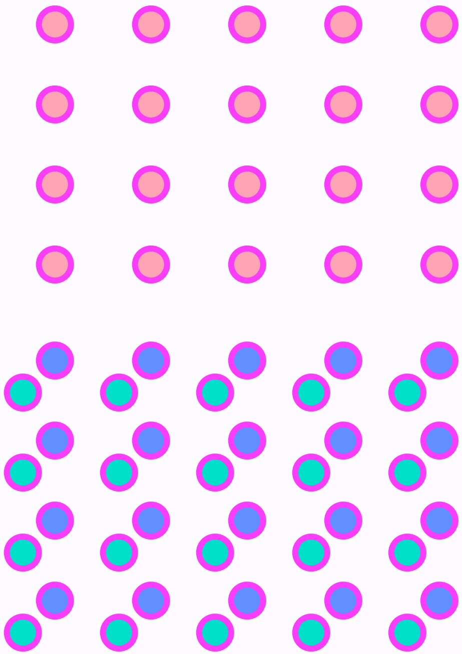
Solid State Physics 460- Lecture 2a
Structure of Crystals
(Kittel Ch. 1)

See many great sites like "Bob's rock shop" with pictures and crystallography info: **http://www.rockhounds.com/rockshop/xtal/index.html**

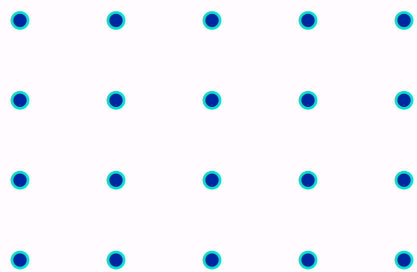
From Last Time

Crystals

- A crystal is a repeated array of atoms
- Crystal ⇔ Lattice + Basis



Crystal



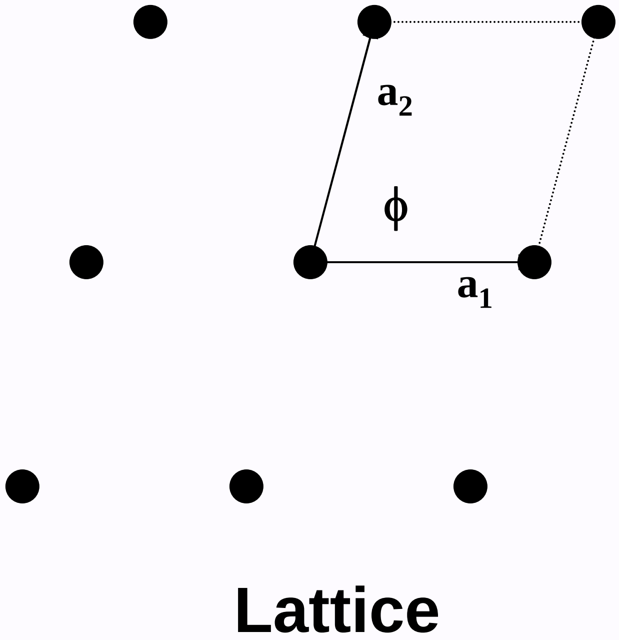
Lattice of points (Bravais Lattice)

Basis of atoms

- Crystals can be classified into a small number of types – See text for more details

From Last Time

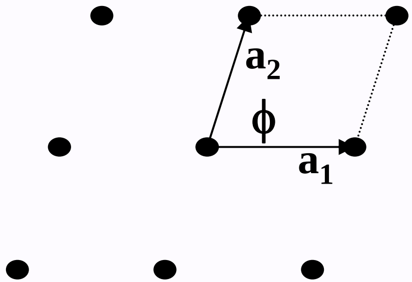
Two Dimensional Crystals



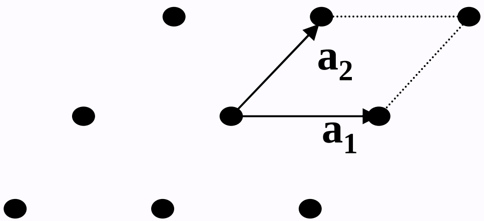
- Infinite number of possible lattices and crystals
- Finite number of possible lattice types and crystal types

