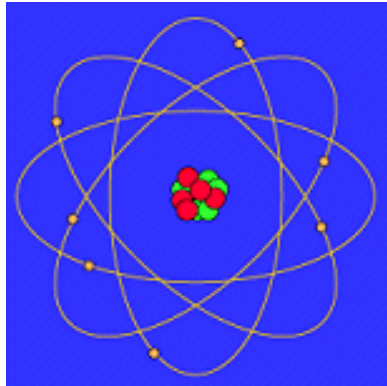


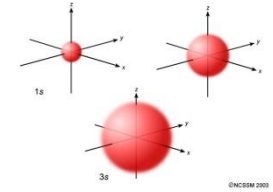
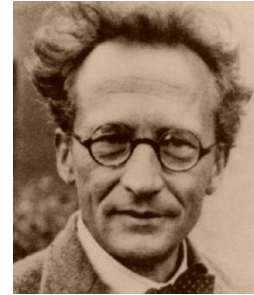
TEMA 5

Principios de Cristaloquímica

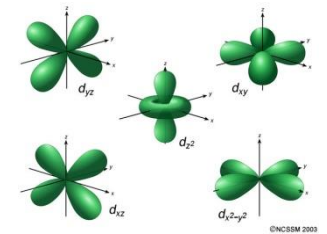
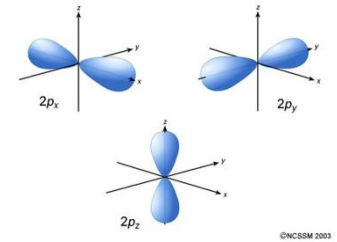
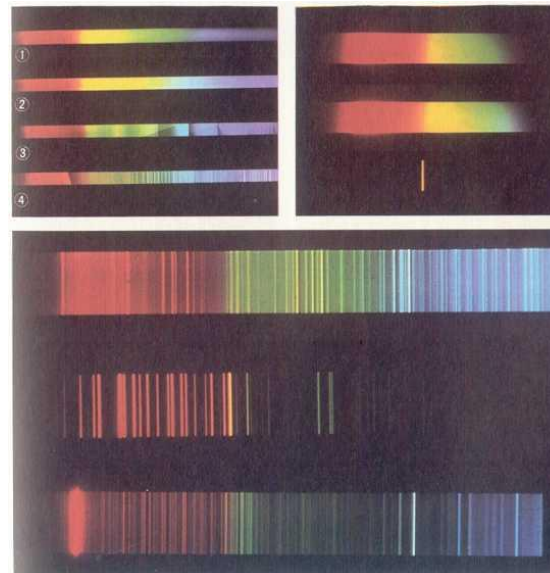
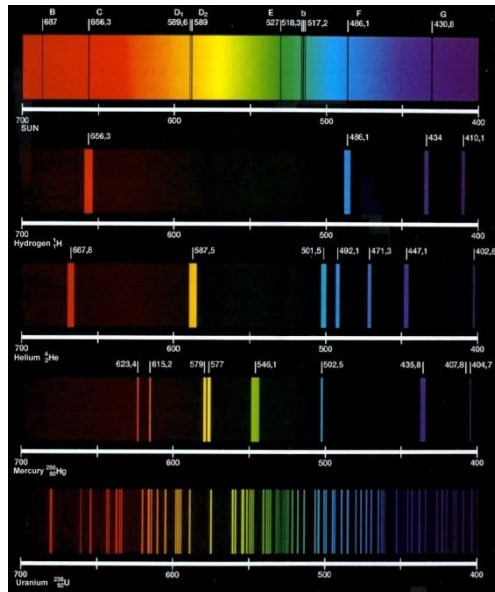
Átomo de Bohr



