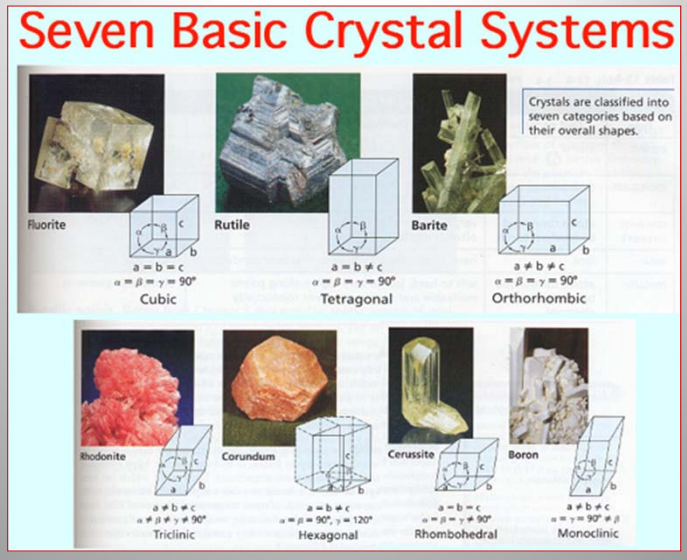
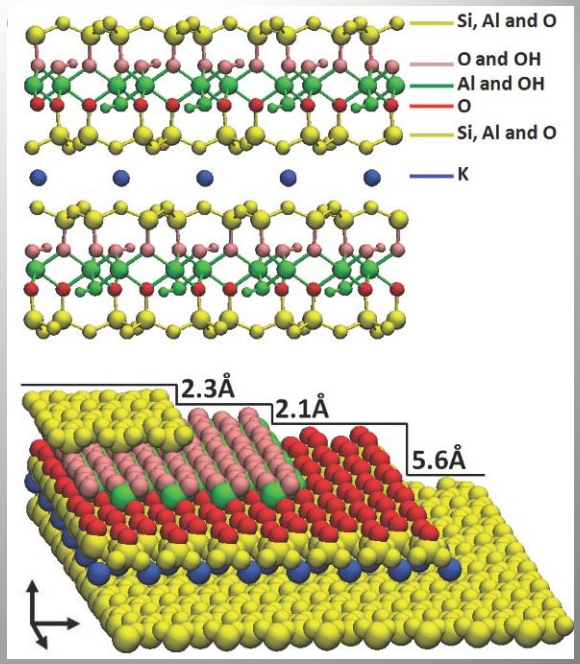


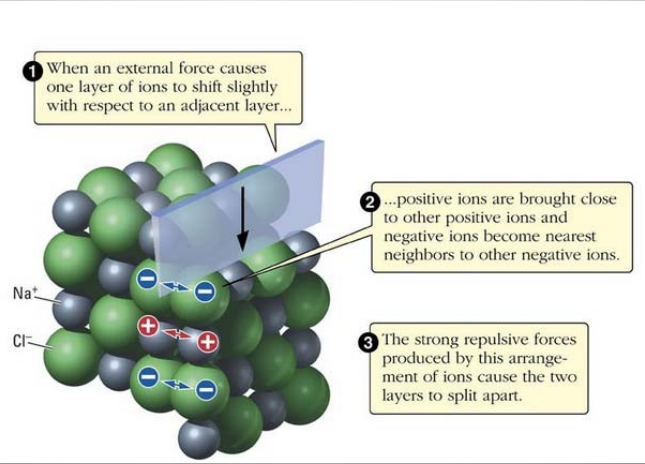
PHYS485
Materials Physics

Dr. Gregory W. Clark
Manchester University

- **$K(Al,Cr,Mn)_3Si_3O_{10}(OH)_2$**
- Muscovite mica: weak *Van der Waal's bonding* along certain crystallographic planes



