



Simple cubic



Body-centered cubic



Face-centered cubic

	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors ^a	6	8	12
Nearest-neighbor distance	a	$3^{1/2}a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	a	a
Packing fraction ^b	$\frac{1}{6}\pi$ = 0.524	$\frac{1}{8}\pi\sqrt{3}$ = 0.680	$\frac{1}{6}\pi\sqrt{2}$ = 0.740

Estructuras cristalinas: ejemplos

Diamante

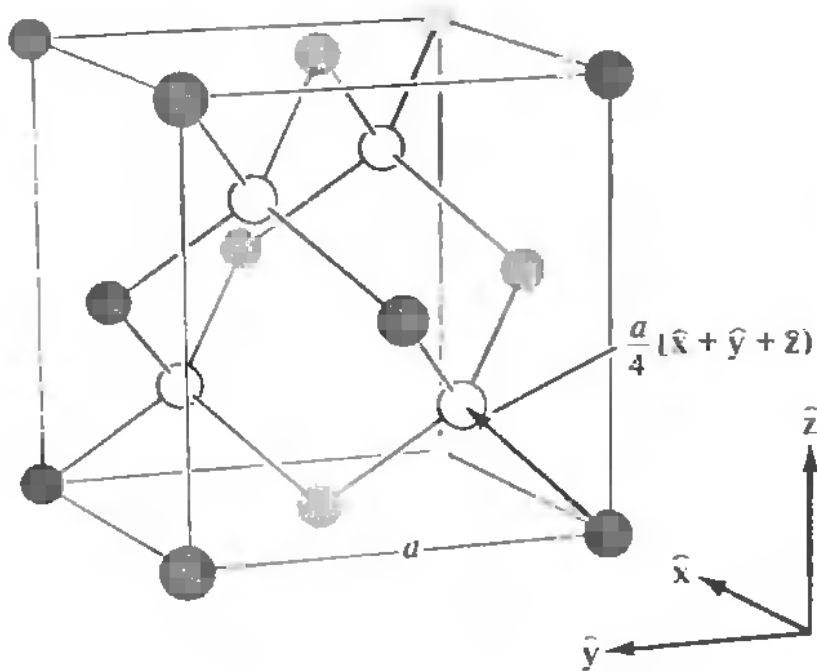


Table 4.3
ELEMENTS WITH THE DIAMOND CRYSTAL
STRUCTURE

ELEMENT	CUBE SIDE a (Å)
C (diamond)	3.57
Si	5.43
Ge	5.66
α -Sn (grey)	6.49

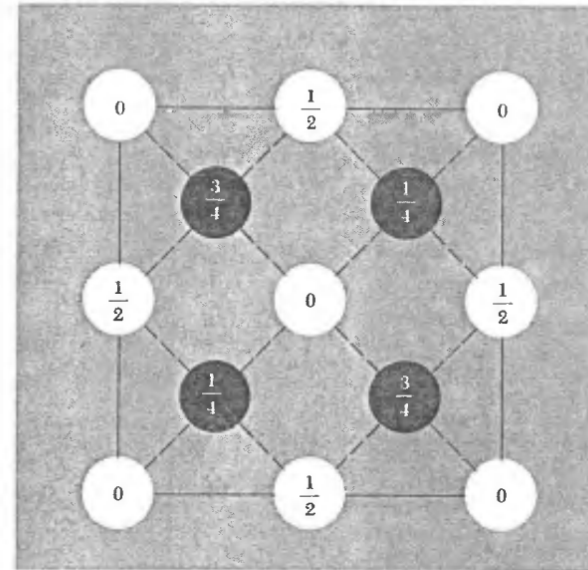


Figure 24 Atomic positions in the cubic cell of the diamond structure projected on a cube face; fractions denote height above the base in units of a cube edge. The points at 0 and $\frac{1}{2}$ are on the fcc lattice; those at $\frac{1}{4}$ and $\frac{3}{4}$ are on a similar lattice displaced along the body diagonal by one-fourth of its length. With a fcc space lattice, the basis consists of two identical atoms at $000; \frac{1}{4}\frac{1}{4}\frac{1}{4}$.

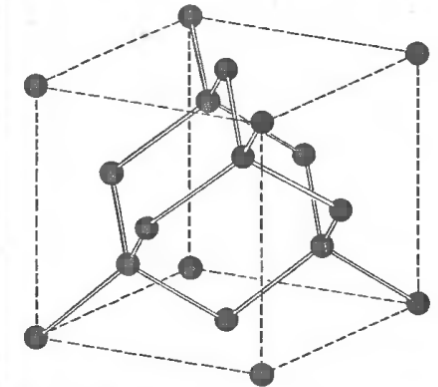
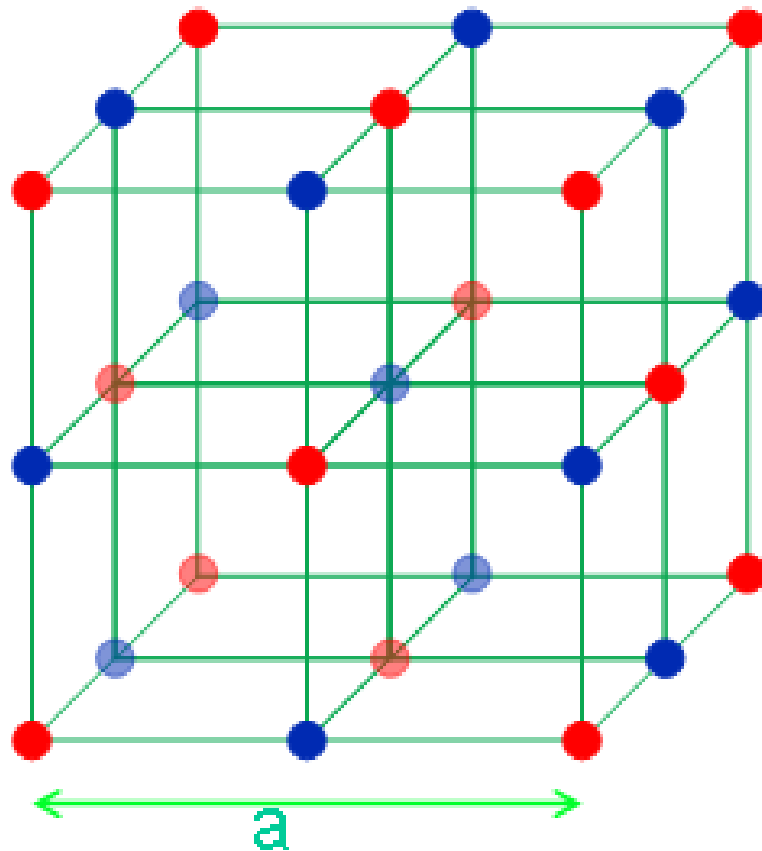
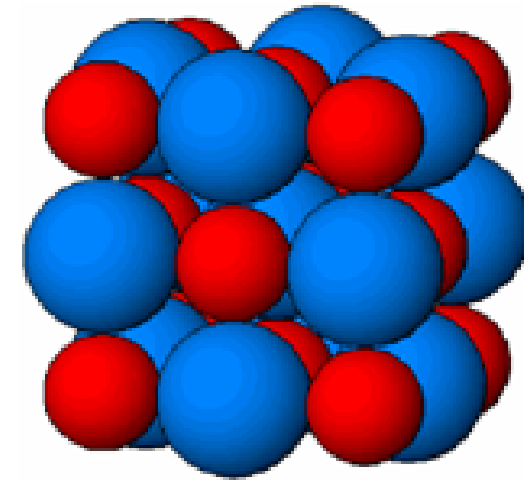