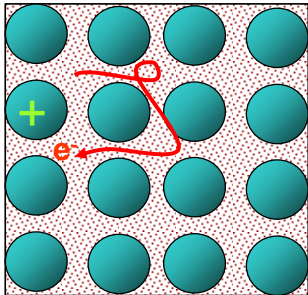
Átomo de Schrödinger



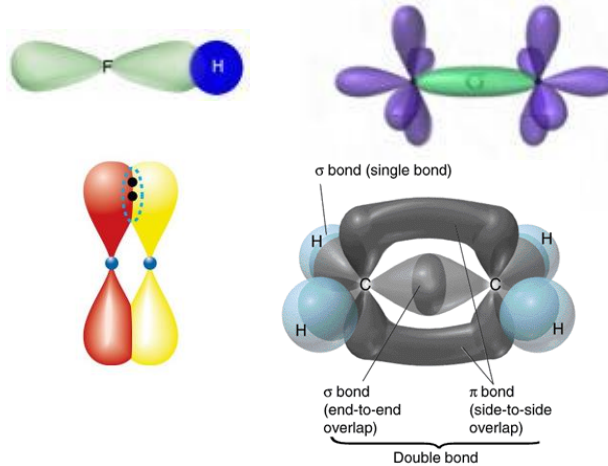
Espectros atómicos



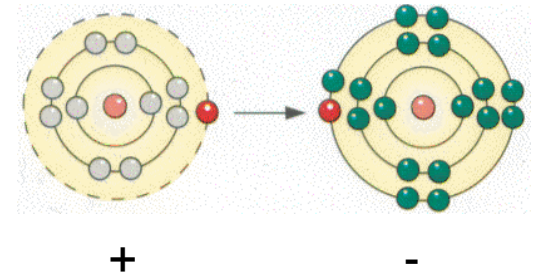
Enlace Metálico



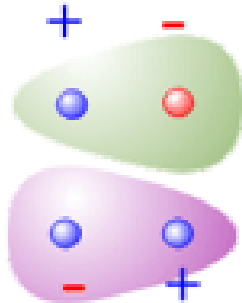
Enlace covalente



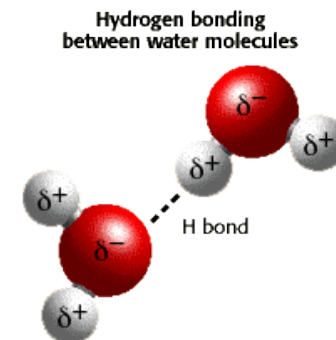
Enlace iónico



Enlace de van der Waals

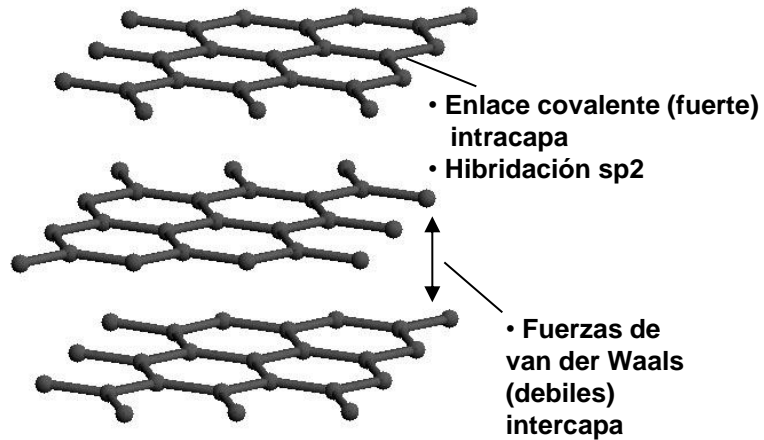


Enlace por puente de hidrógeno

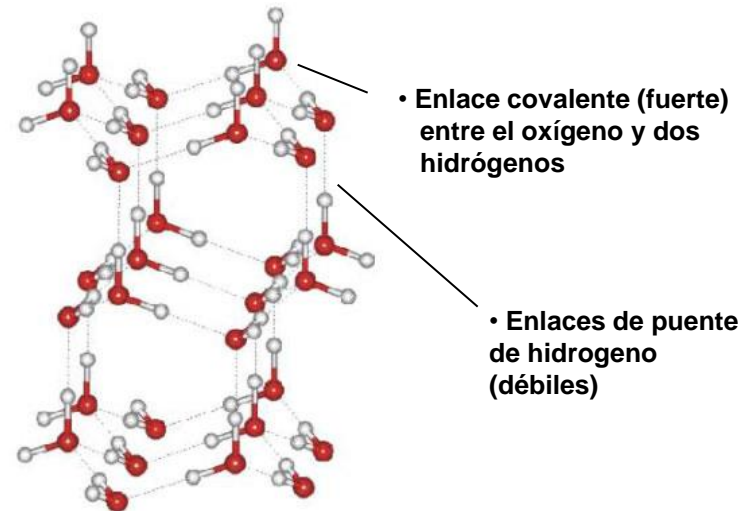


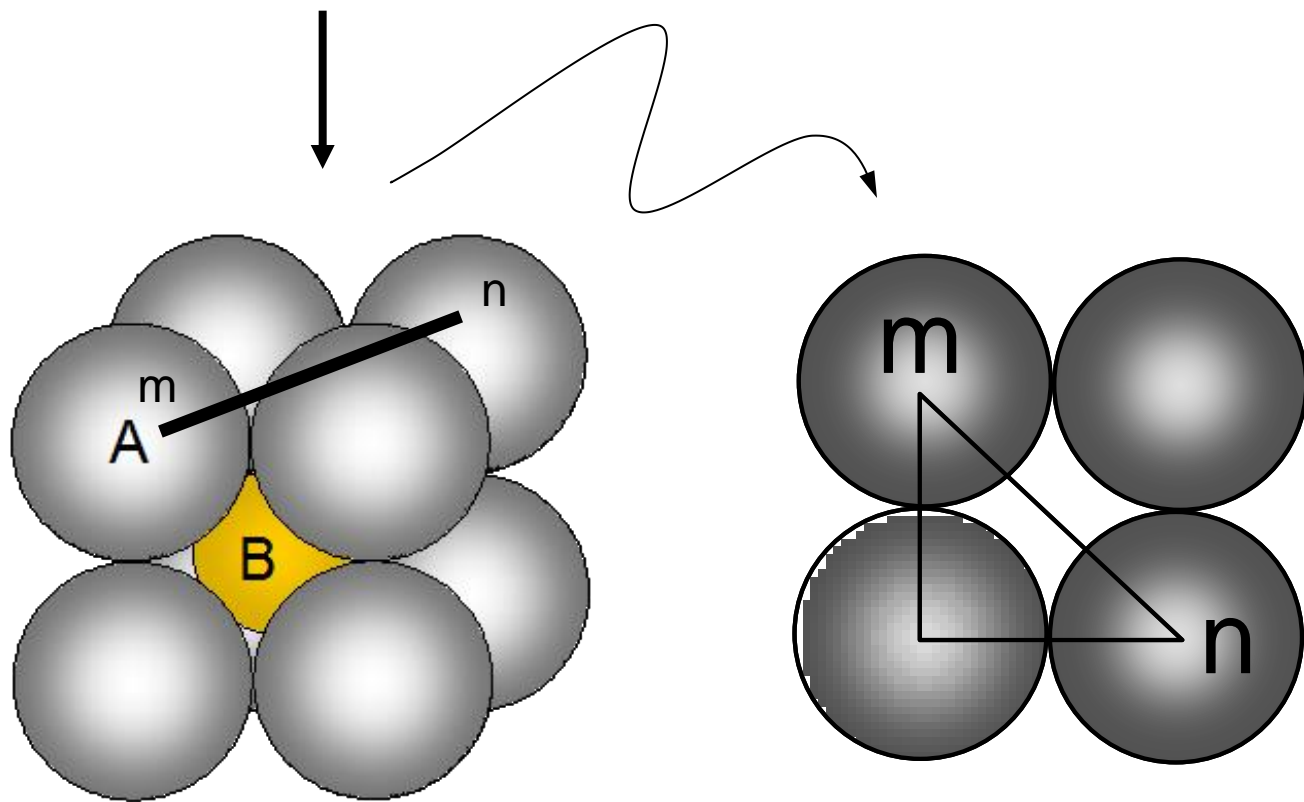
Combinación de enlaces

Grafito. C










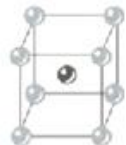




Hielo. H₂O

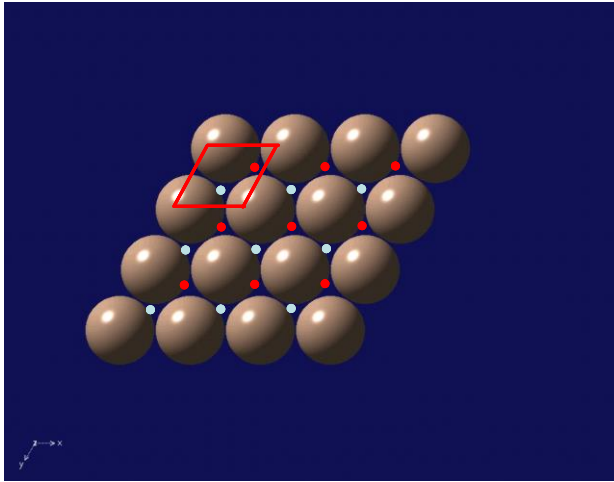




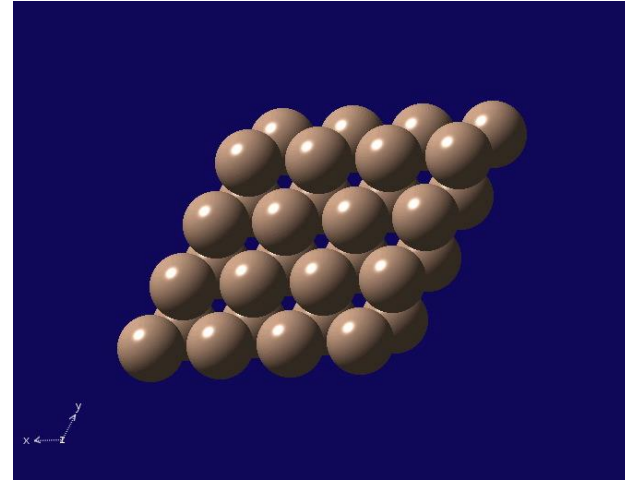
Esquemas de coordinación

Relación R_B/R_A mínima	NC	Geometría		
< 0,155	2	lineal		
0,155	3	triangular		
0,255	4	tetraédrica		
0,414	6	octaédrica		
0,732	8	cúbica		
1,0	12	empaquetamiento compacto		

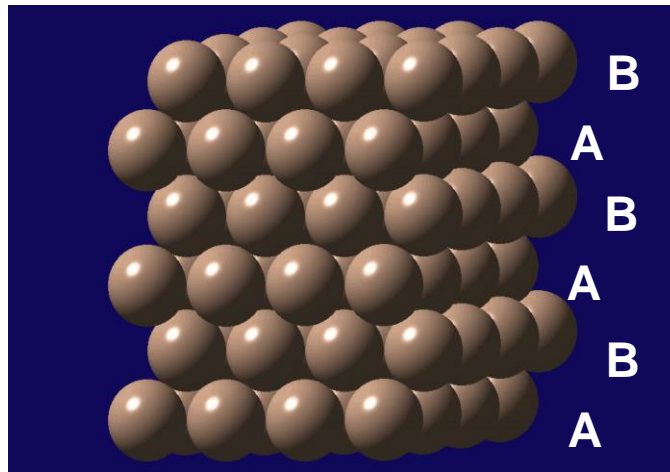
EMPAQUETADOS COMPACTOS



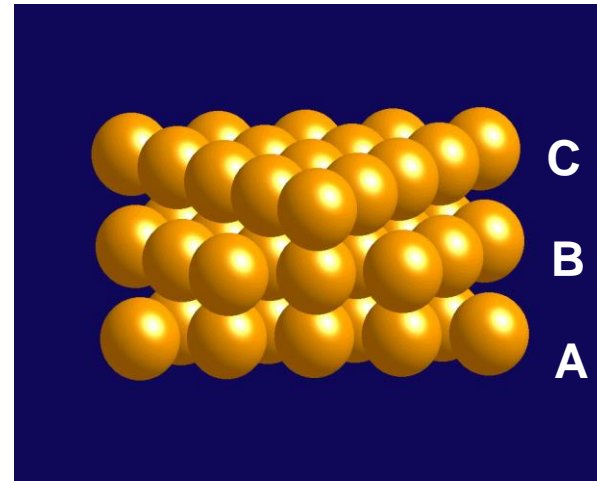
Capa de empaquetamiento hexagonal compacto



