

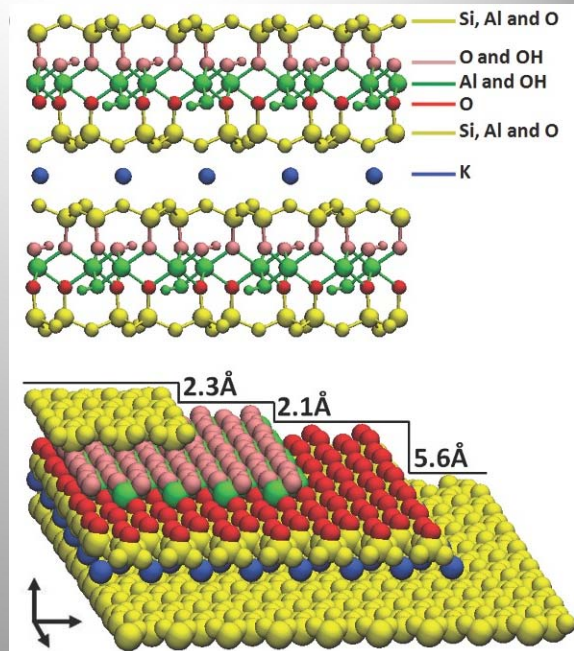
## Seven Basic Crystal Systems



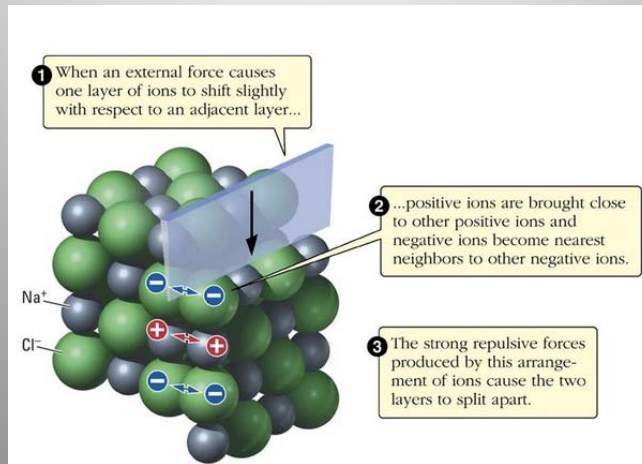
PHYS485  
**Materials Physics**

Dr. Gregory W. Clark  
 Manchester University

- $\text{K}(\text{Al}, \text{Cr}, \text{Mn})_3\text{Si}_3\text{O}_{10}(\text{OH})_2$
- Muscovite mica:  
 weak *Van der Waal's* bonding  
 along certain  
 crystallographic  
 planes



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

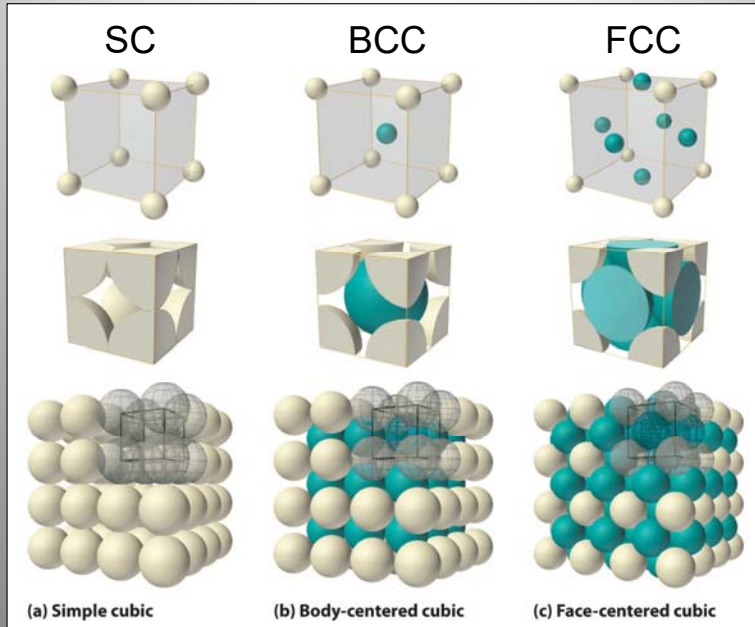


### Atomium in Brussels, Belgium



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

# Cubic lattices



**Percent Ionic Character of a Single Chemical Bond**

Difference in electronegativity	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	
Percent ionic character, %	1.1	1.3	1.6	2.0	2.5	3.1	3.8	4.6	5.5	6.5	7.7	9.0	10.5	12.1	13.8	15.6	17.5	19.5	21.6	23.8	26.1	28.5	31.0	33.6	36.3	39.1	42.0	45.0	48.1	51.3	54.6	58.0	61.5

