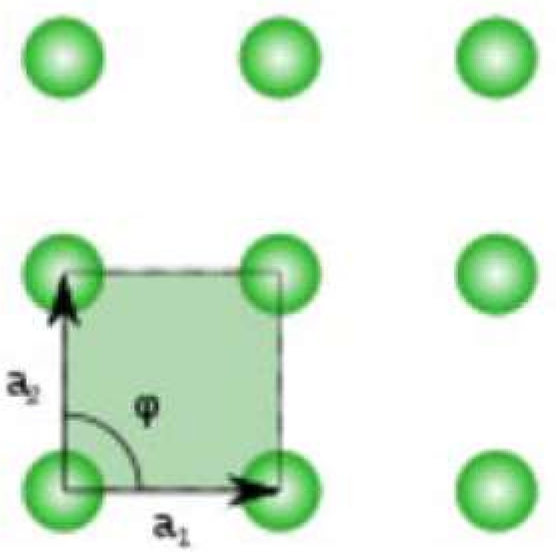
Two dimensional Bravais lattices

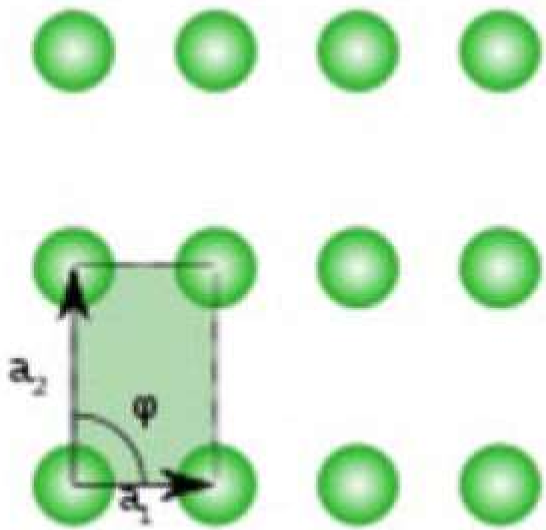
Two dimensional Bravais lattices
Square lattice