Apilamiento de la segunda capa

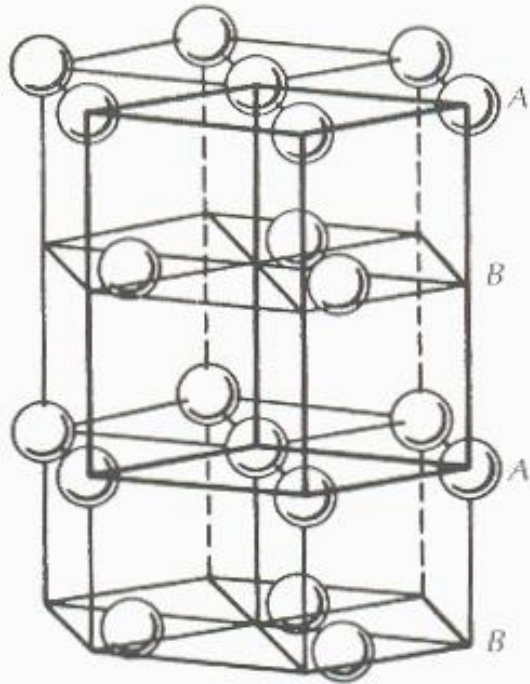


Hexagonal compacto

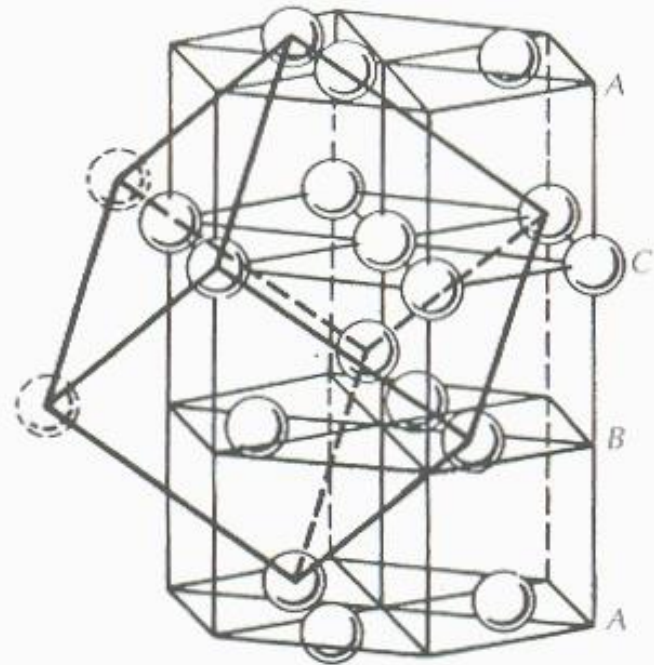


Cúbico compacto

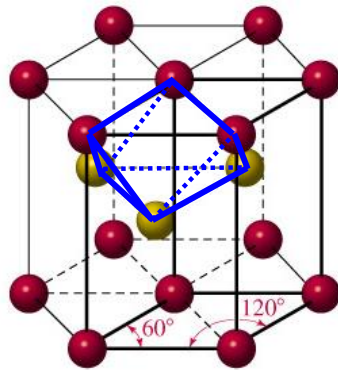
hcp



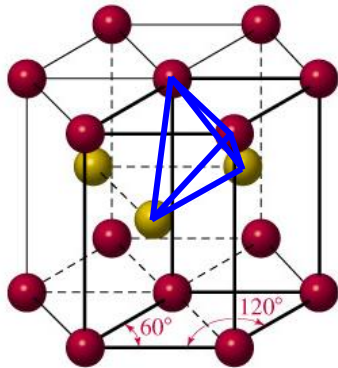
ccp



HCP

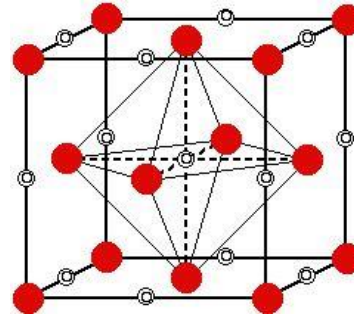


4 posiciones octaédricas

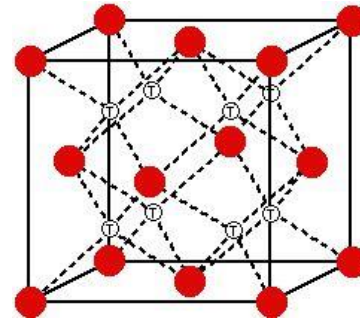


8 posiciones tetraédricas

CCP



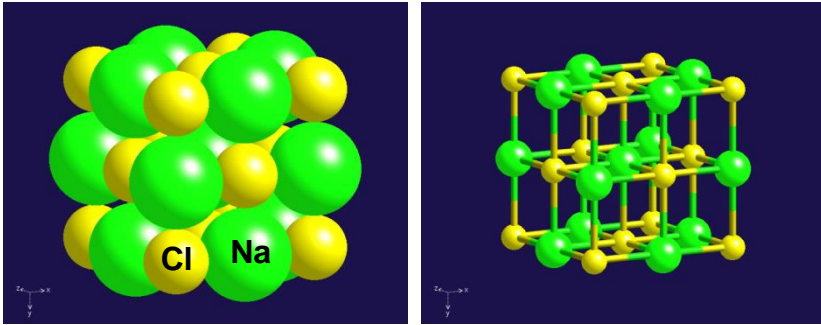
4 posiciones octaédricas



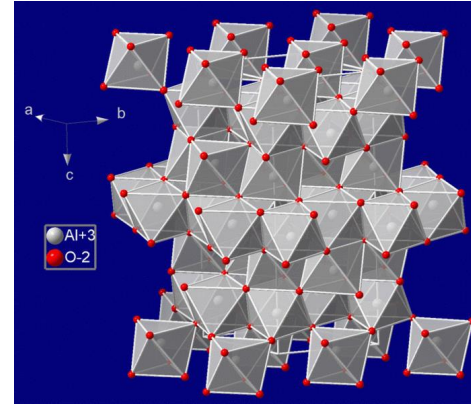
8 posiciones tetraédricas

Huecos octaédricos y tetraédricos en los empaquetados compactos

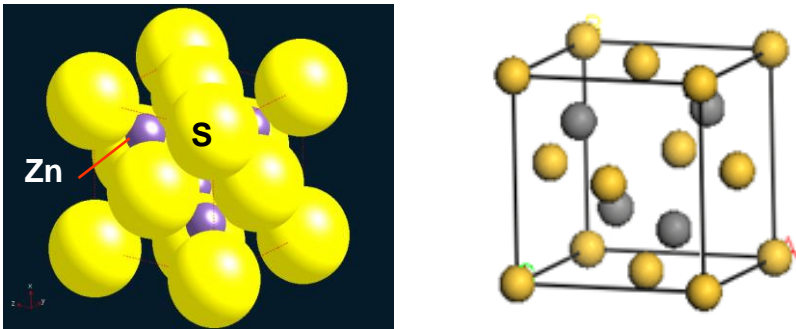
Estructura de la halita (NaCl)



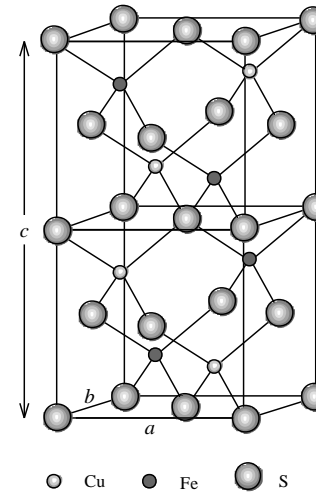
Estructura del corindón (Al_2O_3), el hematites, Fe_2O_3 la ilmenita Fe_2TiO_3



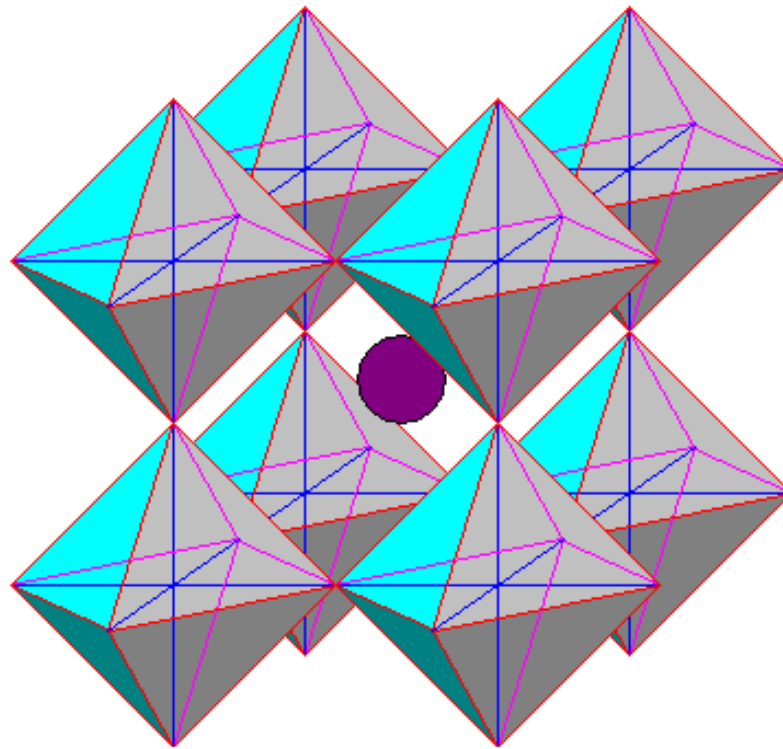
Estructura de la blenda (ZnS)

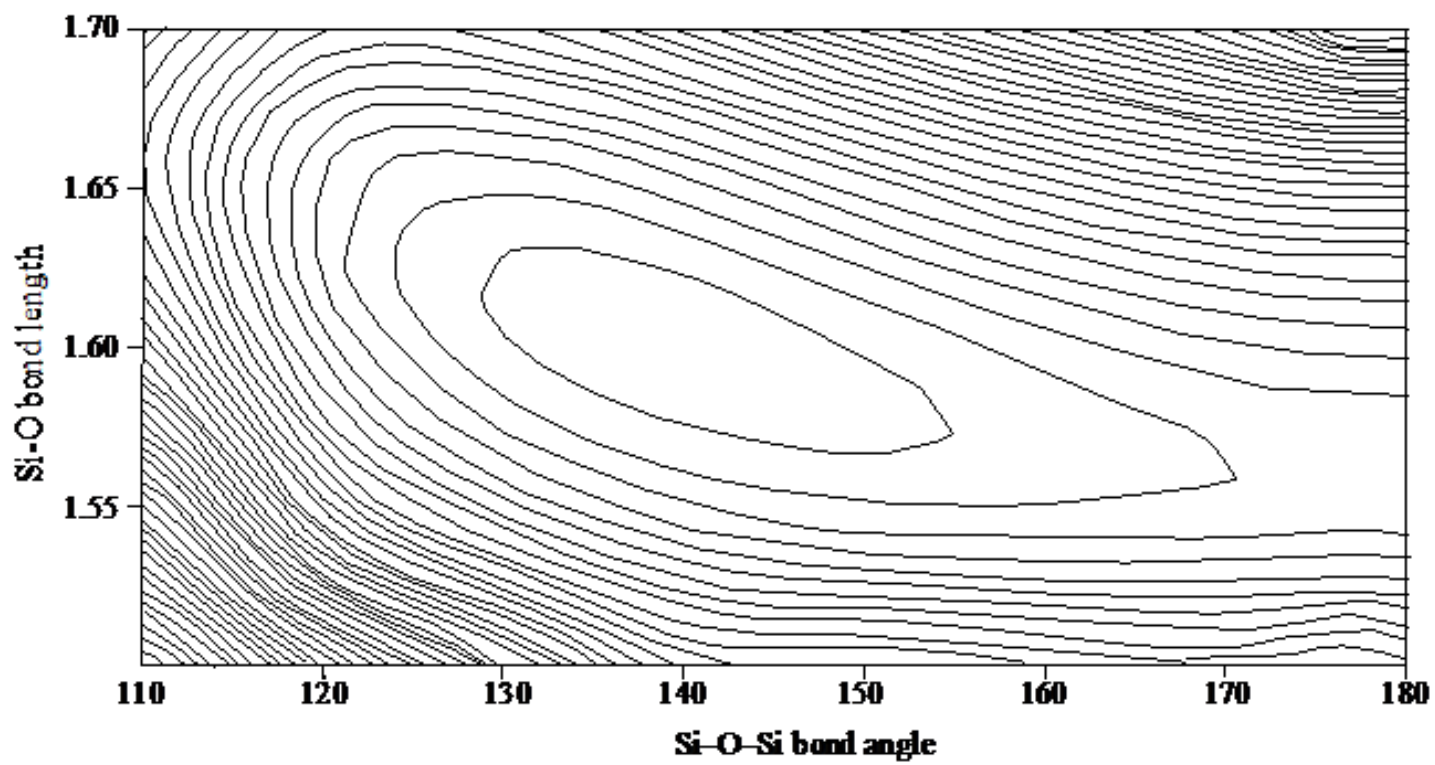
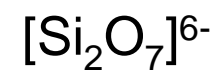
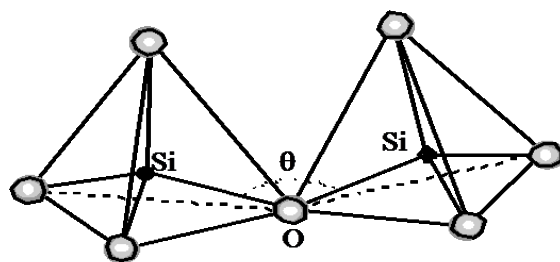