**DATA CONCERNING THE MORE STABLE ELEMENTARY (SUBATOMIC) PARTICLES**

Symbol	Masses	Protons	Electrons	Neutrons	Charge
Atom (mass)	$1.6746 \times 10^{-27}$ kg	1	1	1	0
Electron (mass)	$9.10938 \times 10^{-31}$ kg	0	1	0	-1.602176634 × 10 <sup>-19</sup> C
Neutron (mass)	$1.67493 \times 10^{-27}$ kg	0	0	1	0
Photon (mass)	0	0	0	0	0
Alpha particle	$6.64465 \times 10^{-27}$ kg	2	2	2	0
Deuteron	$3.34358 \times 10^{-27}$ kg	1	1	1	0
Proton	$1.67262 \times 10^{-27}$ kg	1	1	0	0

**PERIODIC TABLE**

The periodic table below shows the A and B subgroup designations for elements in rows 4, 5, 6, and 7. The designations are color-coded: red for s-block, blue for d-block, green for p-block, and purple for f-block.

**KEY**

- CRYSTAL STRUCTURE (SC, BCC, FCC, etc.)
- ADDRESS (Group, Period)
- ELECTRONEGATIVITY (Pauling's)
- HEAT OF VAPORIZATION (kJ/mol)
- HEAT OF FUSION (kJ/mol)
- HEAT OF VAPORIZATION (kJ/mol)
- ATOMIC VOLUME (cm<sup>3</sup>/mol)
- IONIZATION POTENTIAL (eV)
- ELECTRICAL CONDUCTIVITY (10<sup>6</sup> Ω<sup>-1</sup>m<sup>-1</sup>)
- THERMAL CONDUCTIVITY (W/m·K)
- SPECIFIC HEAT CAPACITY (J/kg·K)

**NOTES:**

- (1) For representative oxides (higher valence) of groups 13-16, color is white if color is red, black if color is blue and semitransparent if both colors are shown. Intensity of color indicates relative strength.
- (2) Cubic, face centered;  $\frac{\sqrt{2}}{2}$  cubic, body centered; cubic
- (3) Hexagonal;  $\frac{\sqrt{3}}{2}$  hexagonal; orthorhombic; monoclinic
- (4) At 300 K (27°C)
- (5) Generality at 293 K (20°C)
- (6) From density at 300 K (27°C) for liquid and solid elements; values for gaseous elements refer to liquid state at boiling point
- (7) Quantum mechanical value for free atom

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## Cubic Lattices: densities

( $a$  = lattice parameter)

# nearest neighbors

- **Atomic densities:**

➤ SC:  $\rho_{atm} = 1/a^3$

➤ BCC:  $\rho_{atm} = 2/a^3$

➤ FCC:  $\rho_{atm} = 4/a^3$

- **Mass densities:**

➤ SC:  $\rho = 1 M/a^3$

➤ BCC:  $\rho = 2 M/a^3$

➤ FCC:  $\rho = 4 M/a^3$

- **Coordination number:**

➤ SC: 6

➤ BCC: 8

➤ FCC: 12

- **Atomic radii** (close packing):

➤ SC:  $r = a/2$

➤ BCC:  $r = \sqrt{3} a / 4$

➤ FCC:  $r = \sqrt{2} a / 2$

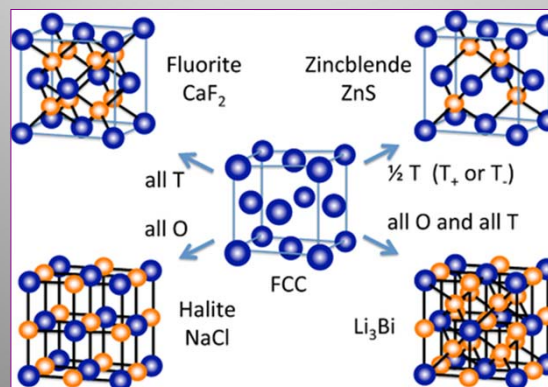
**Packing fraction:** SC = 0.52, BCC = 0.68, FCC = 0.74

[pf = (V of atoms)/(total V)]