Figure 25 Crystal structure of diamond, showing the tetrahedral bond arrangement.

Estructura NaCl



Red: FCC

Base: consiste de 2 átomos

Na: $(0,0,0)$ ●

Cl: $a(1/2, 1/2, 1/2)$ ●

Ejem.: LiH, KCl, PbS, AgBr, MgO, MnO, KBr.

Algunos compuesto con estructura de Cloruro de Sodio

Cristal	a (Å)	Cristal	a (Å)	Cristal	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23
NaBr	5.97	AgCl	5.55	SrTe	6.47
NaI	6.47	AgBr	5.77	BaO	5.52
KF	5.35	MgO	4.21	BaS	6.39
KCl	6.29	MgS	5.20	BaSe	6.60
KBr	6.60	MgSe	5.45	BaTe	6.99
KI	7.07	CaO	4.81		

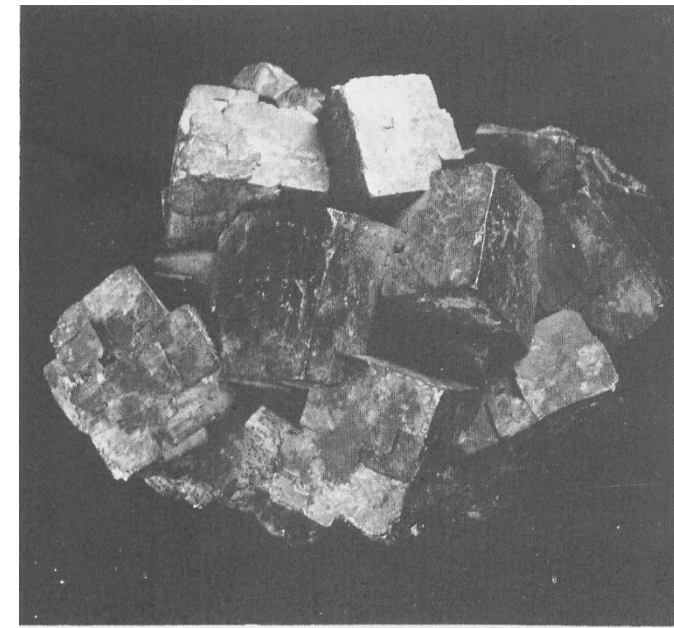
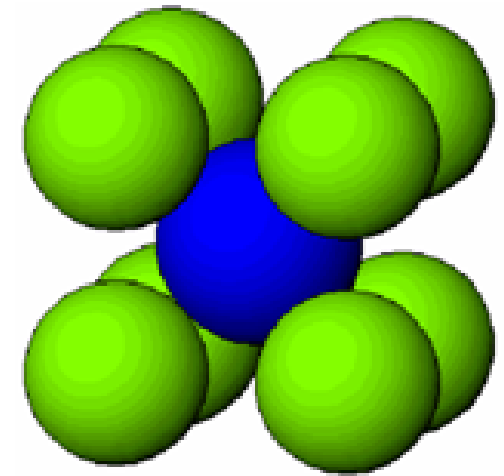
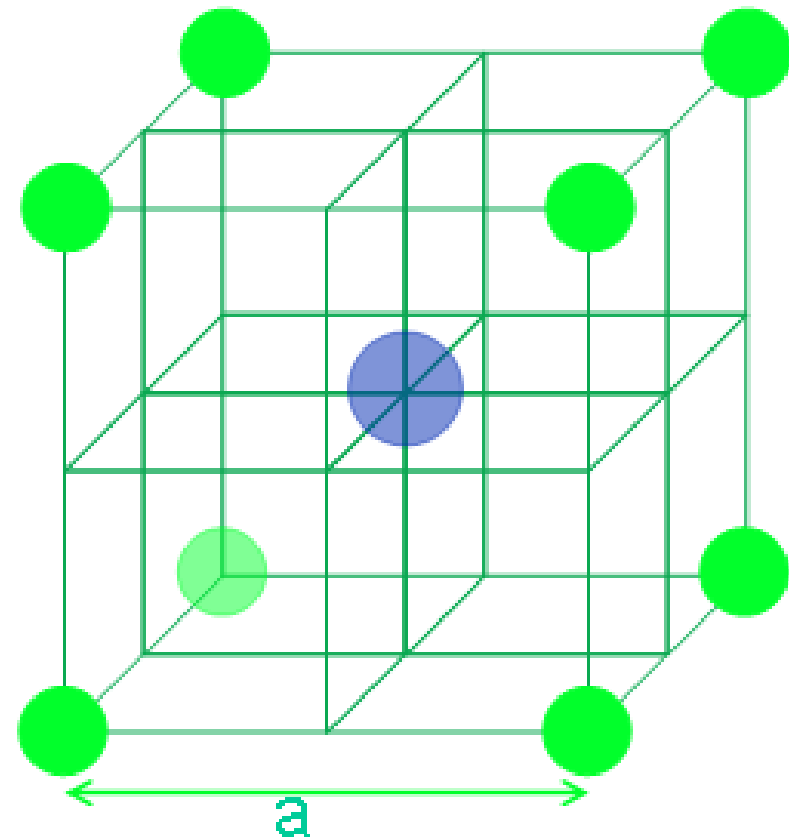


Figure 19 Natural crystals of lead sulfide, PbS, which has the NaCl crystal structure. (Photograph by B. Burleson.)