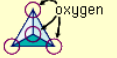
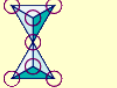
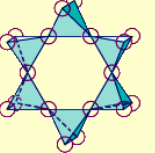
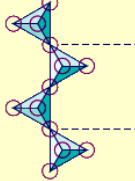
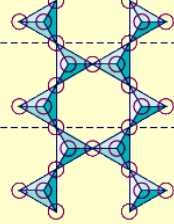
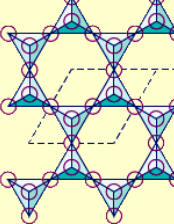
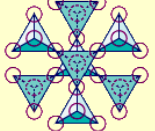
Estructura de la calcopirita (CuFeS)



Estructura de la Perovskita (CaTiO_3)





class	arrangement of SiO ₄ tetrahedrons (central Si ⁴⁺ not shown)	unit composition	mineral example
Nesosilicates		(SiO ₄) ⁴⁻	Olivine, (Mg, Fe) ₂ SiO ₄
Sorosilicates		(Si ₂ O ₇) ⁶⁻	Hemimorphite, Zn ₄ Si ₂ O ₇ (OH) ₂ ·H ₂ O
Cyclosilicates		(Si ₆ O ₁₈) ¹²⁻	Beryl, Be ₃ Al ₂ Si ₆ O ₁₈
Inosilicates (single chain)		(Si ₂ O ₆) ⁴⁻	Pyroxene e.g., enstatite, MgSiO ₃
Inosilicates (double chain)		(Si ₄ O ₁₁) ⁶⁻	Amphibole e.g., anthophyllite, Mg ₇ Si ₈ O ₂₂ (OH) ₂
Phyllosilicates		(Si ₂ O ₅) ²⁻	Mica e.g., phlogopite, KMg ₃ (AlSi ₃ O ₁₀)(OH) ₂
Tectosilicates		(SiO ₂) ⁰	High cristobalite, SiO ₂

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Unidades estructurales del los silicatos

Nesosilicatos: tetraedros SiO₄. Si:O = 1/4

Sorosilicatos: dos tetraedros unidos por un oxígenos. Si:O = 1:3,5

Ciclosilicatos: anillos de varios tetraedros

Inosilicatos:

Piroxenos: Cadenas sencillas de tetraedros. Si:O = 1/3.

Anfíboles: Cadenas dobles de tetraedros. Si:O = 3 y Si:O = 2,5. La relación Si:O total es 1:2,75.

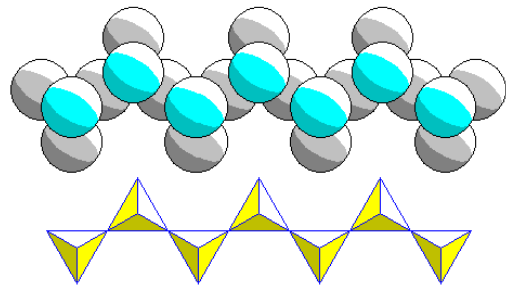
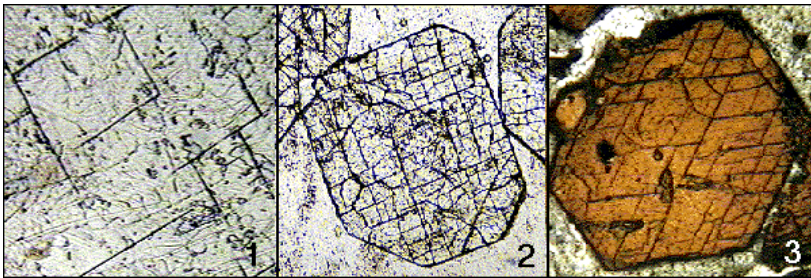
Filosilicatos: láminas con disposición hexagonal de tetraedros Si:O = 1:2,5.

Tectosilicatos: armazones tridimensionales de tetraedros. Si:O = 1/2

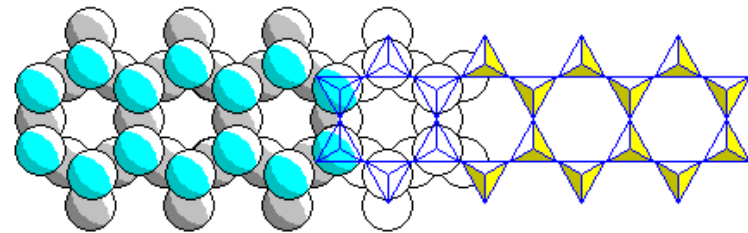
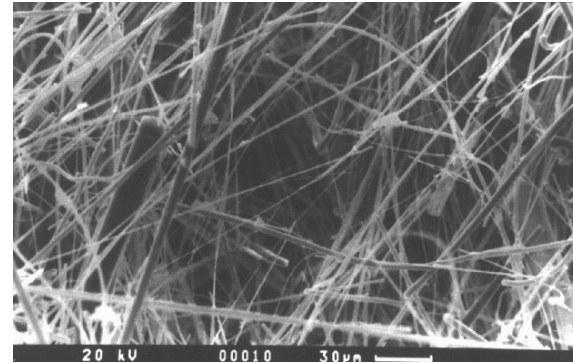
- Los defectos de carga de las unidades estructurales se compensan con la entrada de cationes en las estructuras.

- Las estructura básica de los tectosilicatos no tiene carga. Sin embargo la sustitución de Si⁴⁺ por Al³⁺ genera una carga negativa que se compensa con cationes

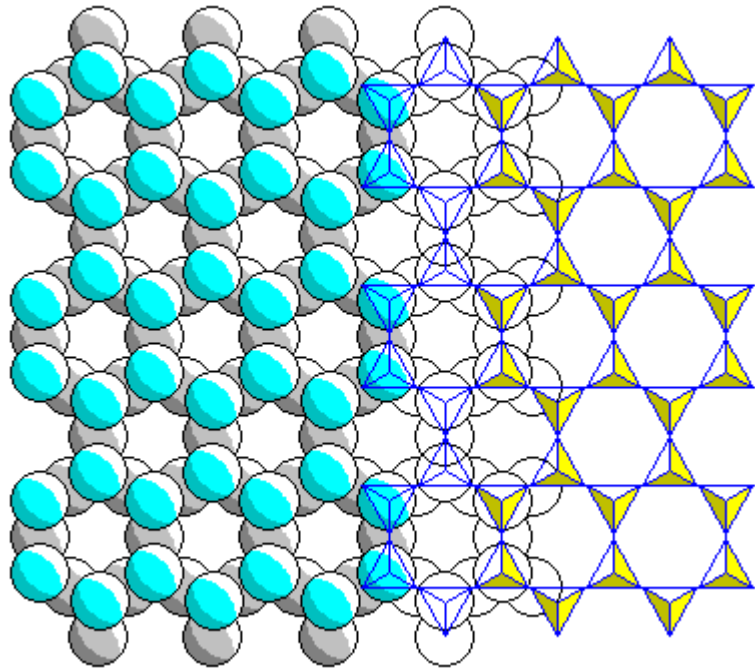
Piroxenos



Anfíboles: asbestos

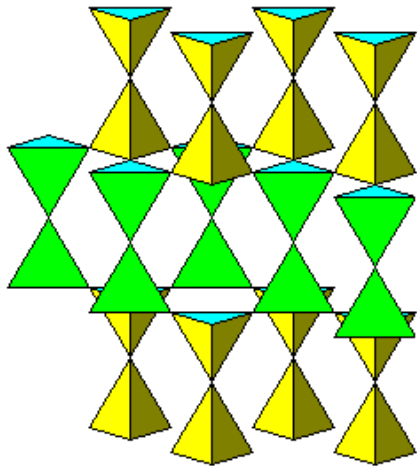


filosilicatos

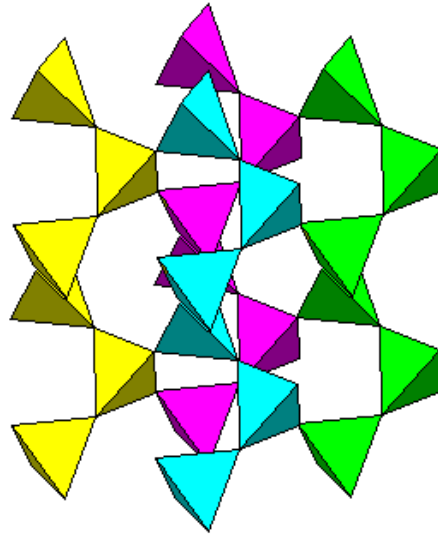


mica

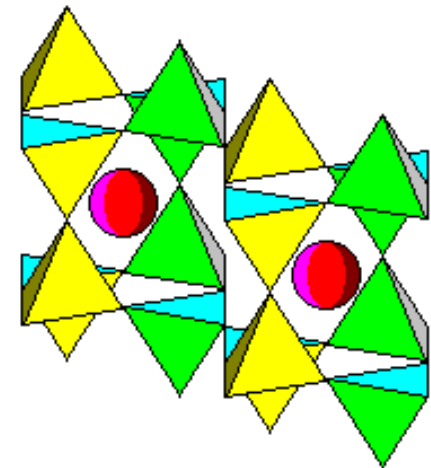
Armazones estructurales tectosilicatos



Tridimita (SiO₂)