From Last Time

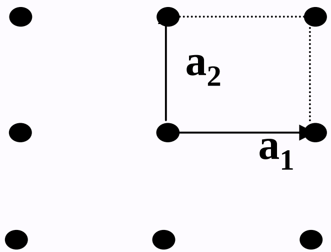
Possible Two Dimensional Lattices



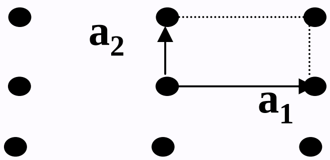
General oblique



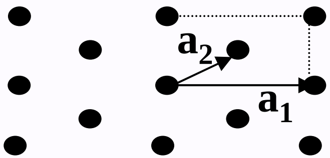
Hexagonal $\Phi = 60$, $a_1 = a_2$
6-fold rotation , reflections



Square
4-fold rot., reflect.



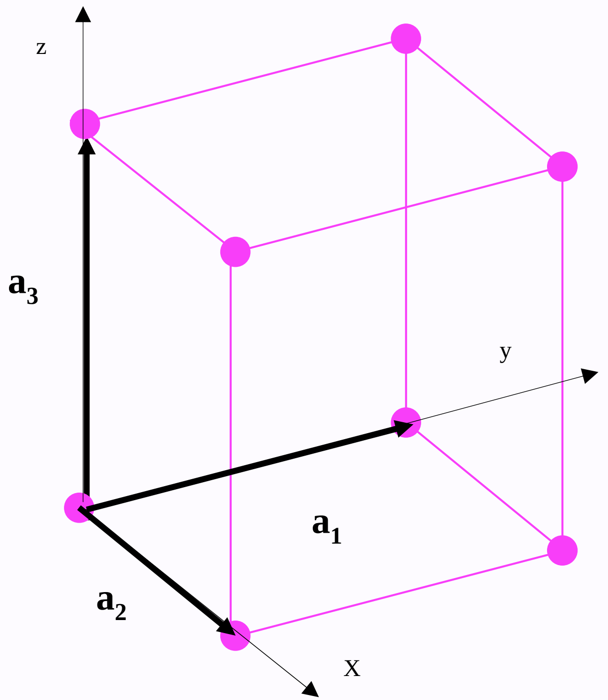
Rectangular
2-fold rot., reflect.



Centered Rectangular
2-fold rot., reflect.

- These are the only possible special crystal types in two dimensions

Three Dimensional Lattices

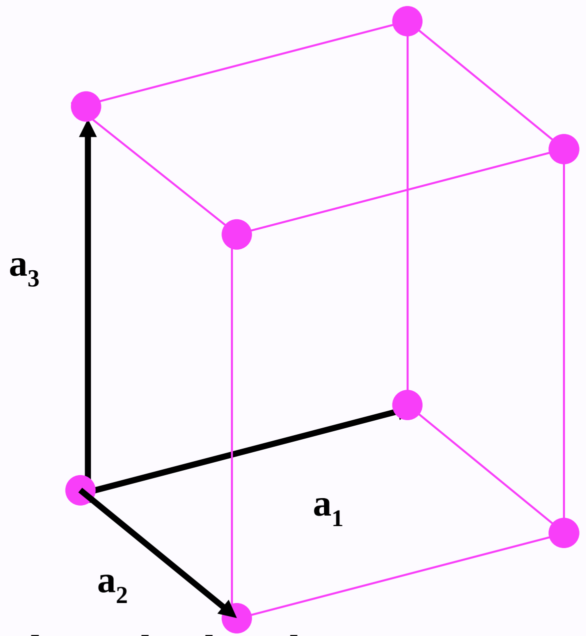


- **Every point on the Bravais lattice is a multiple of 3 primitive lattice vectors**