Estructura CsCl



Red: cúbica

Base: consiste de 2 átomos

Cs: $(0,0,0)$ ●

Cl: $a(1/2, 1/2, 1/2)$ ●

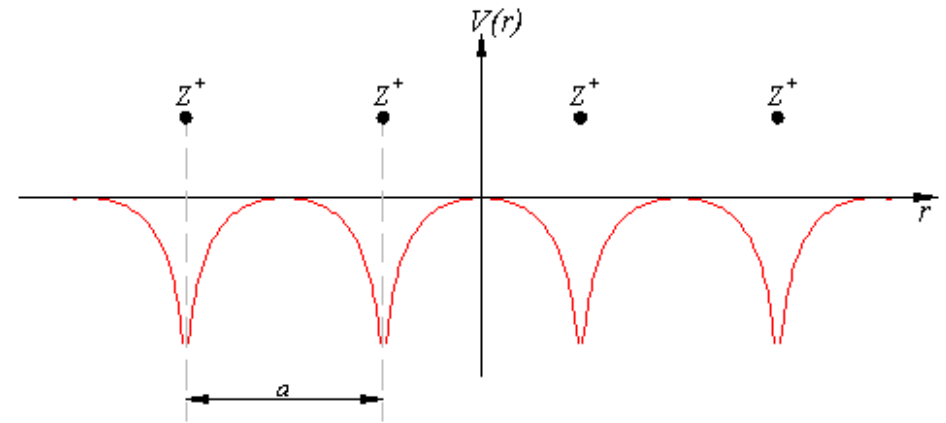
Ejem.: CuZn, CsBr, LiAg.

Representación de Fourier de las propiedades cristalinas

Consideremos una función con la periodicidad de la red (densidad electrónica, potencial cristalino, etc):

$$f(\bar{r} + \bar{R}_l) = f(\bar{r})$$

$$1D: f(x+a) = f(x)$$



Se puede desarrollar en una Serie de Fourier:

$$f(x) = \sum_n f_n e^{i(2\pi/a)nx} \quad \text{ya que}$$

$$f(x+a) = \sum_n f_n e^{i(2\pi/a)nx} e^{i2\pi n} = f(x)$$

$$f_n = \frac{1}{a} \int_0^a f(x) e^{-i(2\pi n/a)x} dx \quad \text{ya que}$$

$$\frac{1}{a} \int_0^a f(x) e^{-i(2\pi n/a)x} dx = \sum_m f_m \underbrace{\frac{1}{a} \int_0^a e^{i(2\pi/a)(m-n)x} dx}_{\delta_{mn}} = f_n$$

Conviene introducir una red (de Bravais) unidimensional, con dimensiones $1/L$, mediante el vector primitivo $\bar{b} = (2\pi/a)\hat{i}$.

$$f(x) = \sum_n f_n e^{i\bar{G}_n \cdot \bar{r}} \quad \text{con } \bar{G}_n = nb\hat{i} \text{ y } \bar{r} = x\hat{i}$$

Para el caso tridimensional tenemos:

$$f(\bar{r}) = \sum_G f_{\bar{G}} e^{i\bar{G} \cdot \bar{r}}$$

como $f(\bar{r} + \bar{R}_l) = f(\bar{r}) \quad \forall \bar{R}_l \in$ red de Bravais

$$\bar{G} \text{ cumple } e^{i\bar{G} \cdot (\bar{r} + \bar{R}_l)} = e^{i\bar{G} \cdot \bar{r}} \Rightarrow e^{i\bar{G} \cdot \bar{R}_l} = 1 \quad (*)$$

Estos \bar{G} definen la Red Reciproca (RR)

$$\bar{G} \cdot \bar{\mathbf{R}}_l = 2\pi \cdot \text{entero} = \sum_{i=1}^3 l_i \bar{a}_i \cdot \bar{G}.$$

$$\therefore \bar{a}_i \cdot \bar{G} = 2\pi n_i$$

Red Reciproca: Definición

La Red Reciproca es una red de Bravais con vectores primitivos \mathbf{b}_i que cumplen:

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

$$\mathbf{G} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3.$$

$$\mathbf{G} \cdot \mathbf{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3).$$

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3.$$

Se los puede construir de la siguiente manera:

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

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

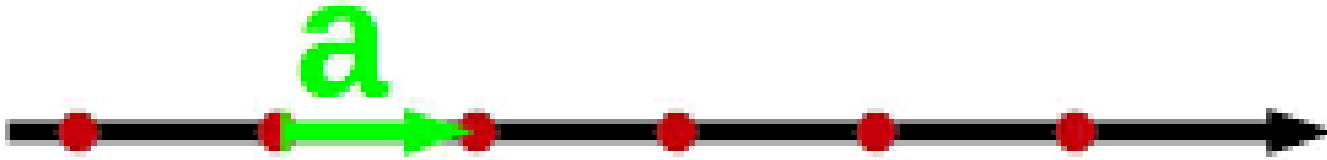
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

Donde:

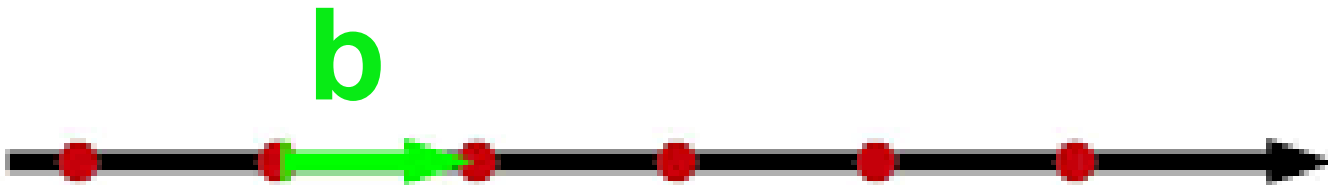
$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

es el volumen de la celda unitaria de la red directa

Ejemplos:

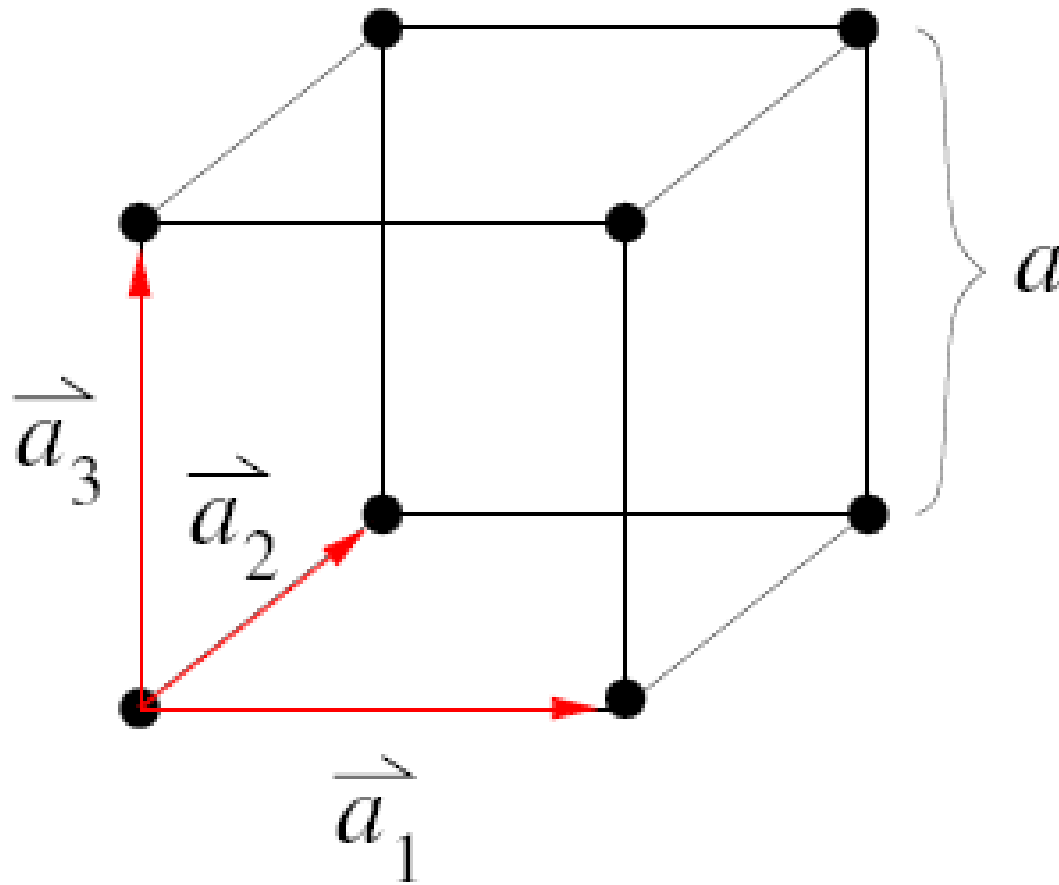


RR ?



$$\mathbf{b} = 2\pi/a$$

Cúbica simple (SC)



$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

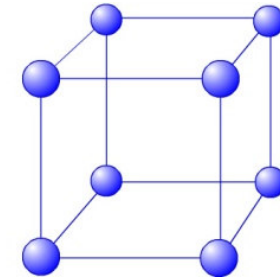
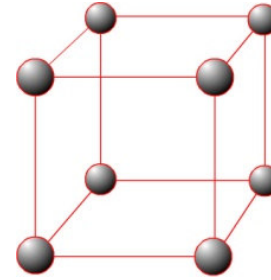
$$\vec{a}_3 = a\hat{z}$$

$$\mathbf{b}_1 = \frac{2\pi}{a} \mathbf{x}, \quad \mathbf{b}_2 = \frac{2\pi}{a} \mathbf{y}, \quad \mathbf{b}_3 = \frac{2\pi}{a} \mathbf{z}. \quad (\text{SC})$$

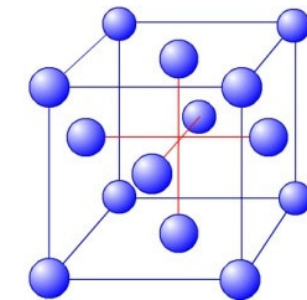
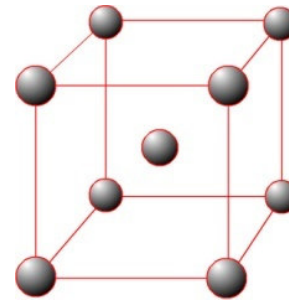
Bravais

Recíproca

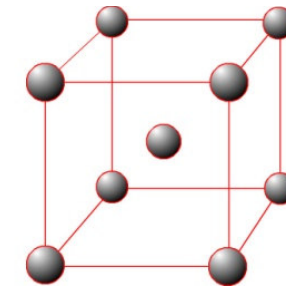
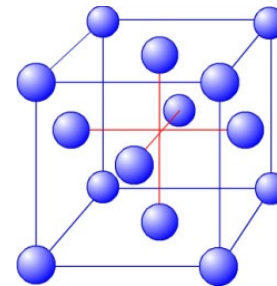
cs [a] \longrightarrow cs [$2\pi/a$]



bcc [a] \longrightarrow fcc [$4\pi/a$]



fcc [a] \longrightarrow bcc [$4\pi/a$]



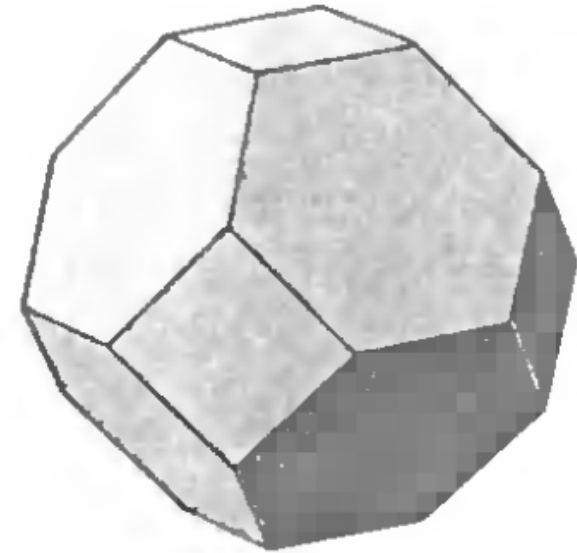
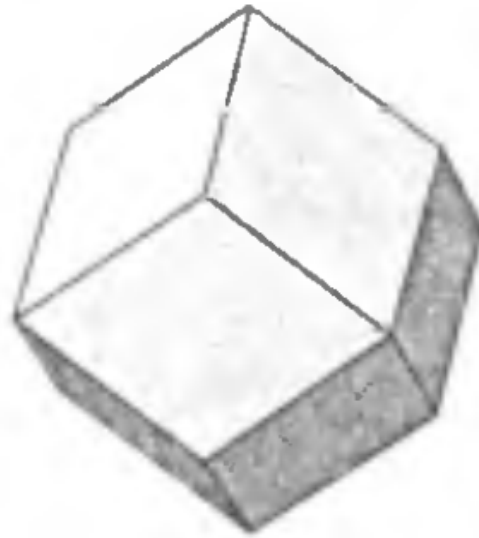
hexagonal [a,c] \longrightarrow hexagonal [$2\pi/\sqrt{3}a, 2\pi/c$]
rotada 30° en torno al eje c