Cuarzo (SiO₂)



Feldespatos

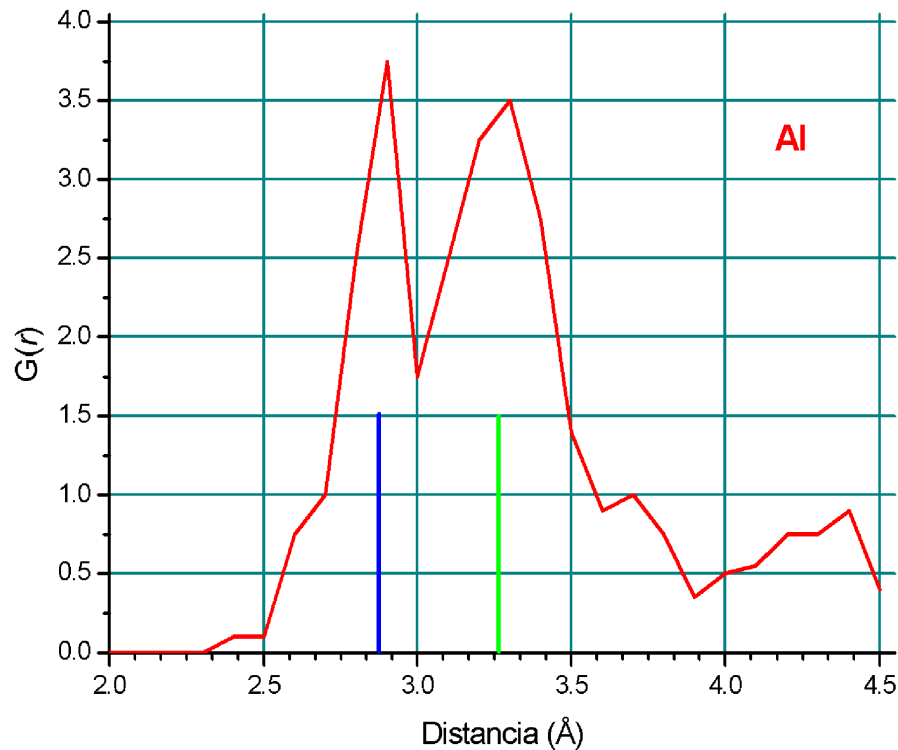
- Feldespatos alcalinos KAlSi_3O_8 - $\text{NaAlSi}_3\text{O}_8$

- Plagioclasas $\text{CaAl}_2\text{Si}_2\text{O}_8$ - $\text{NaAlSi}_3\text{O}_8$

Un modelo cristaloquímico alternativo

Material cedido por el profesor Ángel Vegas

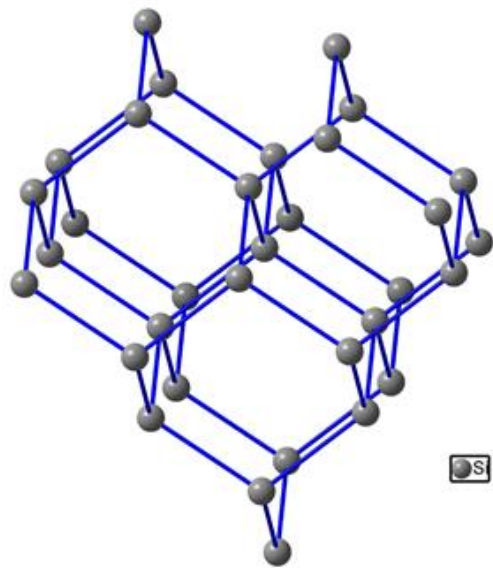
Los óxidos mantienen la topología y las distancias del metal del que provienen



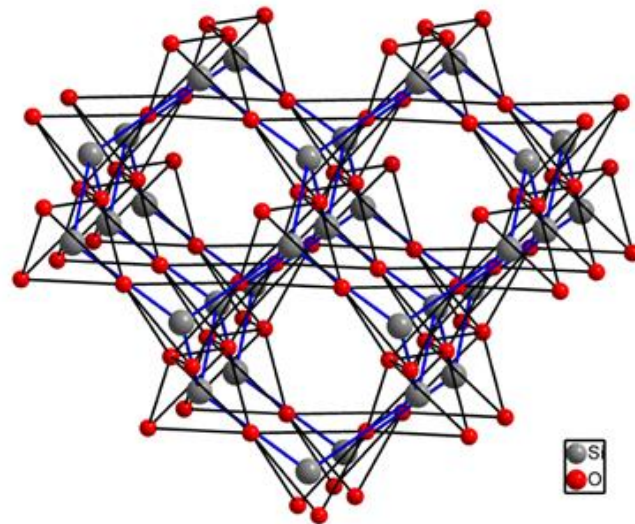
$$fcc-Al, a = 4.04 \text{ \AA}$$
$$d_{Al-Al} = 2.86 \text{ \AA}$$

Alrededor de 2700 compuestos

RAUL ISEA

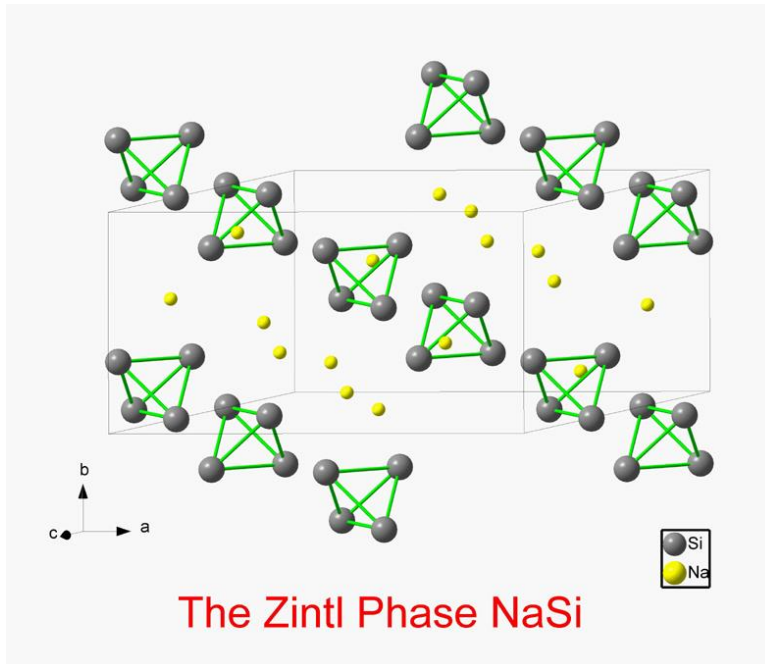


Si

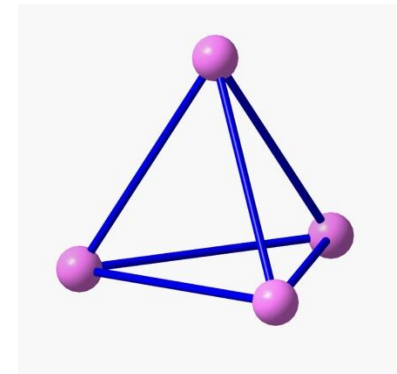


SiO₂ - Cristobalite

El concepto de Zintl-Klemm: Fases de Zintl



NaSi: Si as $\Psi\text{-P}$ (Si_4)⁴⁻

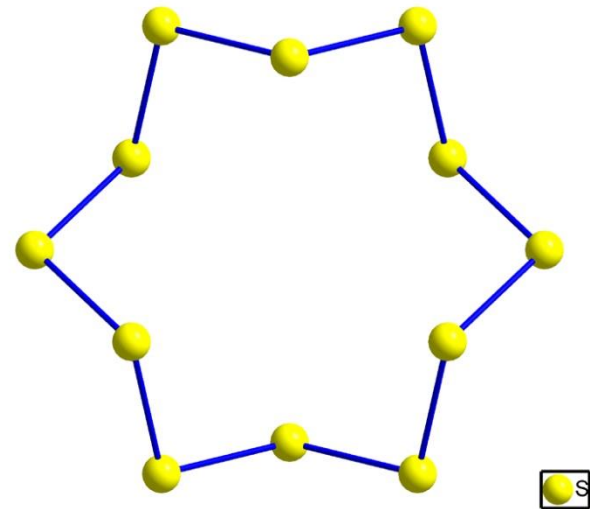
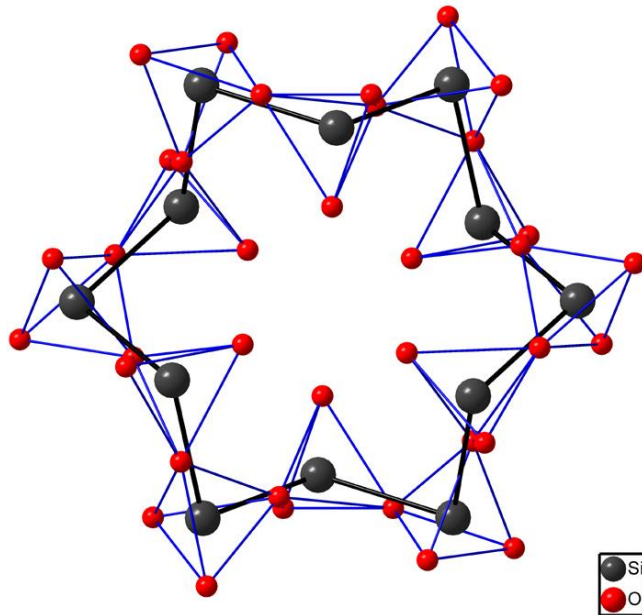