$|a_1| = |a_2|$, $\varphi = 90°$

Symmetries:
reflection about both x and y
rotations by 90^o ,180^o

Two dimensional Bravais lattices
Rectangular lattice

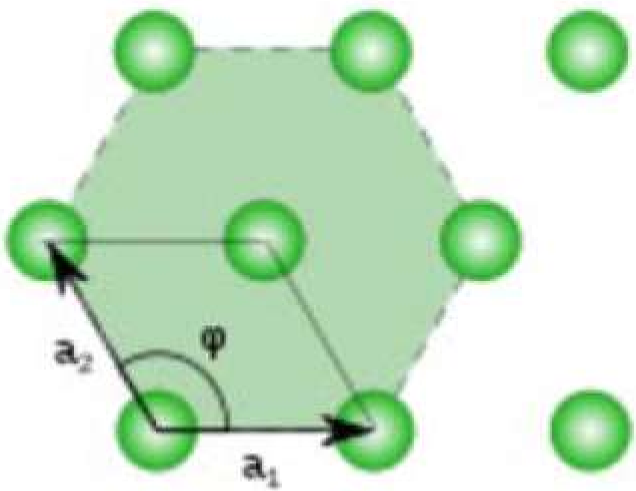


$|a_1| \neq |a_2|,\ \varphi = 90°$

Square lattice compressed along one axis

Symmetries:
reflection about both x and y, rotations by 180^o

Two dimensional Bravais lattices
Triangular (Hexagonal) lattice



$|a_1| = |a_2|$, $\varphi = 120°$

Symmetries:
reflection about both x and y
rotations by 60°

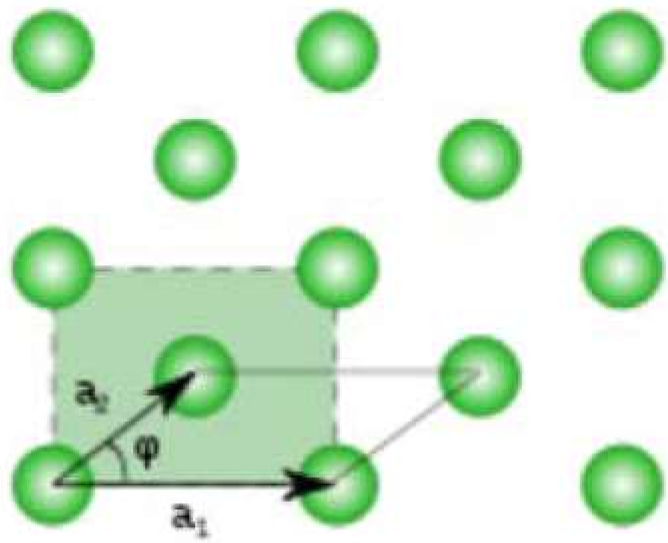
Possible primitive vectors

$$\vec{a}_1 = a\,(1\,,\;0)$$

$$\vec{a}_2 = a\,(-\frac{1}{2}\,,\;\frac{\sqrt{3}}{2})$$

Two dimensional Bravais lattices

Centered rectangular lattice

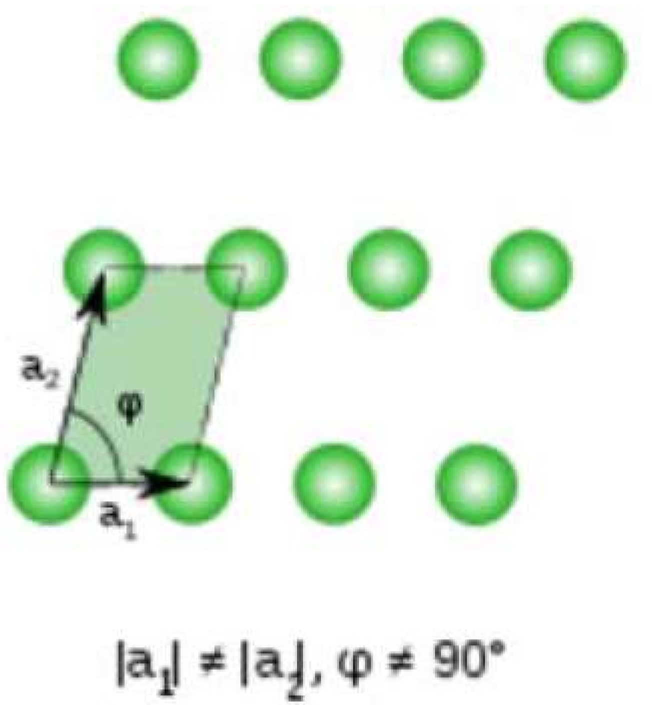


$|a_1| \neq |a_2|$, $\varphi \neq 90°$

Compressed hexagonal lattice

Symmetries:
reflection about both x and y,
rotations by 180^{o}

Two dimensional Bravais lattices
Oblique lattice

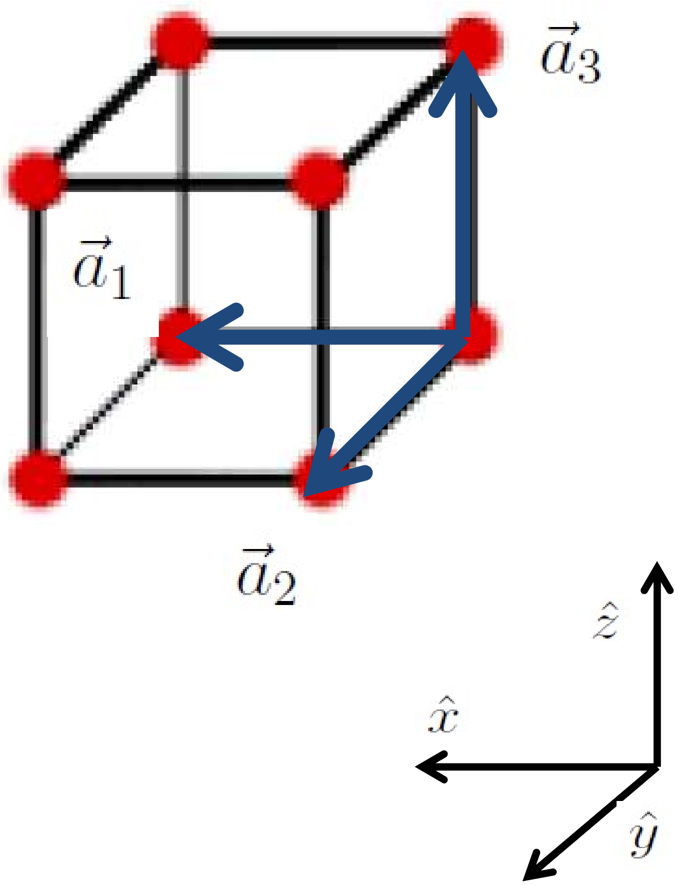


Arbitrary choice
of primitive vectors