Primera zona de Brillouin

Por definición, la Primera Zona de Brillouin es la celda de Wigner-Seitz para la red recíproca.

Figure 5.2

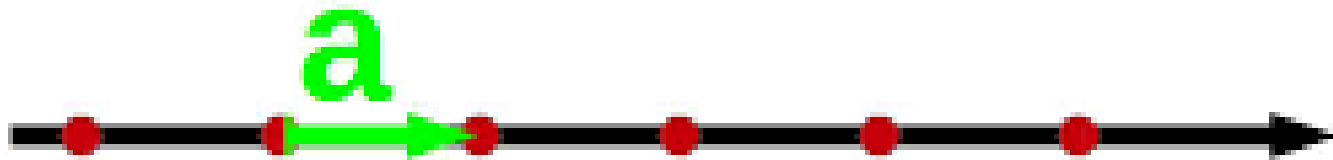
- (a) The first Brillouin zone for the body-centered cubic lattice.
- (b) The first Brillouin zone for the face-centered cubic lattice.



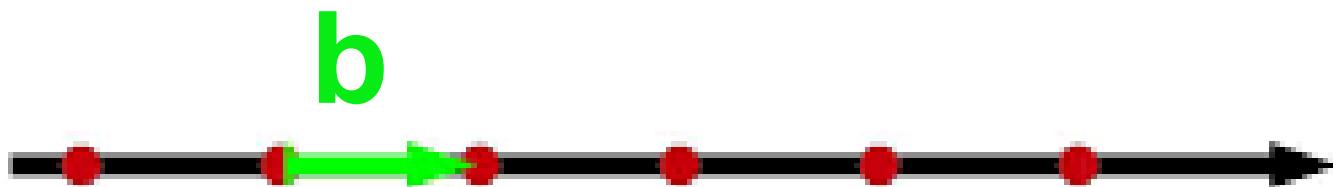
Ejercicio: Demostrar la siguiente propiedad

$$v_r = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{(2\pi)^3}{v}$$

Ejemplo 1D:

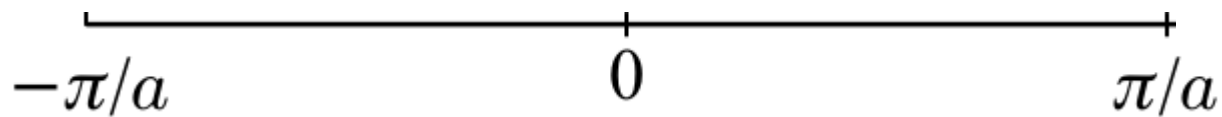


1ZB ?



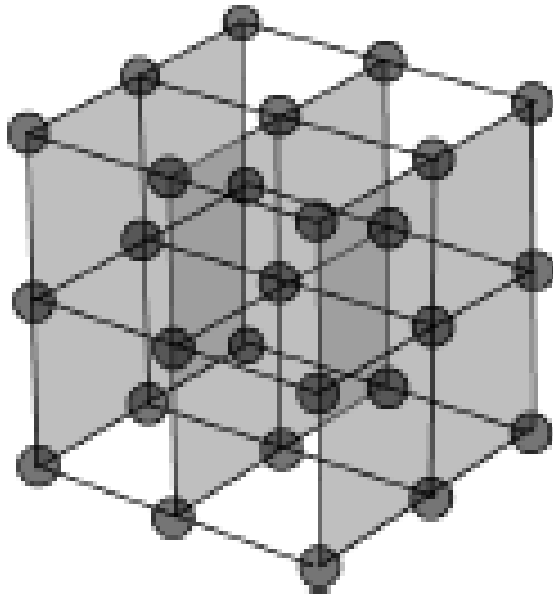
$b = 2\pi/a$

Primer zona de Brillouin

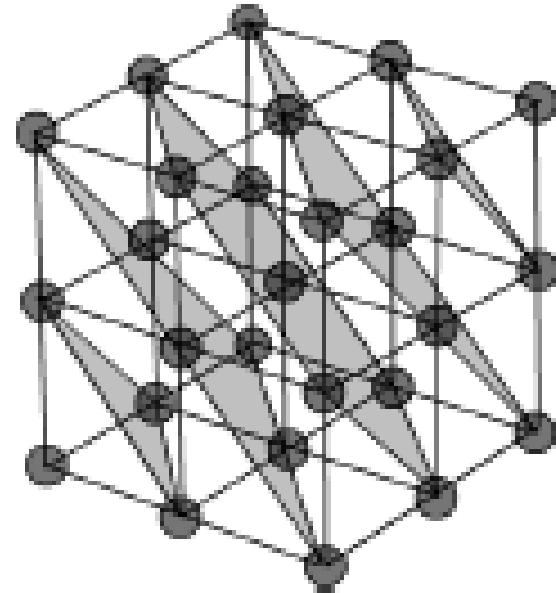


Planos cristalinos

- Es un plano que contiene a lo menos tres puntos no colineales de una red.



Planos cristalinos paralelos a caras principales de la red cúbica simple.