The P_4 molecule

El Si adopta la estructura electrónica del P mediante la donación de electrones del Na al Si. Este pseudo P presenta la estructura del P₄

Aplicación del concepto de Zintl-Klemm a las estructuras de los silicatos

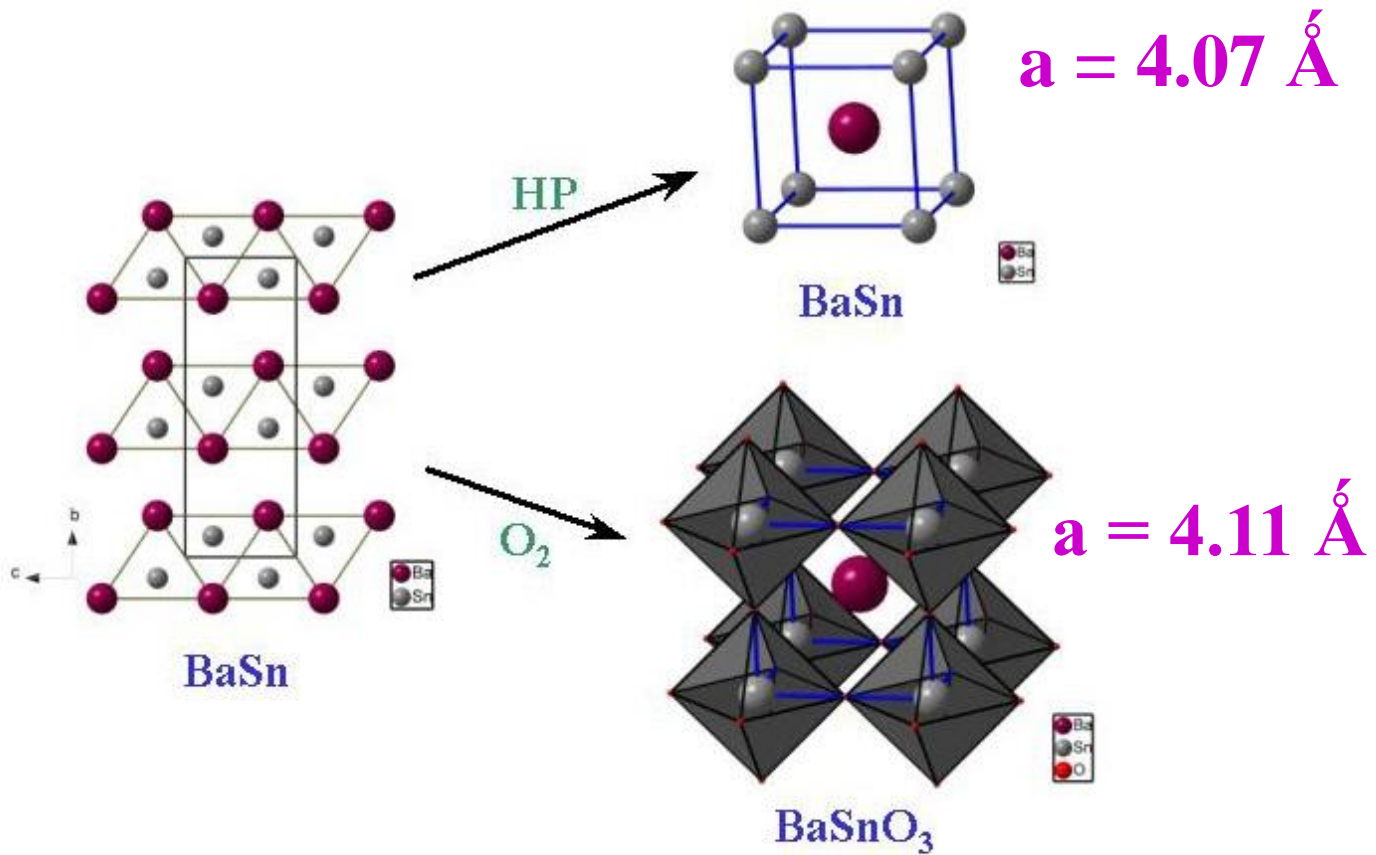
Ejemplo: ciclosilicatos



S_{12}

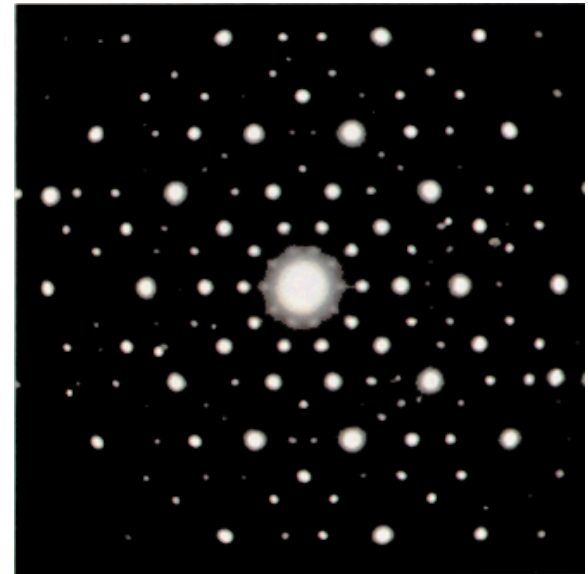
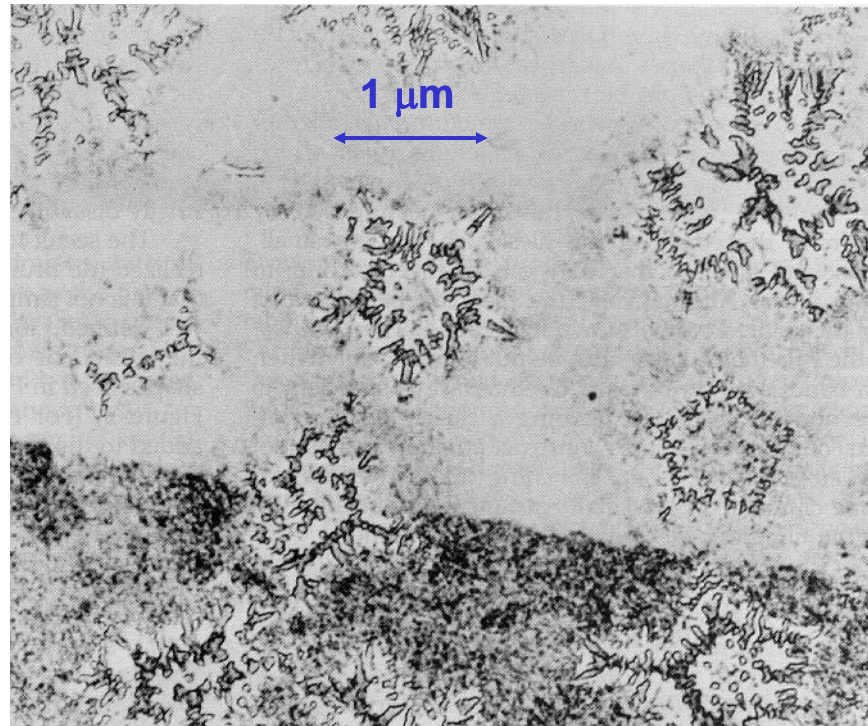
Equivalencia entre oxidación y presión

Beck & Lederer, 1993 → Vegas et al. 1994



CUASICRISTALES

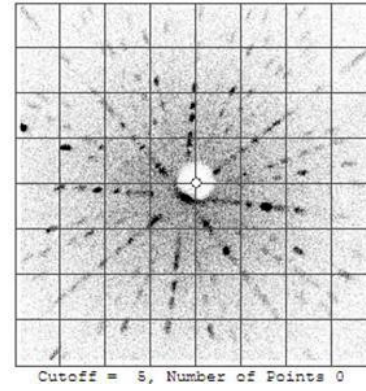
Al_6Mn



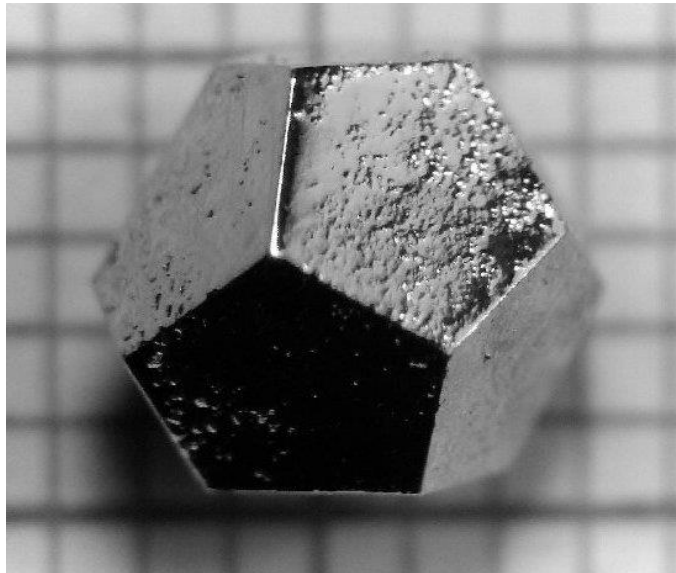
D. Shechtman, I. Blech, D. Gratias, J.W. Cahn (1984)