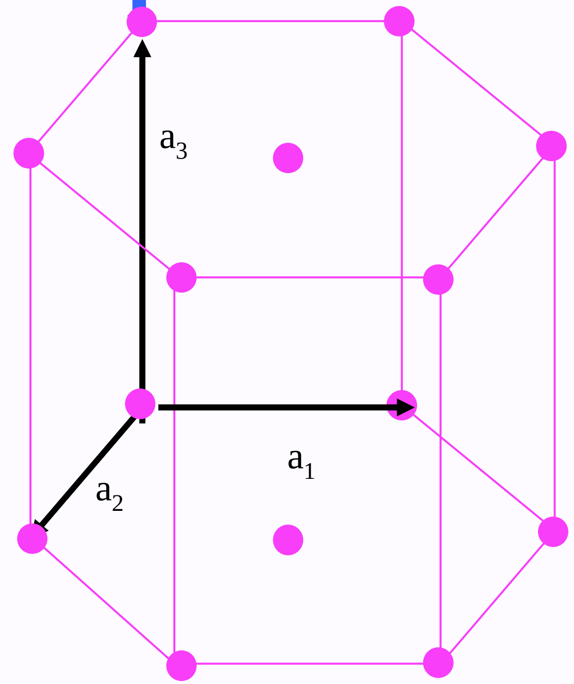
$$T(n_1,n_2,n_3) = n_1\, a_1 + n_2\, a_2 + n_3\, a_3$$