Planos cristalinos perpendiculares a la diagonal principal de una red de Bravais cúbica

Indices de Miller

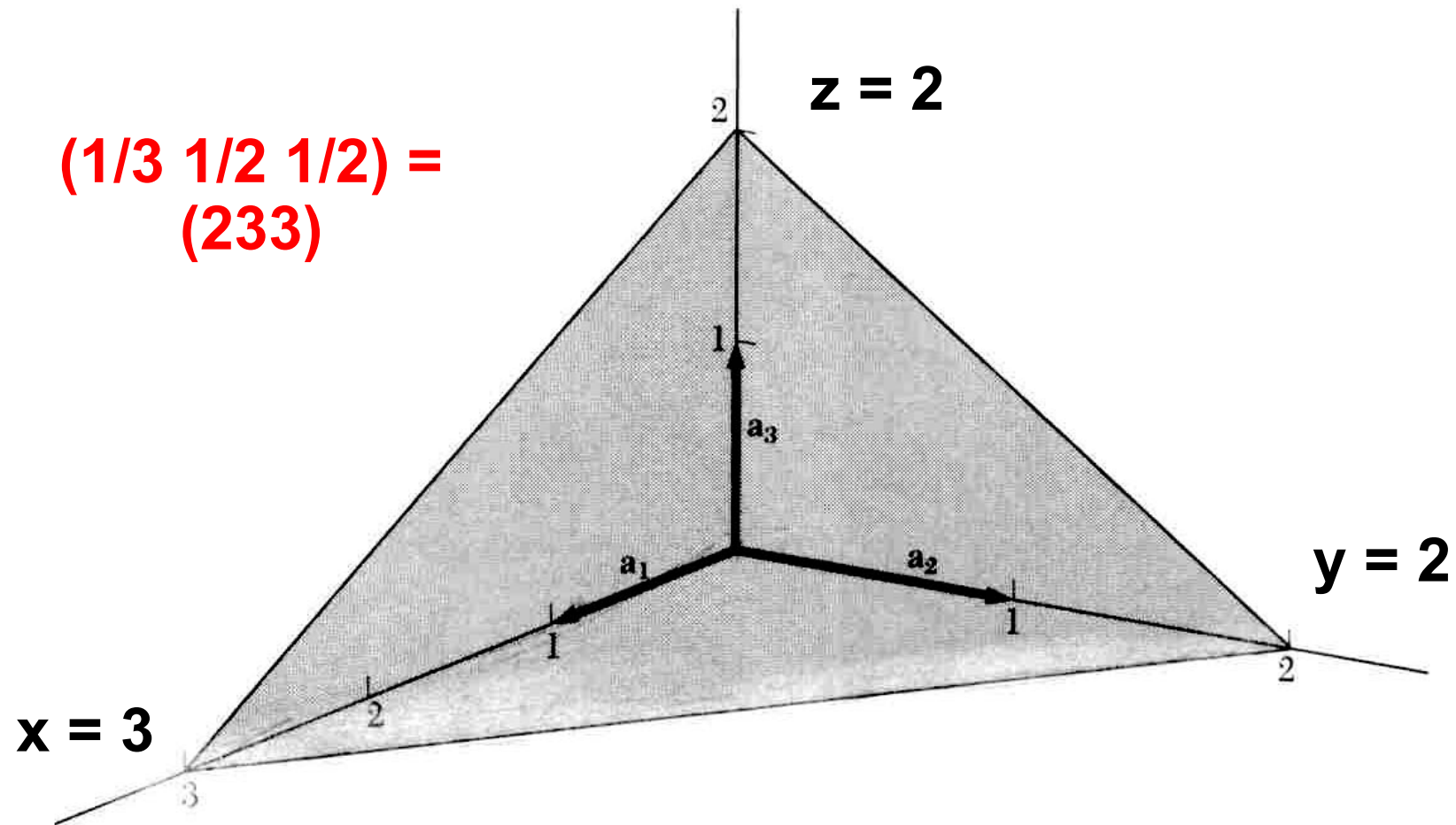
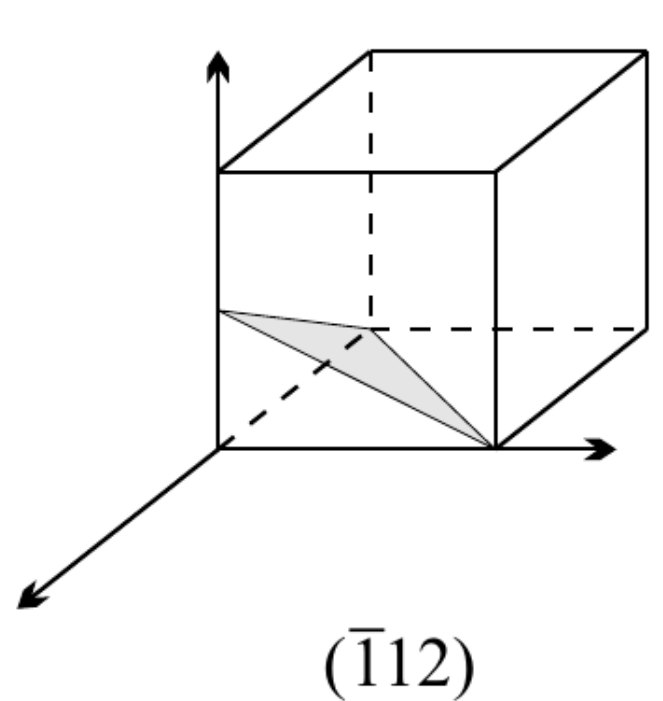
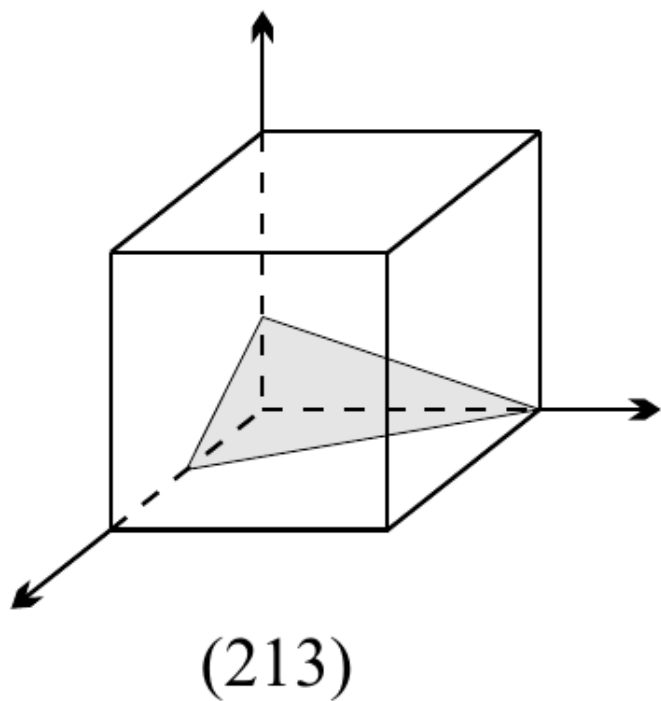