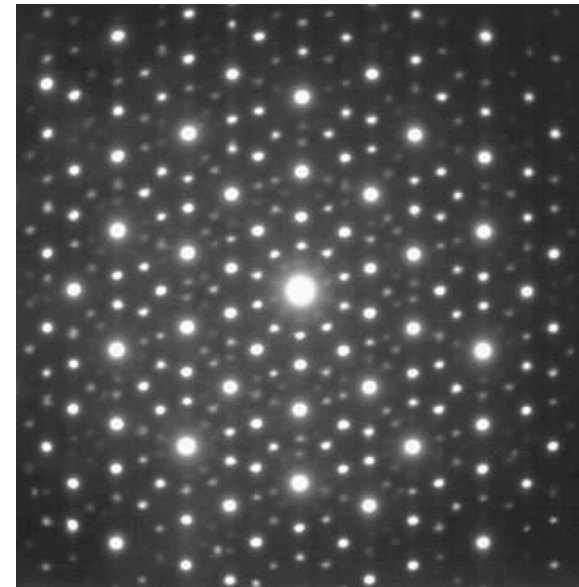
Pirita (FeS_2)



Patrón de difracción de un cristal de pirita



$\text{Zn}_{56.8} \text{Mg}_{34.6} \text{Ho}_{8.7}$



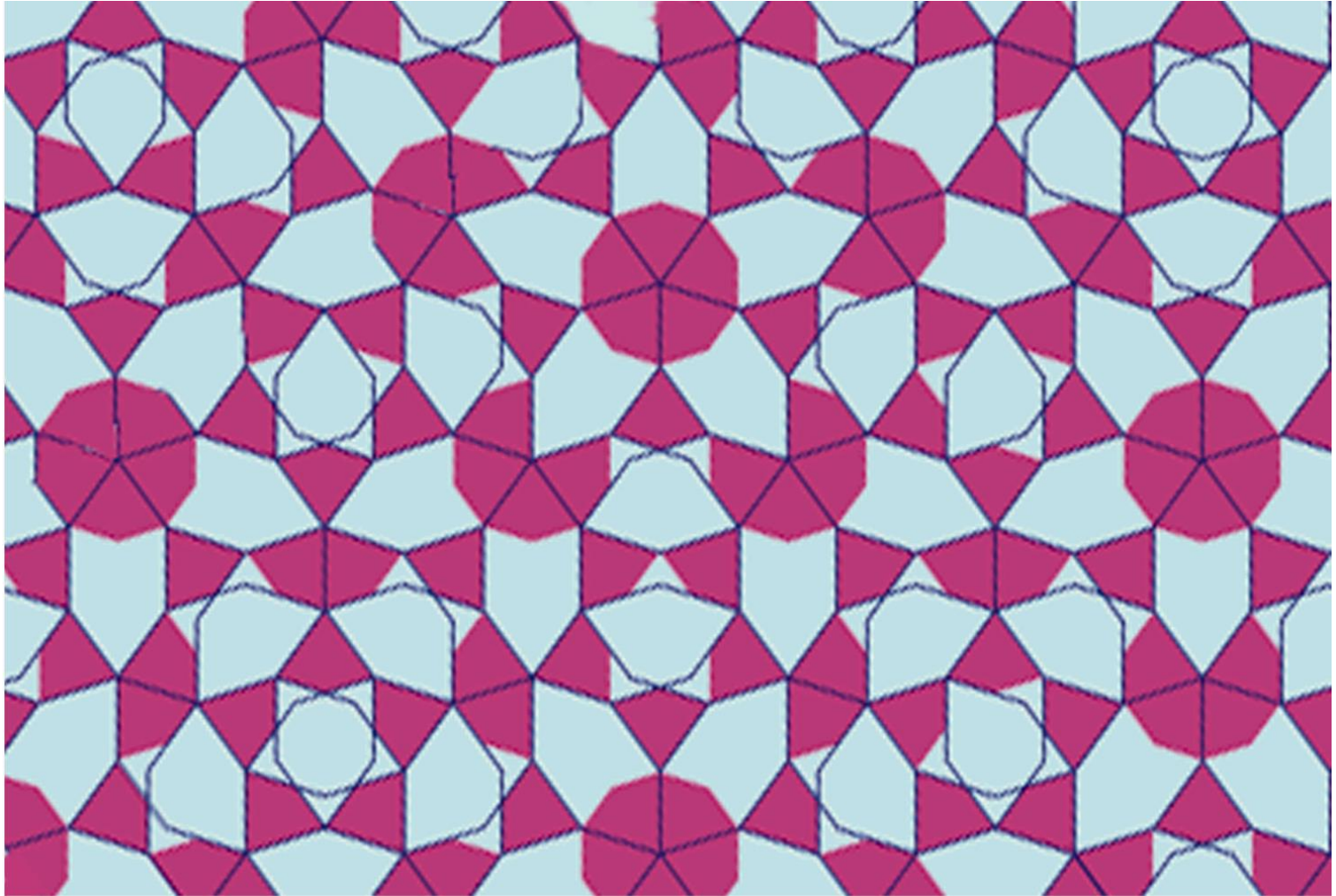
Patrón de difracción de un cristal de HoMgZn

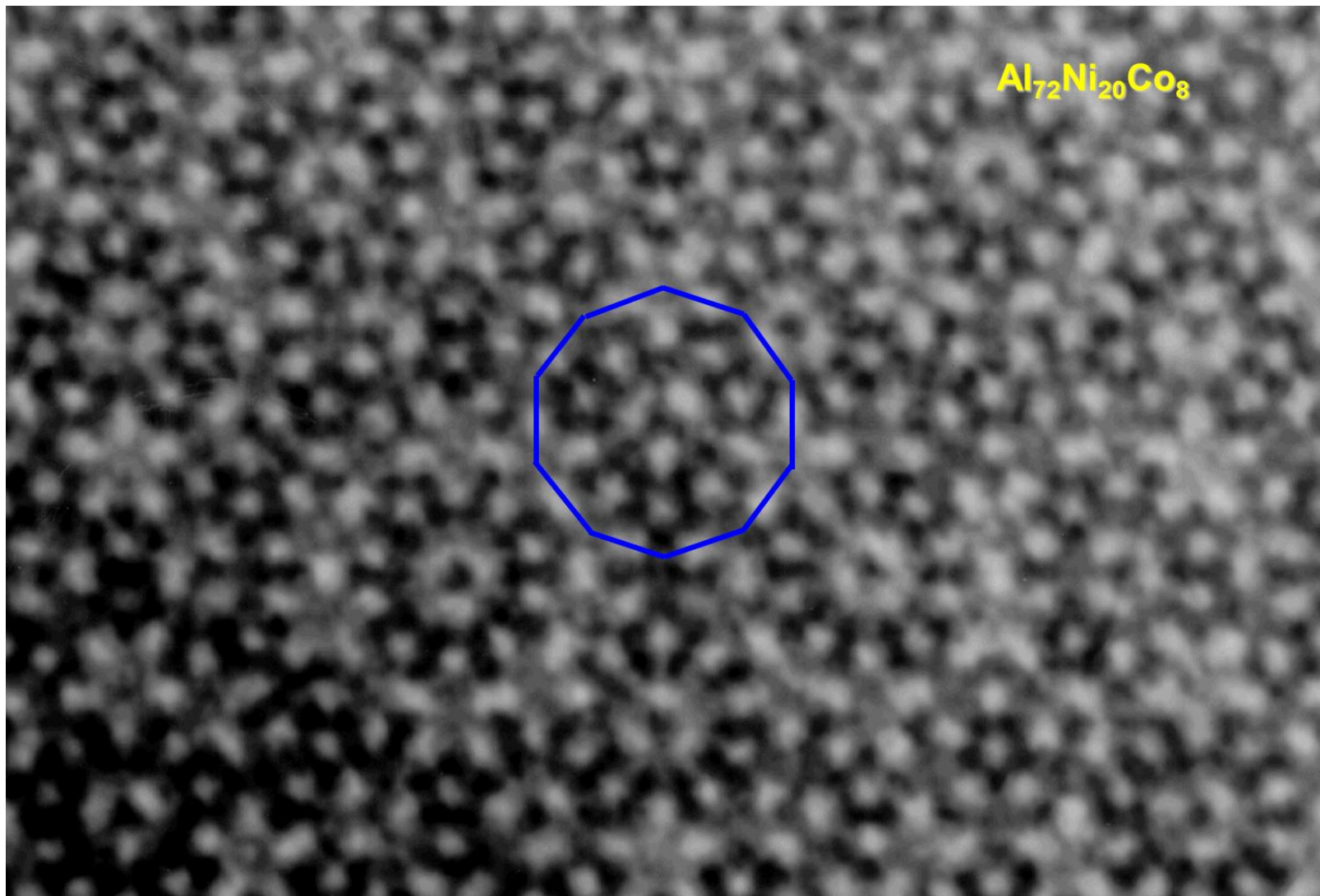
¡ Los cuasicristales no cumplen
la condición $2\cos\alpha = Z!$