No symmetries

Three dimensional Bravais lattices

Three dimensional Bravais lattices
Simple cubic lattice



Possible primitive vectors

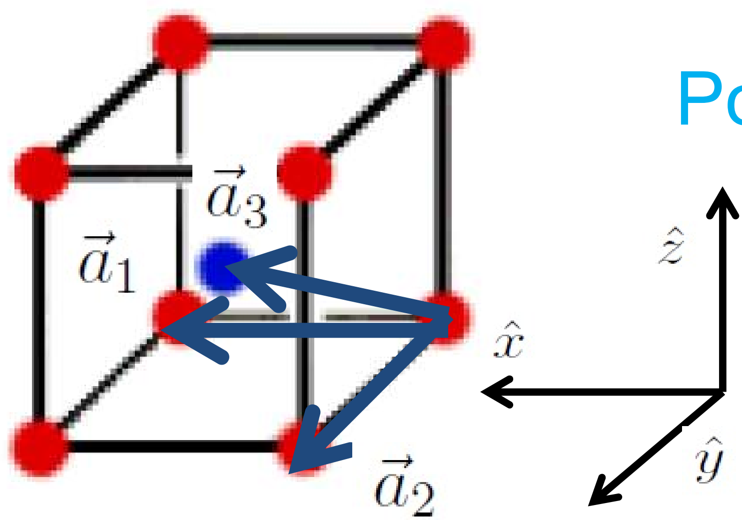
$$\vec{a}_1 = a \cdot \hat{x}$$

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

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

Three dimensional Bravais lattices

Body-centered cubic lattice

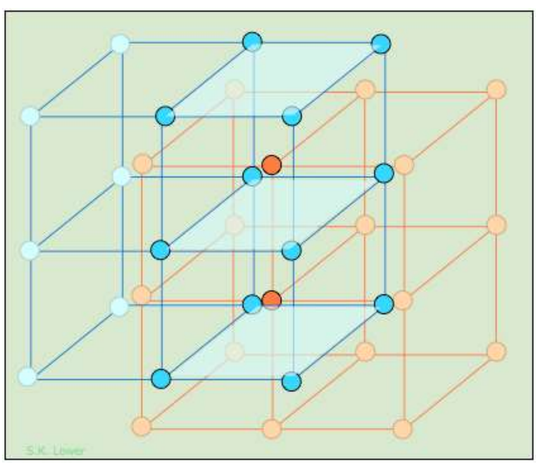


Possible primitive vectors

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

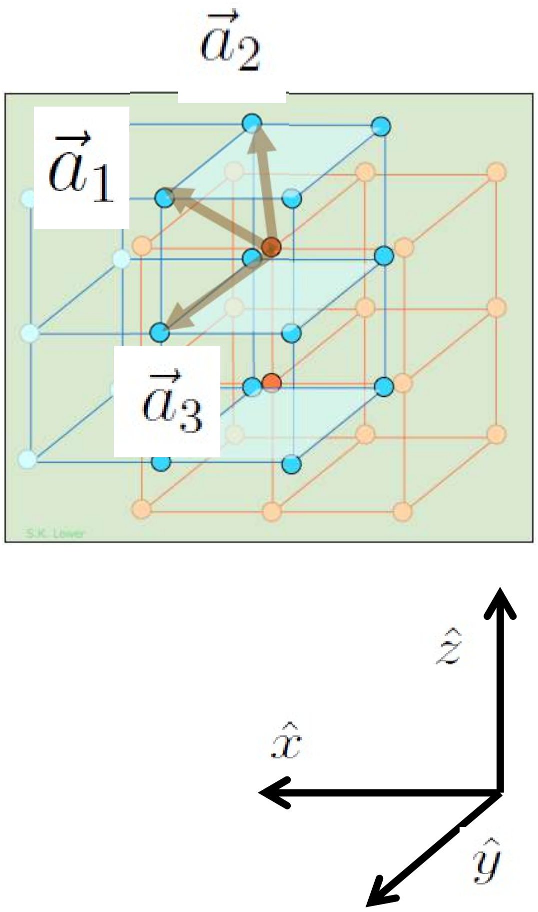
$$\vec{a}_2 = a \cdot \hat{y}$$

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



Three dimensional Bravais lattices

Body-centered cubic lattice



Another possible choice of primitive vectors

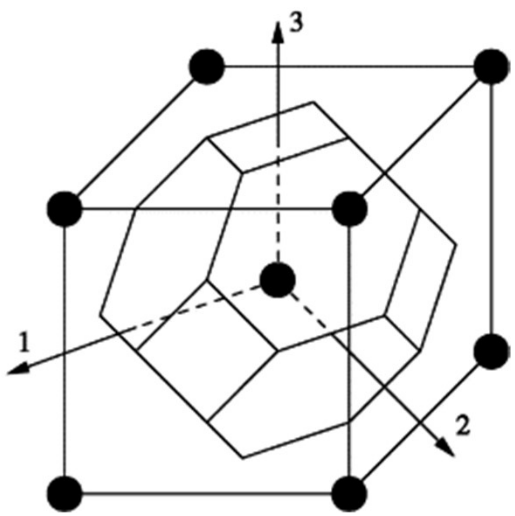
$$\vec{a}_1 = \frac{a}{2} \cdot (\hat{x} + \hat{y} + \hat{z})$$

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

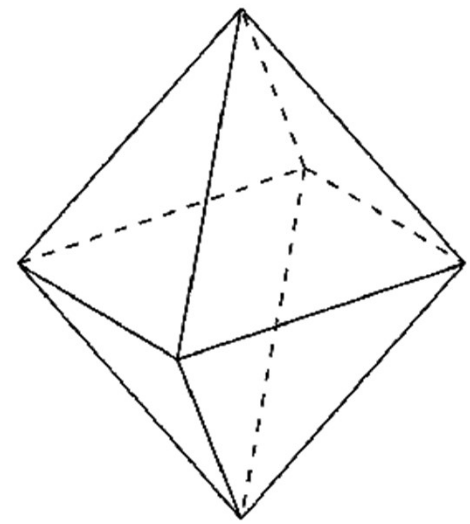
$$\vec{a}_3 = \frac{a}{2} \cdot (\hat{x} + \hat{y} - \hat{z})$$