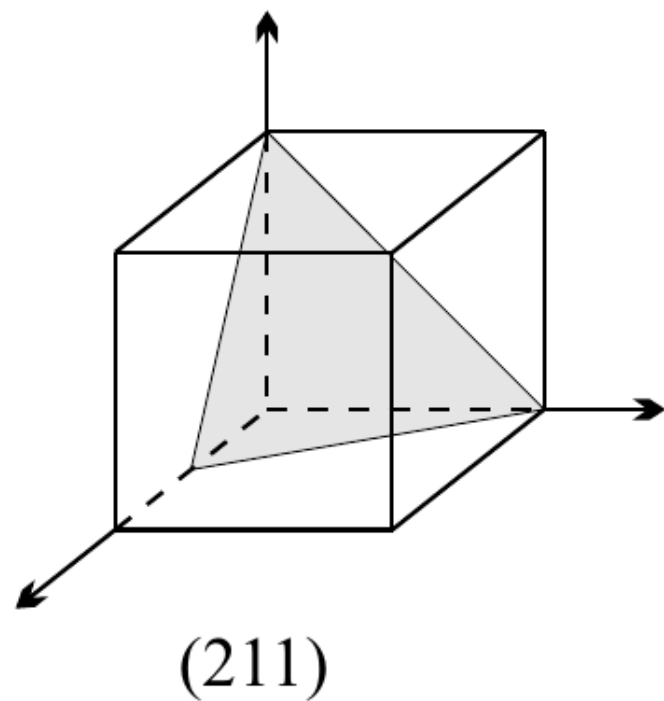
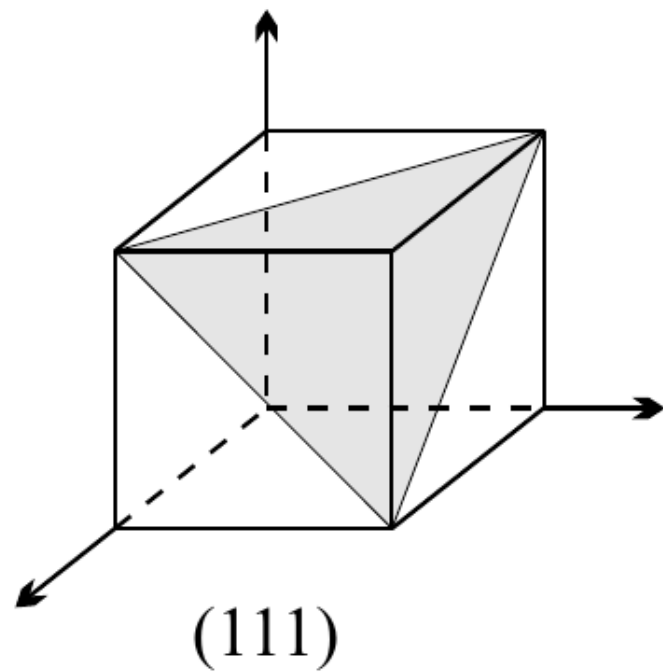
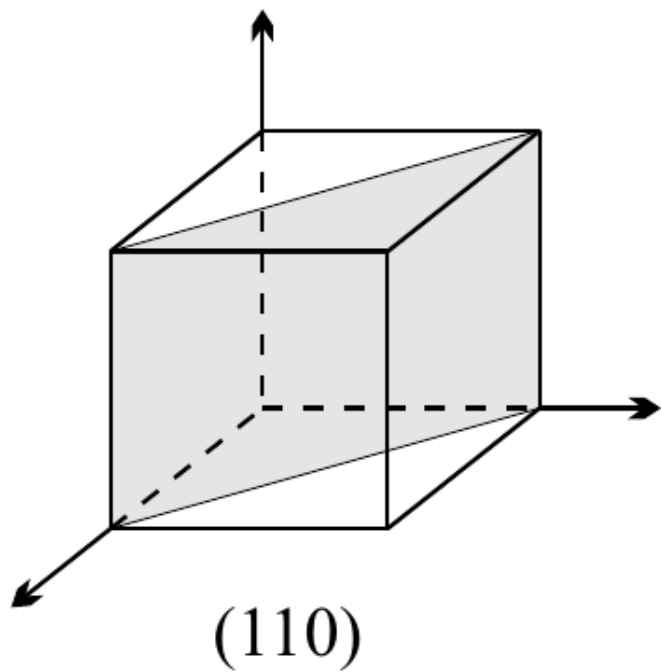
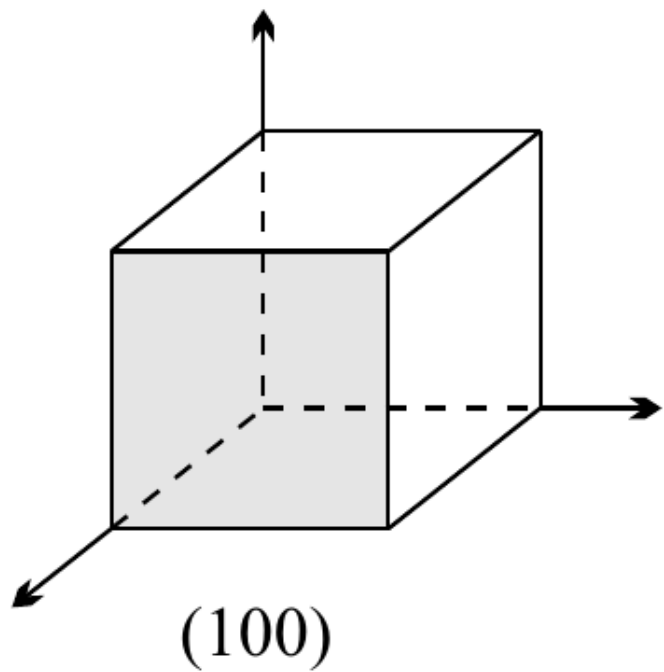
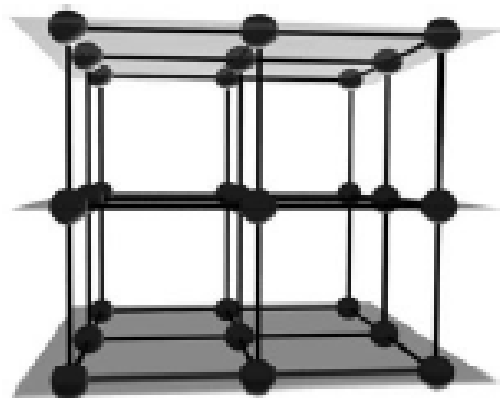
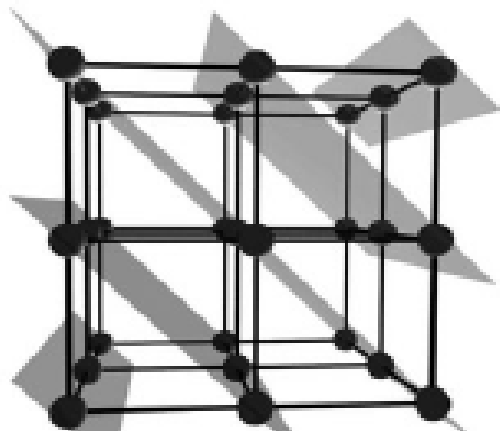