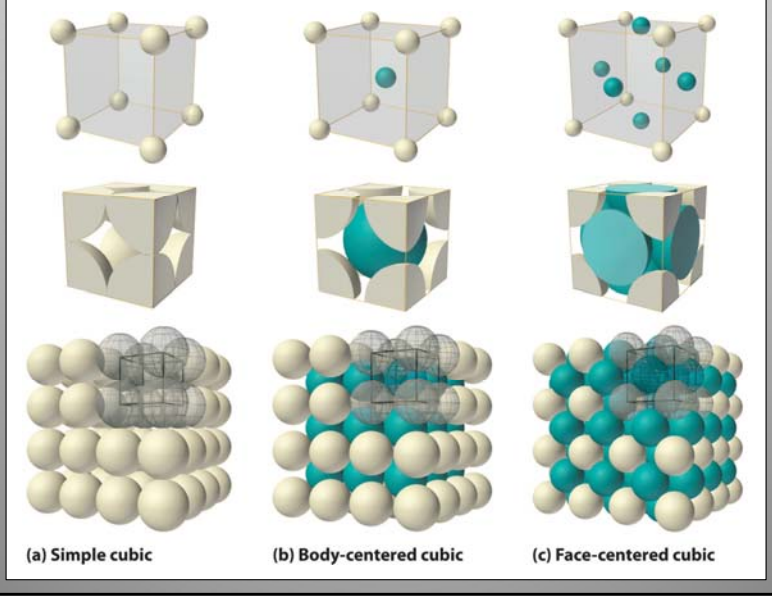
- **NaCl**
- Halite: *strong ionic bonding*, but cleaves easily along certain crystallographic planes

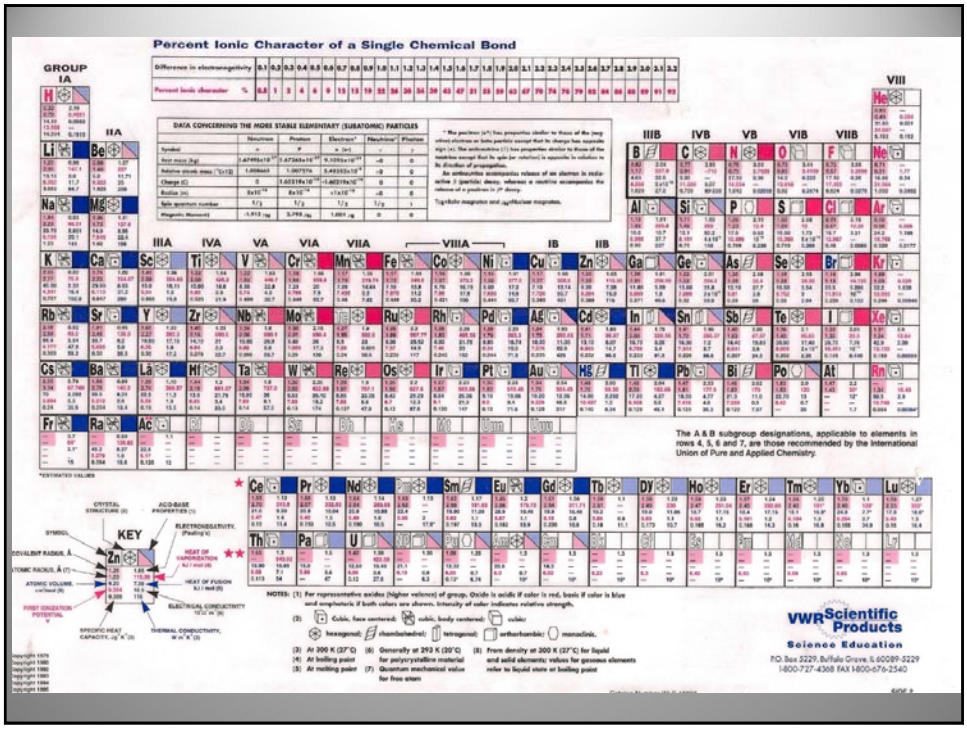


Atomium in Brussels, Belgium

Fe structure, BCC – magnified 165 billion times; Expo 1958.

Cubic lattices





Cubic Lattices: densities

(a = lattice parameter)