Three dimensional Bravais lattices

The Wigner-Seitz cell for Body-centered cubic lattice

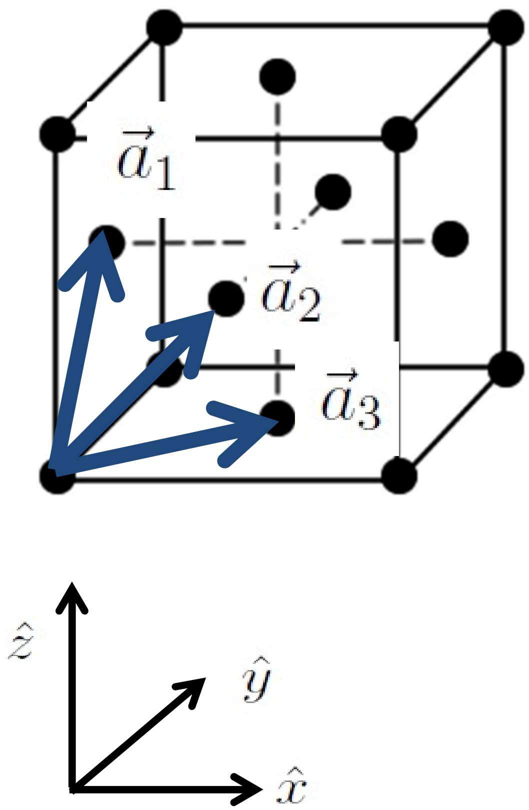


Truncated octahedron



Regular octahedron

Three dimensional Bravais lattices
Face-centered cubic lattice



Possible primitive vectors

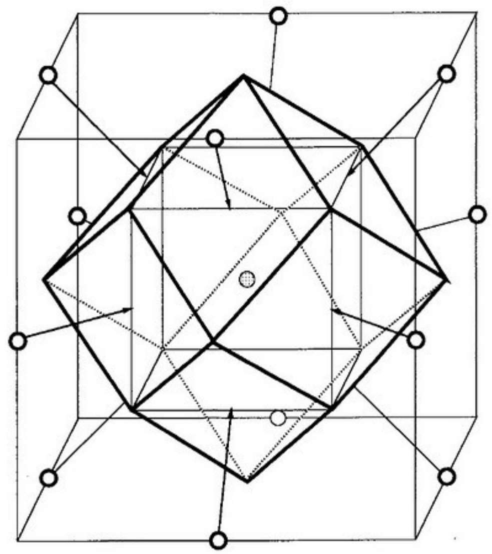
$$\vec{a}_1 = \frac{a}{2} \cdot (\hat{y} + \hat{z})$$

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

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

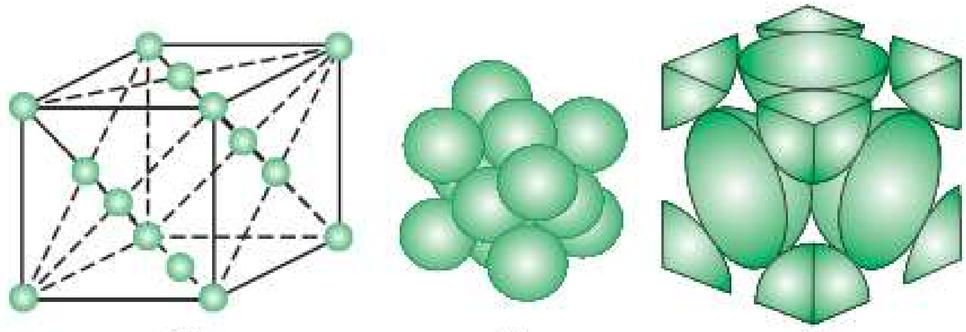
Three dimensional Bravais lattices

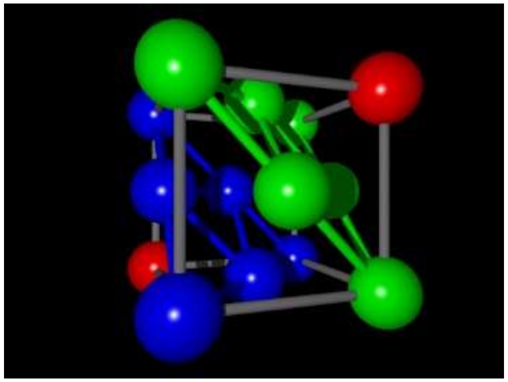
The Wigner-Seitz cell for Face-centered cubic lattice