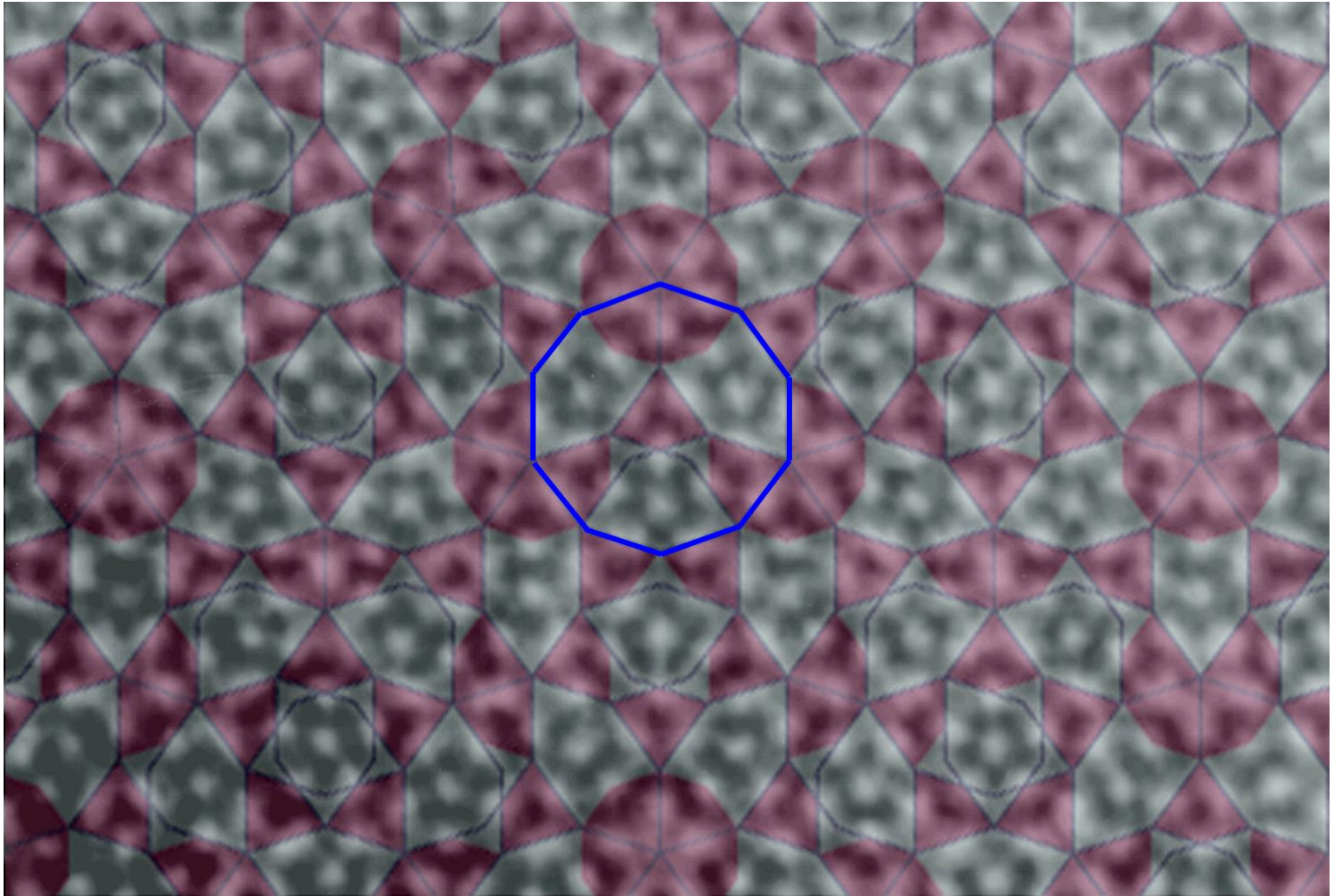
El grito (detalle)
de Edvard Munch

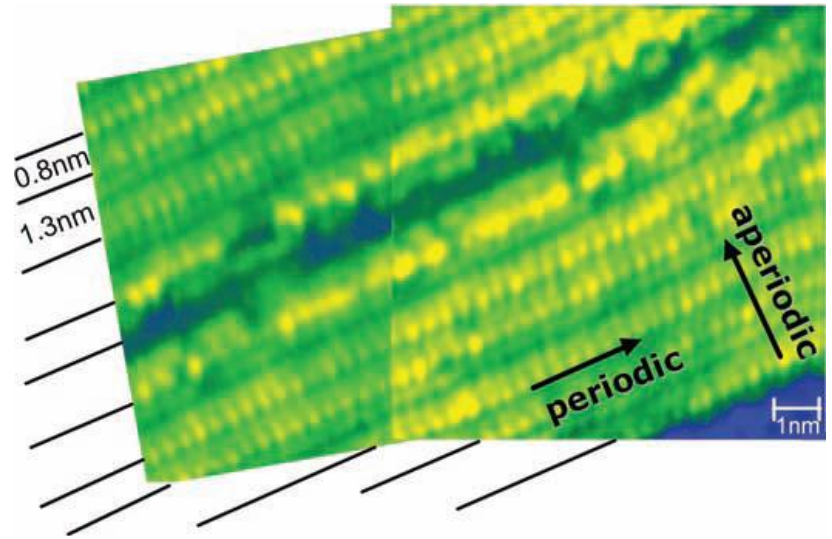
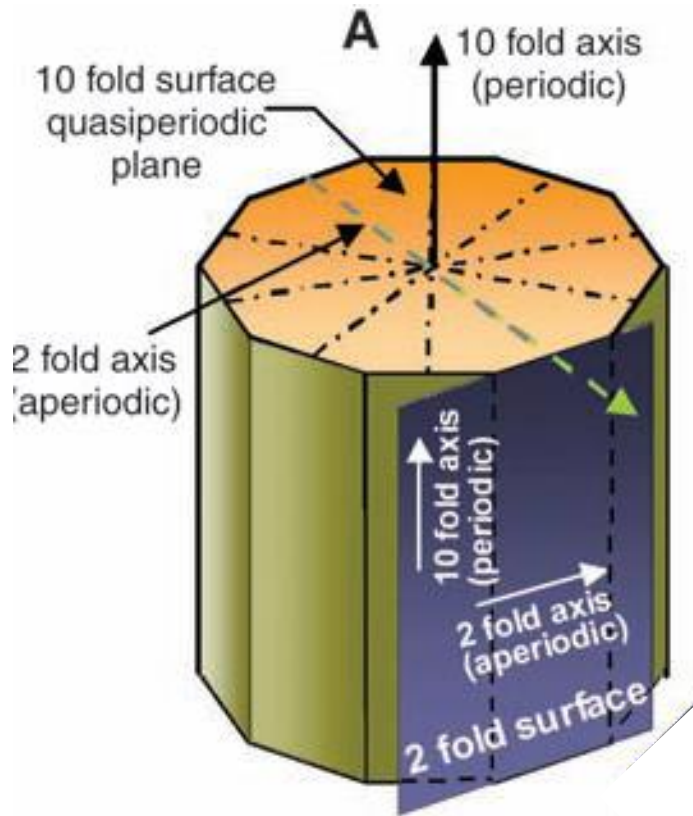
TESELADOS DE PENROSE



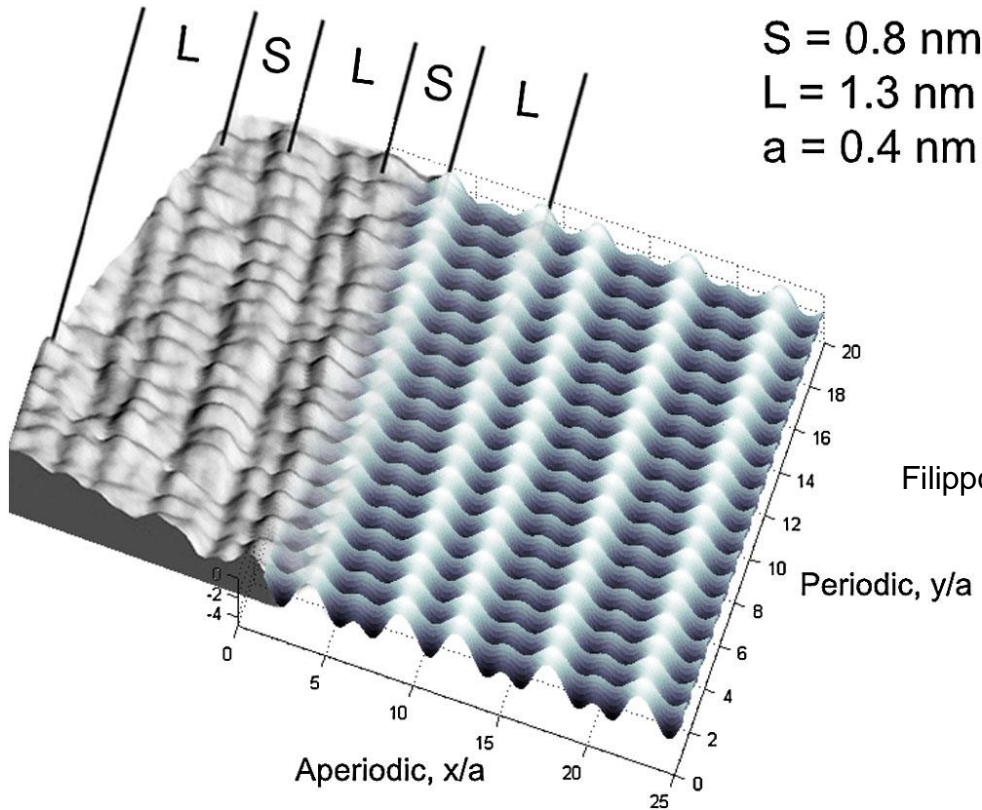


P.J. Steinhardt, H.-C. Jeong, K. Saitoh, M. Tanaka, E. Abe, A.P. Tsai
Nature 396, 55-57 (1998)





Park et al, Science 2005



Filippov et al PRL 2010

SLLSLLSLSLLSLLSLSLLSLSL

Secuencia de Fibonacci

- S
- L
- LS
- LSL
- LSLLS
- LSLLSLSL
- LSLLSLSLLSLLSLSLLSLSL



Nobelpriset 2011

The Nobel Prize in Chemistry 2011



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VETENSKAPS-
AKADEMIEN

THE ROYAL SWEDISH ACADEMY OF SCIENCES



Daniel Shechtman

Technion – Israel Institute of Technology,
Haifa, Israel

"för upptäckten av kvasikrystaller"
"for the discovery of quasicrystals"

Cybernox Collection



**A commercial application:
Cookware with Quasicrystal Coating
(nearly as slippery as Teflon)**