nearest neighbors

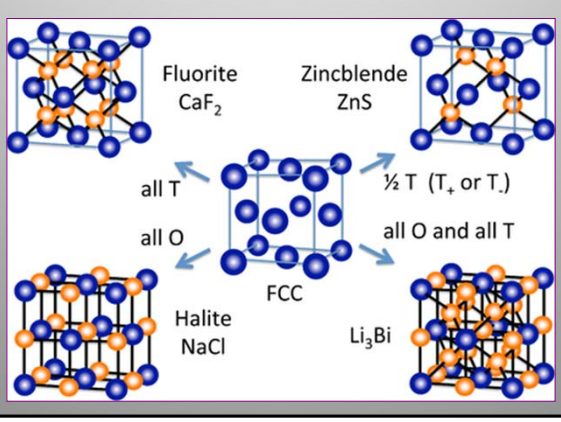
- Atomic densities:
  - SC: $\rho_{atm} = 1/a^3$
  - BCC: $\rho_{atm} = 2/a^3$
  - FCC: $\rho_{atm} = 4/a^3$
- Coordination number:
  - SC: 6
  - BCC: 8
  - FCC: 12
- Mass densities:
  - SC: $\rho = 1\ M/a^3$
  - BCC: $\rho = 2\ M/a^3$
  - FCC: $\rho = 4\ M/a^3$
- Atomic radii (close packing):
  - SC: $r = a/2$
  - BCC: $r = \sqrt{3}\ a\ /\ 4$
  - FCC: $r = \sqrt{2}\ a\ /\ 2$

Packing fraction: SC = 0.52, BCC = 0.68, FCC = 0.74
[pf = *(V of atoms)/(total V)*]

http://ocw.tudelft.nl/fileadmin/ocw/courses/SolidStatePhysics/res00020/ch1_1.swf

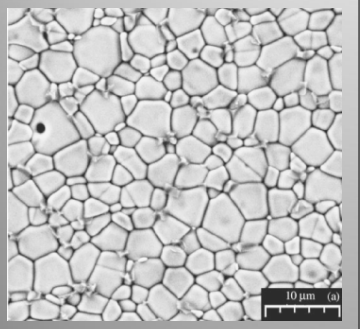
Some variations on the cubic lattices:

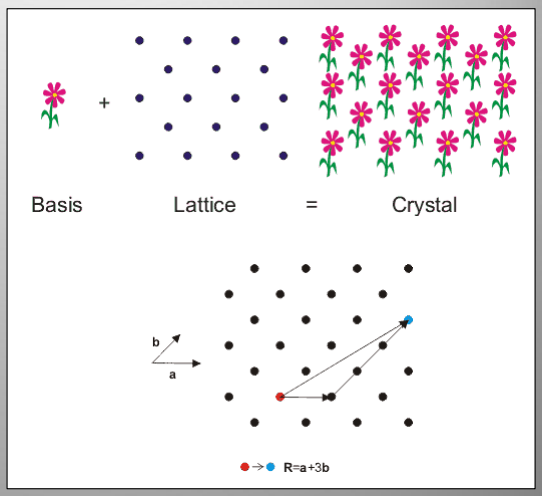
- NaCl structure (FCC-like)
- CaCl structure (BCC-like)
- ZnS [zinc blende] structure (FCC-like)
- Diamond (FCC-like)
- CaF_2 [fluorite] structure (FCC-like)



Crystals

- A **basis** is the "building block" of a crystal
- Basis + Bravais lattice = crystal





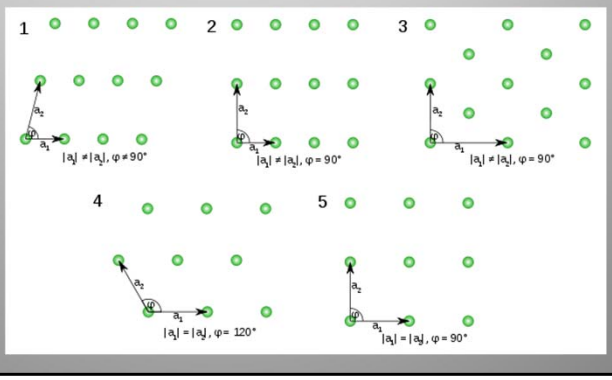
Wallpaper patterns as crystals

Find the lattice and basis of these two wallpaper patterns. What symmetries do the patterns have?

http://www.phys.psu.edu/~ralbert/phys412/chapter1.pdf

Bravais Lattices

- An infinite array of points, determined by lattice vectors, $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ such that all n_i are integers and all the a_i are primitive vectors
- In 2-D

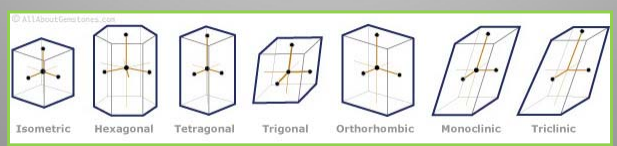


- **# possible different shapes of unit cell?**

We must be able to fill all space by translational symmetry, with no gaps.