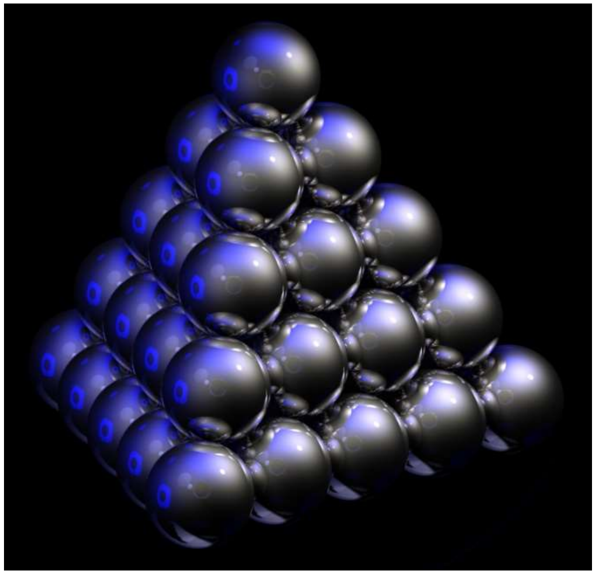


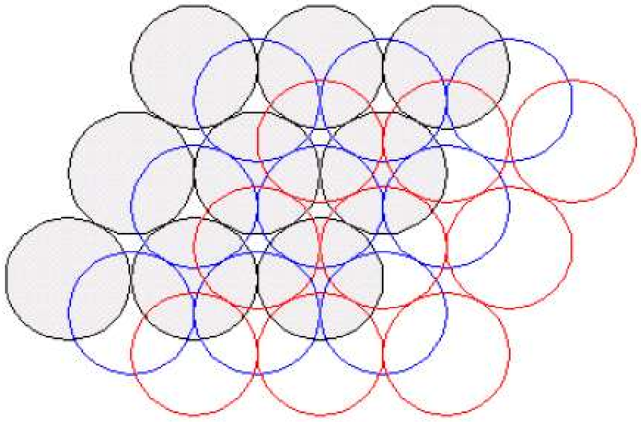
Rhombic dodecahedron

Face-centered cubic lattice is cubic close packed



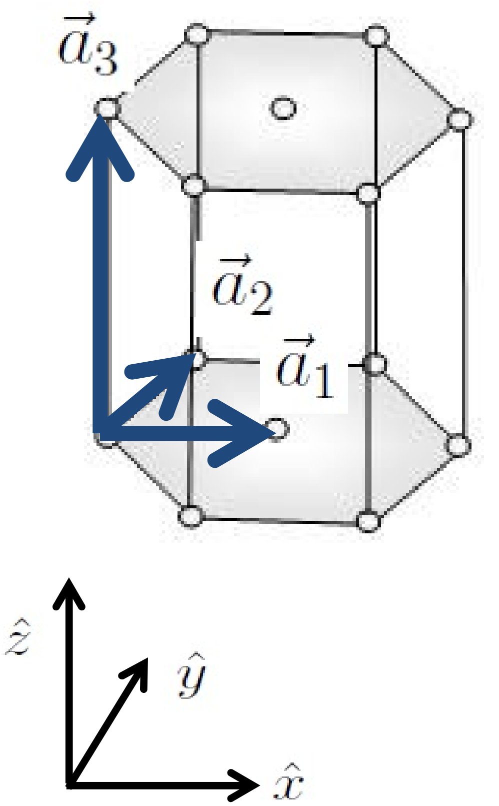






Three dimensional Bravais lattices

The simple hexagonal lattice



Possible primitive vectors

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

$$\vec{a}_2 = \frac{a}{2} \cdot x + \frac{\sqrt{3}}{2} a \cdot \hat{y}$$

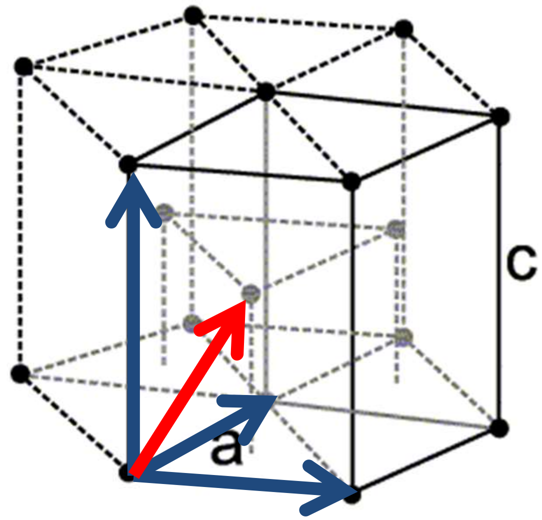
$$\vec{a}_3 = c \cdot \hat{z}$$

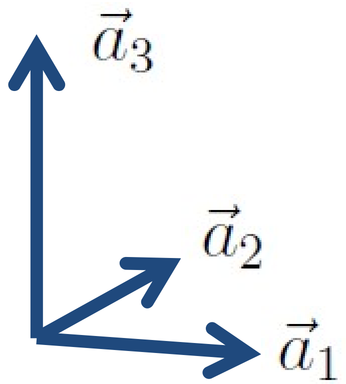
Three dimensional lattices with bases

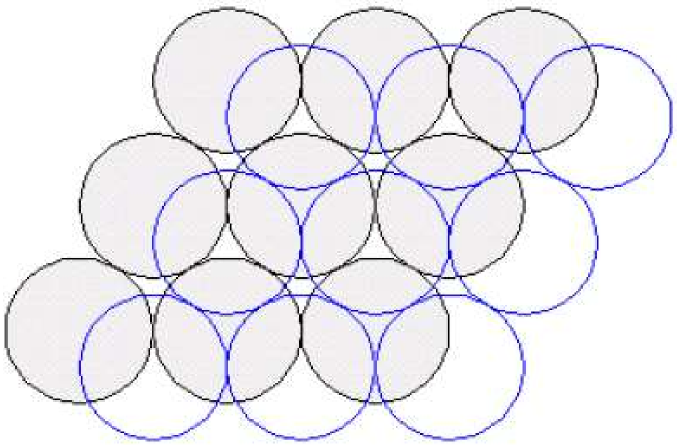
The hexagonal closed-packed hexagonal structure