[http://ocw.tudelft.nl/fileadmin/ocw/courses/SolidStatePhysics/res00020/ch1\\_1.swf](http://ocw.tudelft.nl/fileadmin/ocw/courses/SolidStatePhysics/res00020/ch1_1.swf)

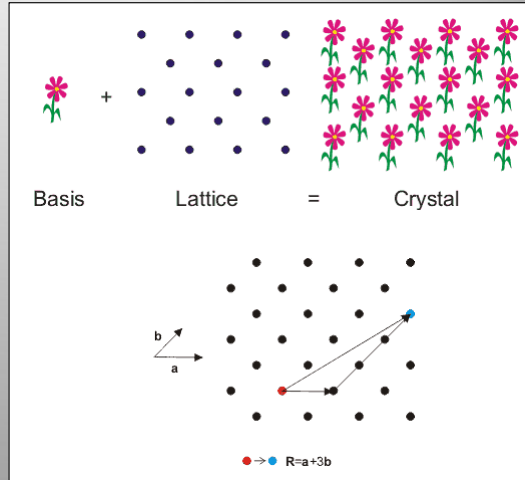
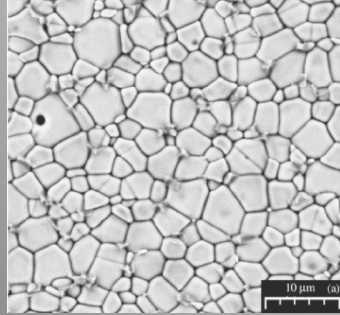
## Some variations on the cubic lattices:

- NaCl structure (FCC-like)
- CaCl structure (BCC-like)
- ZnS [zinc blende] structure (FCC-like)
- Diamond (FCC-like)
- CaF<sub>2</sub> [fluorite] structure (FCC-like)



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

## Crystals



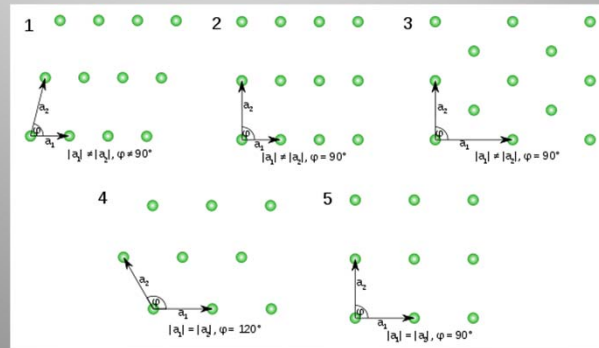
### Wallpaper patterns as crystals



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

## 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

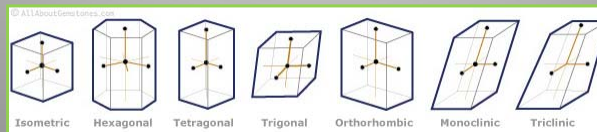


### # possible different shapes of unit cell?

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

We get 7 crystal systems:

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



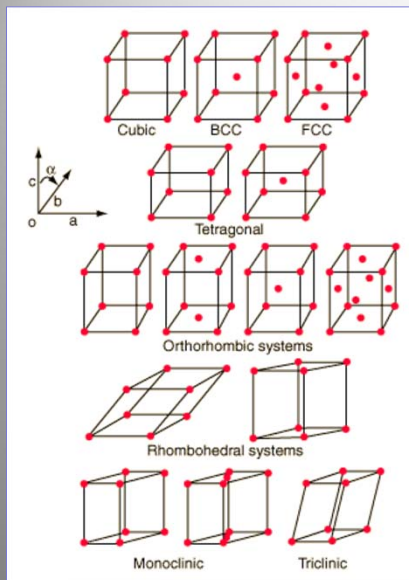
$a, b, c$  represent lengths of lattice vectors  
 $\alpha, \beta, \gamma$  represent angles between lattice vectors

## • 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	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$
Tetragonal	2	P, I	$a=b \neq c$ $\alpha=\beta=\gamma=90^\circ$
Orthorhombic	4	P, C, I, F	$a \neq b \neq c$ $\alpha=\beta=\gamma=90^\circ$
Monoclinic	2	F, C	$a \neq b \neq c$ $\alpha=\beta=90^\circ \neq \gamma$
Triclinic	1	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Trigonal	1	R	$a=b=c$ $\alpha=\beta=\gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	P	$a=b \neq c$ $\alpha=\beta=90^\circ \neq \gamma=120^\circ$

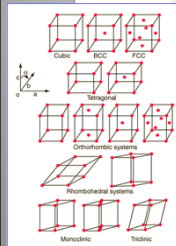
Table 1. Seven crystal systems make up fourteen Bravais lattice types in three dimensions.