where the n's are integers

Three Dimensional Lattices Simplest examples



Simple Orthorhombic Bravais Lattice

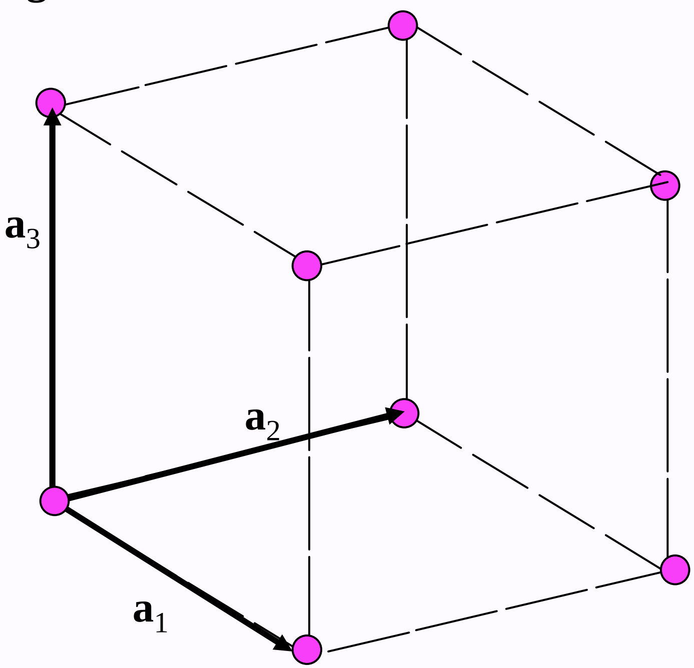


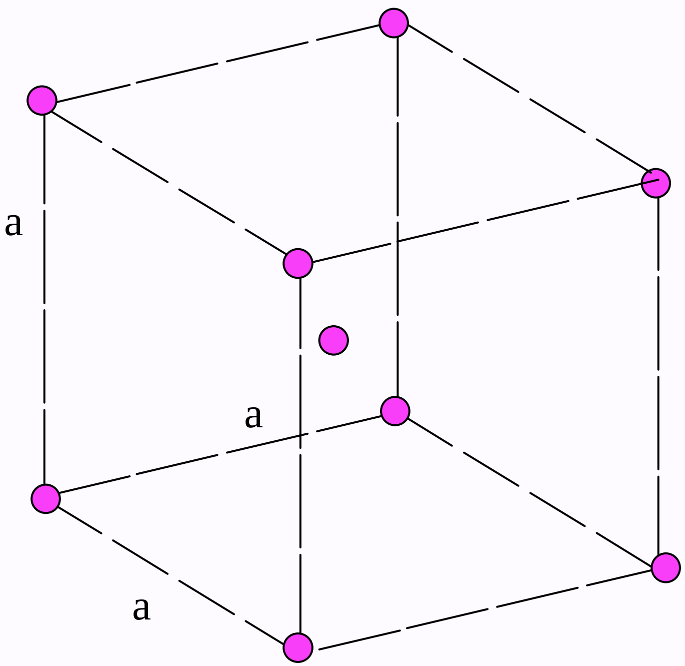
Hexagonal Bravais Lattice

- **Orthorhombic: angles 90 degrees, 3 lengths different**
  Tetragonal: 2 lengths same
  Cubic: 3 lengths same
- **Hexagonal: a_3 different from a_1, a_2 by symmetry**

Cubic Lattices

Length of each side - a





Simple Cubic

Primitive lattice vectors

$\mathbf{a_1}$ = (1,0,0) a

$\mathbf{a_2}$ = (0,1,0) a

$\mathbf{a_3}$ = (0,0,1) a

One atom per cell at position (0,0,0)

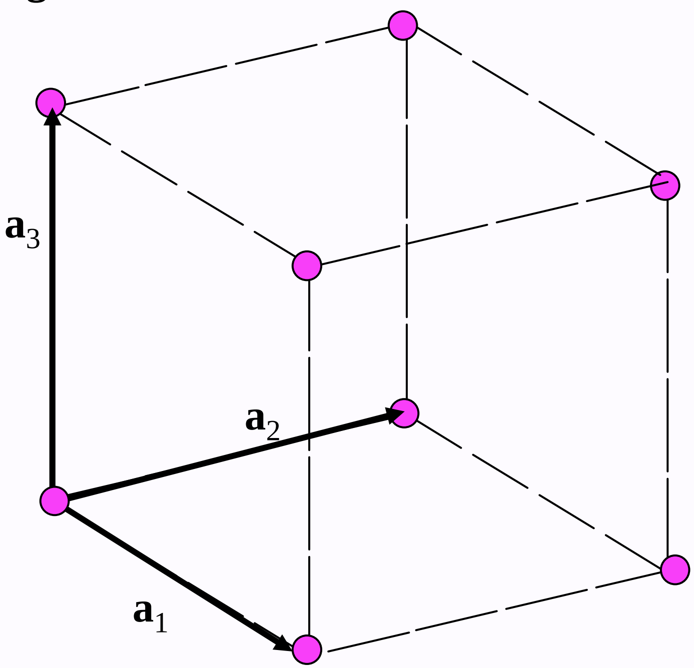
Body Centered Cubic (BCC)

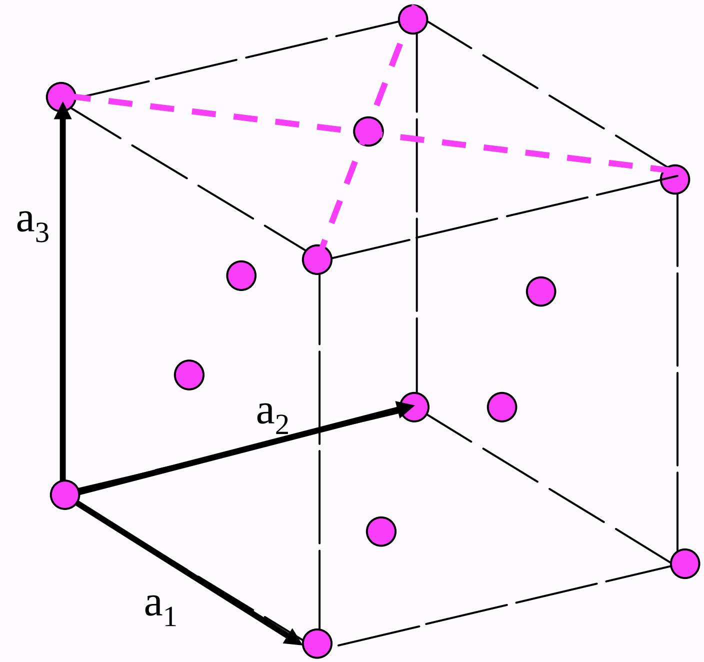
Conventional Cell with 2 atoms at positions