Consists of two interpenetrating simple hexagonal lattices, displaced from one another by

$$\frac{\vec{a}_1}{2} + \frac{\vec{a}_2}{2} + \frac{\vec{a}_3}{2}$$

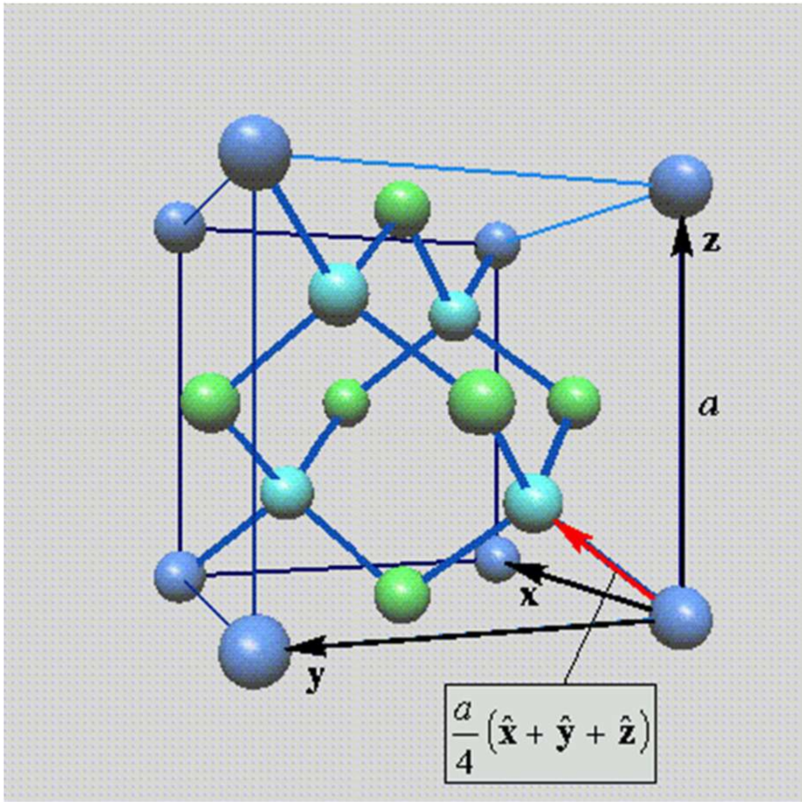






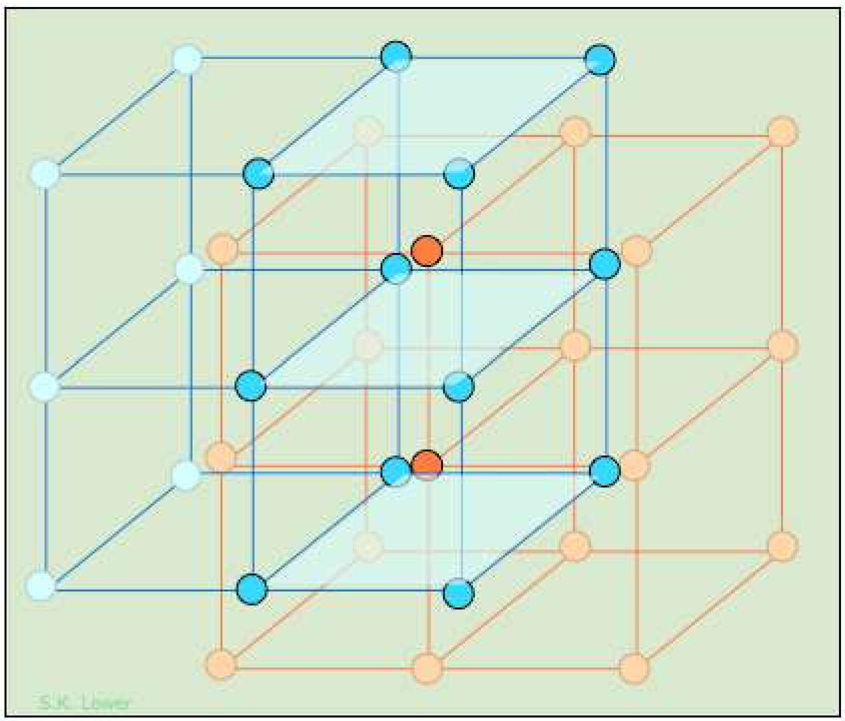
The diamond lattice

Consists of two interpenetrating face-centered cubic lattices



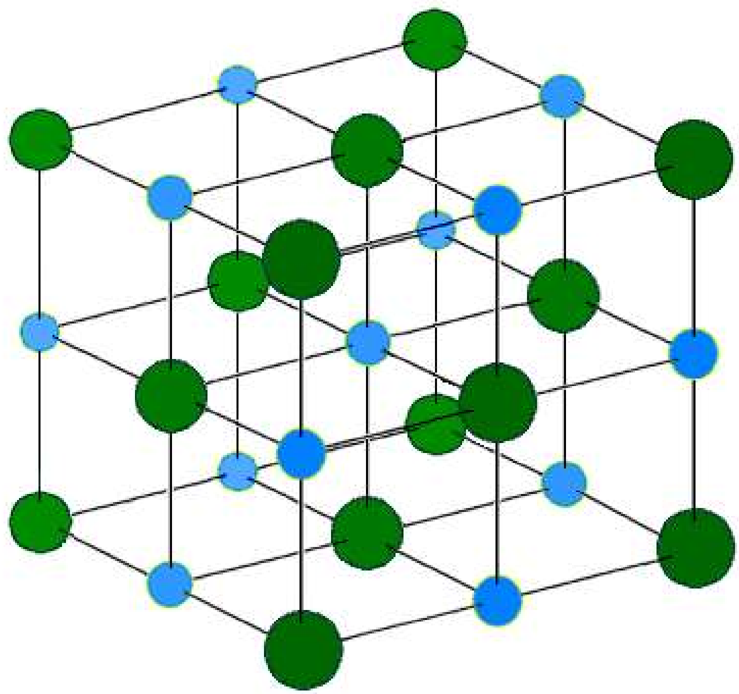
The Cesium-Chloride structure

Simple cubic lattice consisting of one Cs and one Cl ions. Individually Cs and Cl ions form interpenetrating simple cubic lattices. Together ions are placed at the points of a body centered cubic lattice