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

## The Fourteen Bravais Lattices

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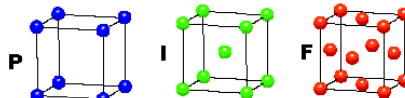
System	Number of Lattices	Lattice Symbol	Restriction on crystal cell angle
Cubic	3	P or sc, I or bcc, F or fcc	$a=b=c$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	P, I	$a=b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Orthorhombic	4	P, C, I, F	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Monoclinic	2	F, C	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$
Triclinic	1	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Trigonal	1	R	$a=b=c$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	P	$a=b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

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
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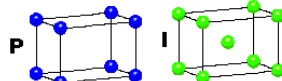
### CUBIC

$a = b = c$   
 $\alpha = \beta = \gamma = 90^\circ$



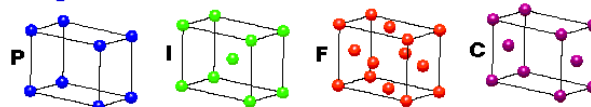
### TETRAGONAL

$a = b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$



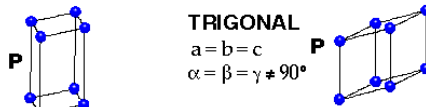
### ORTHORHOMBIC

$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$



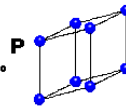
### HEXAGONAL

$a = b \neq c$   
 $\alpha = \beta = 90^\circ$   
 $\gamma = 120^\circ$



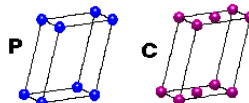
### TRIGONAL

$a = b = c$   
 $\alpha = \beta = \gamma \neq 90^\circ$



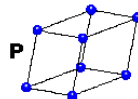
### MONOCLINIC

$a \neq b \neq c$   
 $\alpha = \gamma = 90^\circ$   
 $\beta \neq 120^\circ$



### TRICLINIC

$a \neq b \neq c$   
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$



#### 4 Types of Unit Cell

- P = Primitive
- I = Body-Centred
- F = Face-Centred
- C = Side-Centred

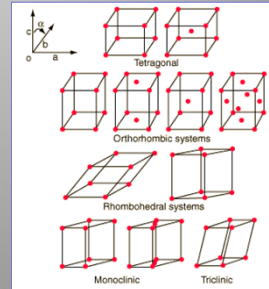
+ 7 Crystal Classes

→ 14 Bravais Lattices

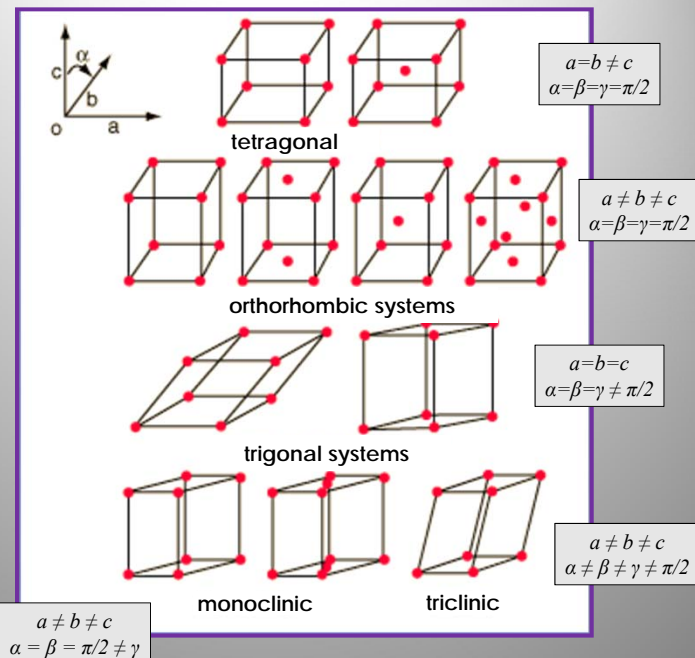


## The non-cubic structures

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

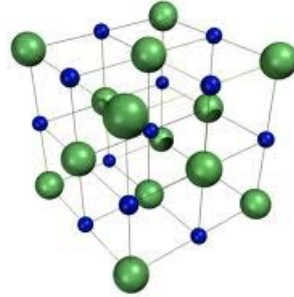


## The non-cubic structures



## 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>