We get 7 crystal systems:

System	Lattice Parameters	
Cubic/Isometric	$a = b = c$	$\alpha = \beta = \gamma = 90°$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
Rhombohedral/Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$
Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90°, \gamma \neq 90°$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$



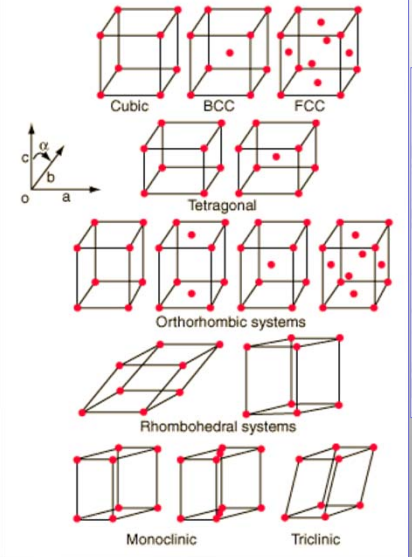
a, b, c represent lengths of lattice vectors
α, β, γ represent angles between lattice vectors

- **Bravais Lattices**

Every lattice point must have the same environment. These don't have to be just at the corner of the cell. Variations possible on the seven crystal systems:

Symbol	Name	Lattice points / cell
P	**primitive** ('corners only')	1
I	**body-centered** ('corner + cube-centre')	2
F	**face-centred** ('centre of all faces + corner')	4
C	**base-centred** ('centre of one face + corners')	2

Bravais Lattices – 3D



The Fourteen Bravais Lattices

The ways in which we can specify the lattice points in space and keep translational symmetry is limited. In 1848, Auguste Bravais demonstrated that there are in fact only fourteen possible point lattices and no more. For his efforts, the term Bravais lattice is often used in place of point lattice.

System	Number of Lattices	Lattice Symbol	Restriction on crystal cell angle
Cubic	3	P or sc, I or bcc, F or fcc	a=b=c α =β =γ=90°
Tetragonal	2	P, I	a=b≠c α=β =γ=90°
Orthorhombic	4	P, C, I, F	a≠b≠ c α=β =γ=90°
Monoclinic	2	P, C	a≠b≠ c α=β=90 °≠β
Triclinic	1	P	a≠b≠ c α≠β≠γ
Trigonal	1	R	a=b=c α=β =γ <120° ,≠90°
Hexagonal	1	P	a=b≠c α =β =90° γ=120°

Table 1. Seven crystal systems make up fourteen Bravais lattice types in three dimensions.

P - Primitive: simple unit cell
F - Face-centred: additional point in the centre of each face
I - Body-centred: additional point in the centre of the cell
C - Centred: additional point in the centre of each end
R - Rhombohedral: Hexagonal class only

Bravais Lattices

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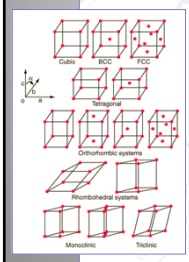