The Sodium-Chloride structure

The FCC Bravais lattice with a basis consisting of one Na and one Cl ions. Individually they form interpenetrating FCC lattices. Cl ions sit at the centers of conventional cubic cells of Na and vice versa.



Classification of Bravais lattices

Important for

- explaining sharp peaks in Xray and Neutron scattering
- solution of Schroedinger equation requires knowledge of the symmetries of crystal potential

The Space group

From the point of view of symmetry, a Bravais lattice is characterized by the specification of all rigid body motions that take the lattice into itself. This set of operations is known as the symmetry group or the space group of the Bravais lattice

The full symmetry of a Bravais lattice contains only operations of the following form

1. Translations through Bravais lattice vectors
   (Translation group)
2. Operations that leave a particular point of the lattice fixed
   (Point group)
3. Operations that can constructed by successive applications of the operations of type (1) or (2)

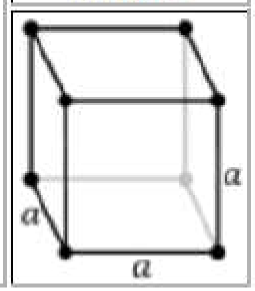
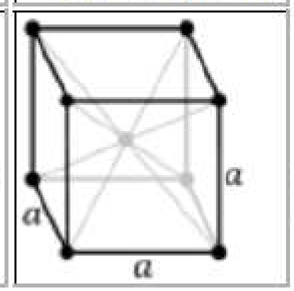
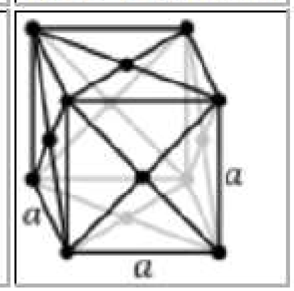
Translation and point groups provide important subgroups of the space group. Generally the space group is not a product of the translation and point groups

Seven distinct point groups

In d=3 there is only seven distinct point groups (and 14 space groups) that a Bravais lattice can have. Any crystal structure belongs to one of these seven point groups of the underlying Bravais lattice.

Cubic system

Contains Bravais lattices whose symmetries are those of a cube

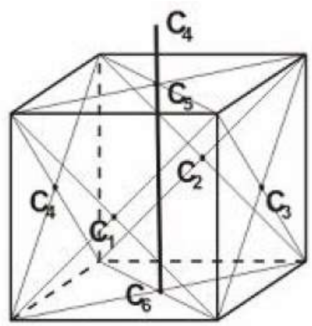
	simple	body-centered	face-centered
cubic (isometric; cube)			

This is a single class from the point of view of point group.
But it includes three different types of Bravais lattices

Symmetries of a cube

Contains those Barvais lattices whose point group is just the symmetry group of the cube.

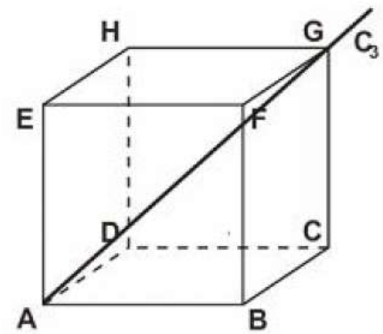
Symmetries of the cube. We fix the center of the cube



– three rotations by 90° (C_4)

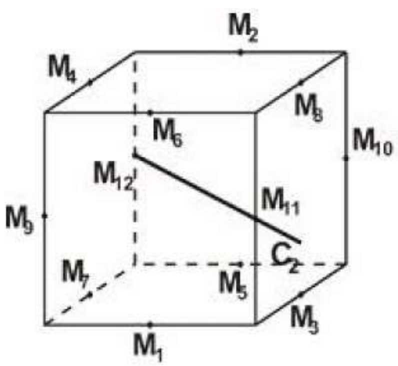
– three rotations by 180° (C_4^2)

– three rotations by 270° (C_4^3)



– four rotations by 120° (C_3)

– four rotations by 240° (C_3^2)