Figure 15 This plane intercepts the a_1 , a_2 , a_3 axes at $3a_1$, $2a_2$, $2a_3$. The reciprocals of these numbers are $\frac{1}{3}$, $\frac{1}{2}$, $\frac{1}{2}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233) .

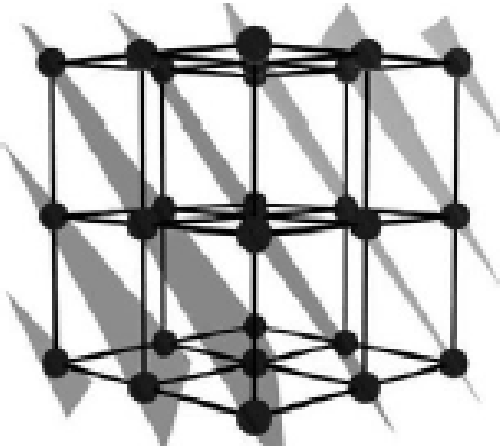




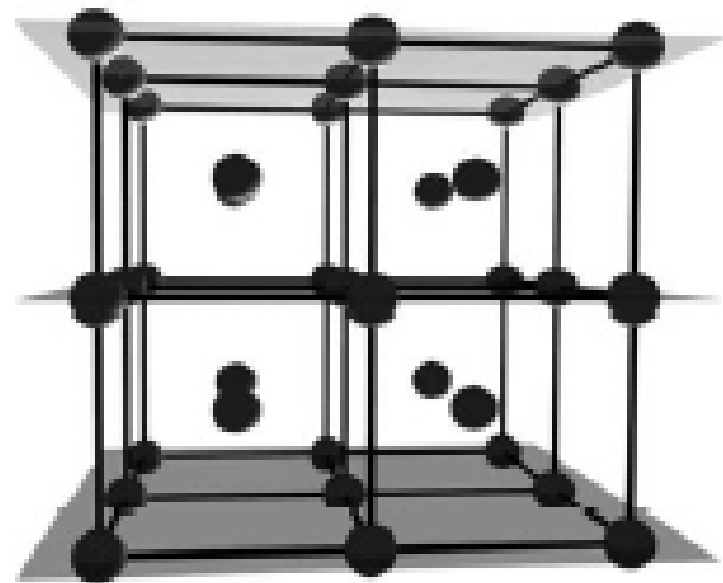
(010) family of lattice planes



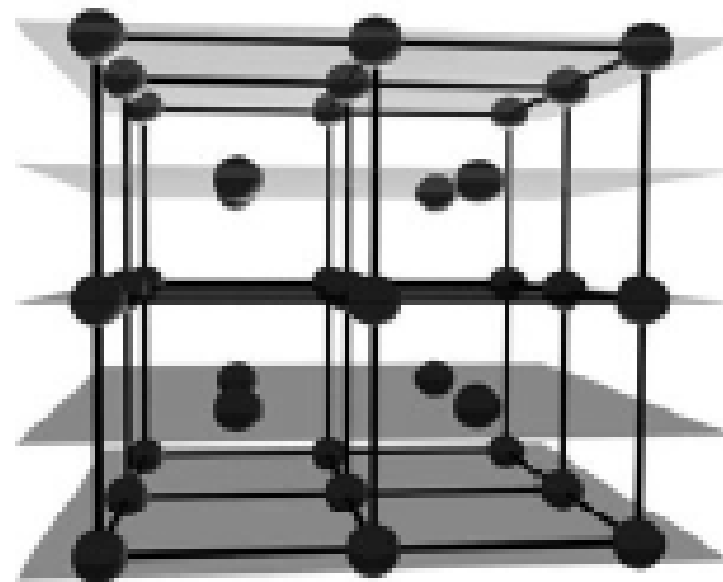
(110) family of lattice planes



(111) family of lattice planes



*(010) family of planes
(not all lattice points included)*



(020) family of lattice planes

Equivalencia familia de planos RD y vectores RR

-Para cualquier familia de planos separados una distancia d , existen vectores en la RR perpendiculares a los planos. El más corto de ellos tiene modulo $2\pi/d$.

-Inversamente, para cualquier vector \mathbf{G} de la RR, existe una familia de planos normales a \mathbf{G} y separados una distancia d , donde $2\pi/d$ es la longitud del vector de la RR más corto paralelo \mathbf{G} .

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

$\mathbf{G}_{hkl} \perp$ familia de planos (hkl) separados por una distancia d

\mathbf{G} es un múltiplo entero de un vector $\mathbf{G}_0 / |\mathbf{G}_0| = 2\pi/d$, $G = n 2\pi/d$

Es posible entonces etiquetar una familia de planos en la RB con tres enteros 'índices de Miller' (hkl) de forma que $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ sea el vector de la RR más corto perpendicular a la familia.

Las redes cúbicas (sc, fcc o bcc) es conveniente describirlas como cúbicas (eventualmente) con motivo. Como todo plano de la fcc o bcc lo es de la sc subyacente podemos definir los índices de Miller para esta última