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Tetragonal	2	P, I	a=b≠c α=β =γ=90°
Orthorhombic	4	P, C, I, F	a≠b≠ c α=β =γ=90°
Monoclinic	2	F, C	a≠b≠ c α=β=90 °≠β
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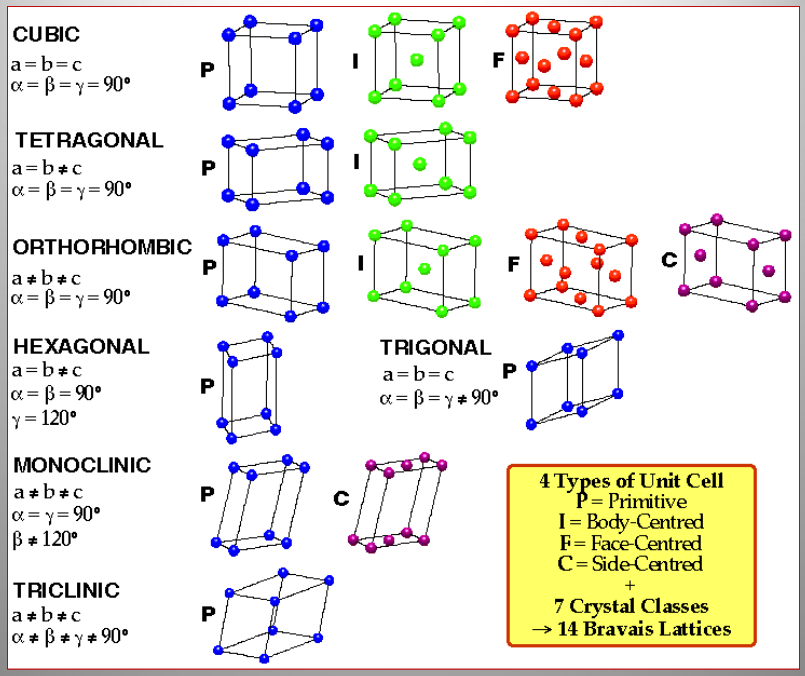
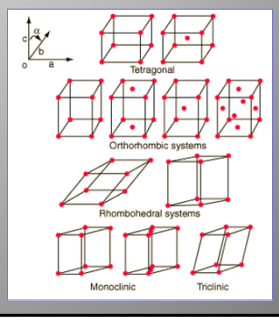
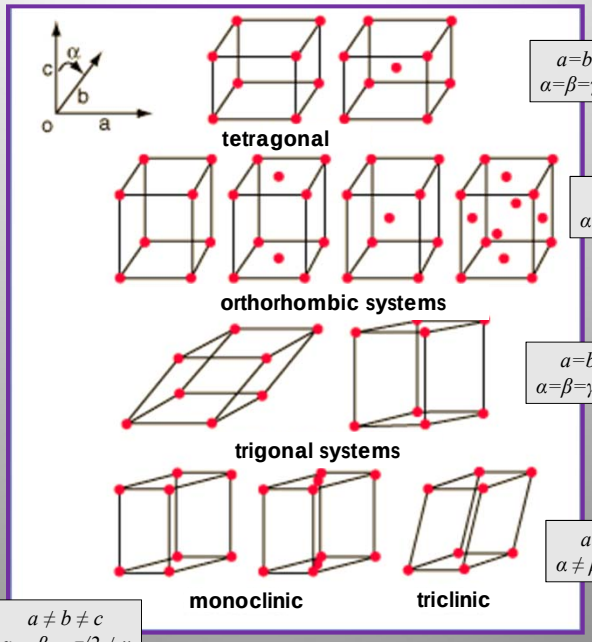


The non-cubic structures

- tetragonal (square, rectangular prism) $a=b\neq c$ $\alpha=\beta=\gamma=\pi/2$
  - *e.g.* white tin (β tin), In; minerals: zircon & rutile
- orthorhombic (rectangular, rectangular prism) $a\neq b\neq c$ $\alpha=\beta=\gamma=\pi/2$
  - *e.g.*, Ga, S, Cl (113K), Br (123K); minerals: barite, aragonite
- trigonal (diagonally stretched cube) $a=b=c$ $\alpha=\beta=\gamma\neq\pi/2$
  - *e.g.*, Hg, Sb, Bi, SM, As;
  - minerals: rose, smoky & amethyst quartz
- triclinic $a\neq b\neq c$ $\alpha\neq\beta\neq\gamma\neq\pi/2$
  - *e.g.*, minerals: turquoise, axinite
- monoclinic (top & faces) $a\neq b\neq c$ $\alpha=\beta=\pi/2\neq\gamma$
  - *e.g.*, minerals: azurite, orthoclase, gypsum



The non-cubic structures



$a=b\neq c$ $\alpha=\beta=\gamma=\pi/2$

$a\neq b\neq c$ $\alpha=\beta=\gamma=\pi/2$

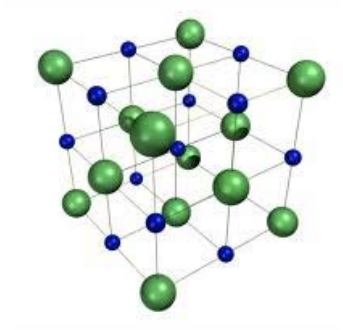
$a=b=c$ $\alpha=\beta=\gamma\neq\pi/2$

$a\neq b\neq c$ $\alpha\neq\beta\neq\gamma\neq\pi/2$

$a\neq b\neq c$ $\alpha=\beta=\pi/2\neq\gamma$

NaCl Structure

- Most alkali halides (group 1)
- Most oxides alkaline earths (group 2)
- Many nitrides, carbides, hydrides (*e.g.* ZrN, TiC, NaH)



Lattice + basis?
What Bravais lattice?
What basis?

http://www.phys.psu.edu/~ralbert/phys412/chapter1.pdf