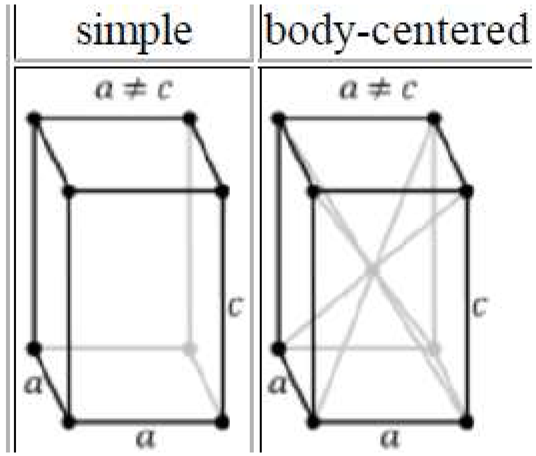
– the picture on the left shows only $\overline{M_{11}M_{12}}$, other possible 2-fold axes are $\overline{M_1M_2}$, $\overline{M_3M_4}$, $\overline{M_5M_6}$, $\overline{M_7M_8}$ and $\overline{M_9M_{10}}$, thus altogether six

Total number of rotations (including “do nothing”) 1+9+8+6=24
When we add inversion we find 24*2=48

Seven distinct point groups

Tetragonal system

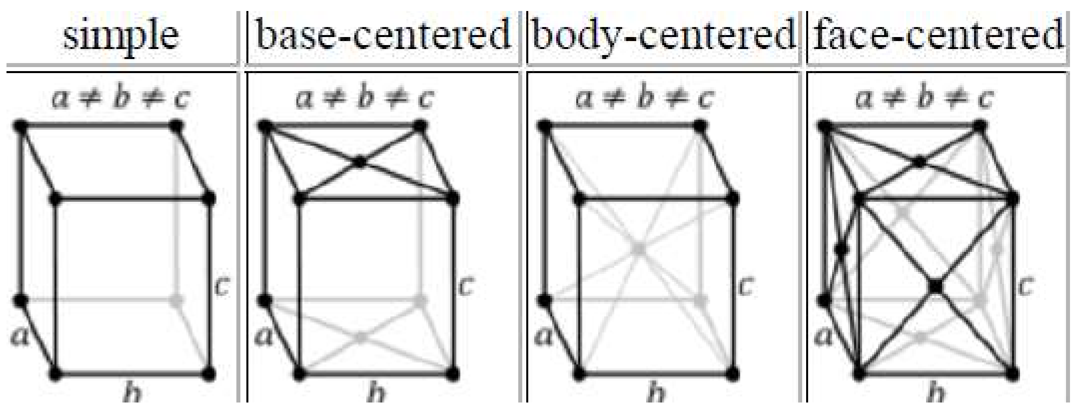
Reduce the symmetry of the cube by pulling on two opposite faces



Seven distinct point groups

Orthorombic system

Deform the tetragonal system by deforming the square faces

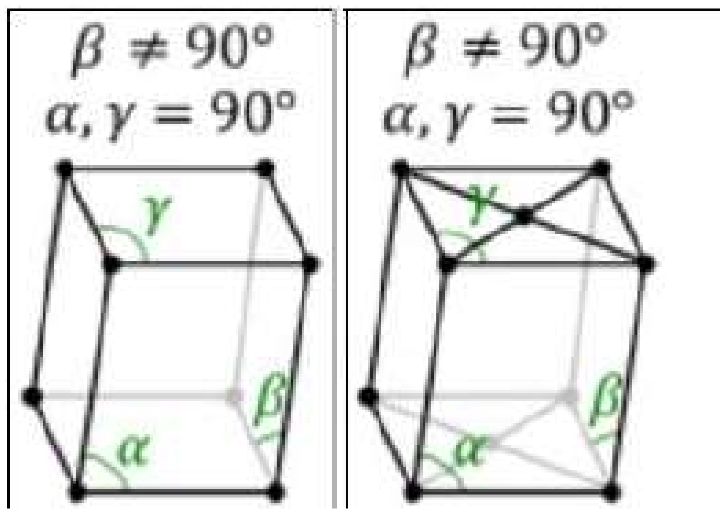


Seven distinct point groups

Monoclinic system

Distort the orthorombic system by distorting rectangular faces

primitive
monoclinic

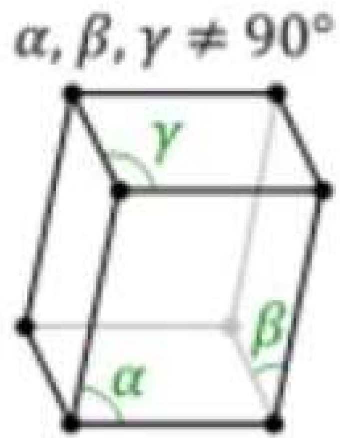


base centered
monoclinic

Seven distinct point groups

Triclinic system

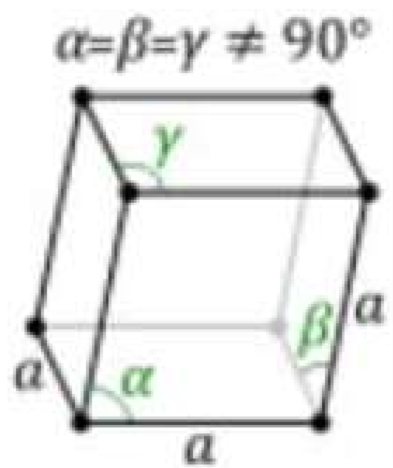
“Complete” the destruction of the cube by tilting the c-axis



Seven distinct point groups

Trigonal system

The trigonal point group describes the symmetry of the object produced by stretching a cube along body diagonal



Seven distinct point groups

Hexagonal system

The right prism with hexagons in the base