(000), (1/2,1/2,1/2) a

Cubic Lattices

Length of each side - a





Simple Cubic

Primitive lattice vectors

$\mathbf{a_1}$ = (1,0,0) a

$\mathbf{a_2}$ = (0,1,0) a

$\mathbf{a_3}$ = (0,0,1) a

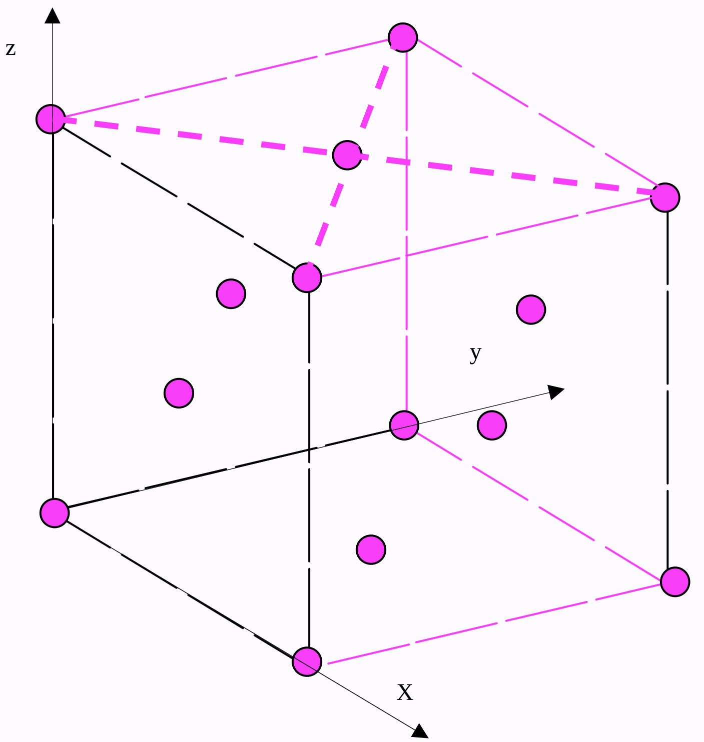
One atom per cell at position (0,0,0)

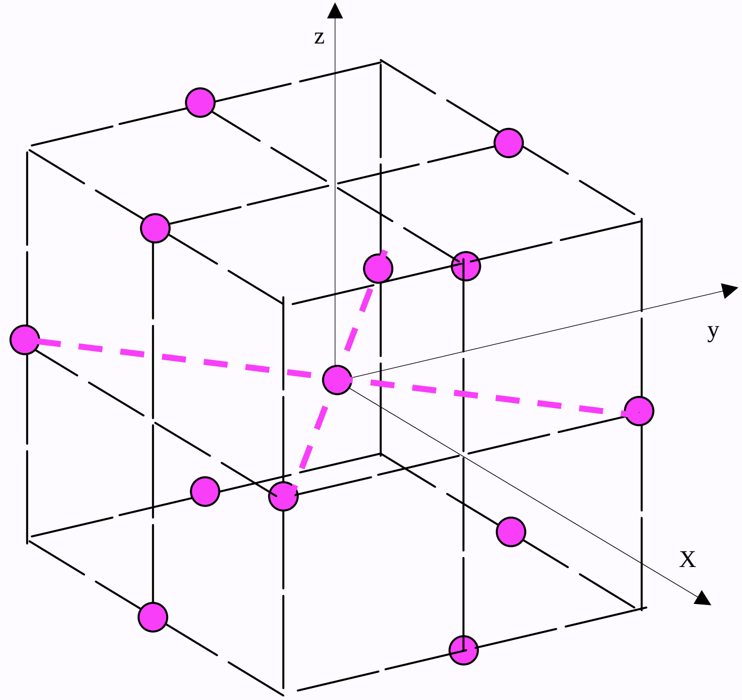
Face Centered Cubic (FCC)

Conventional Cell with 4 atoms at positions

(000), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0)a

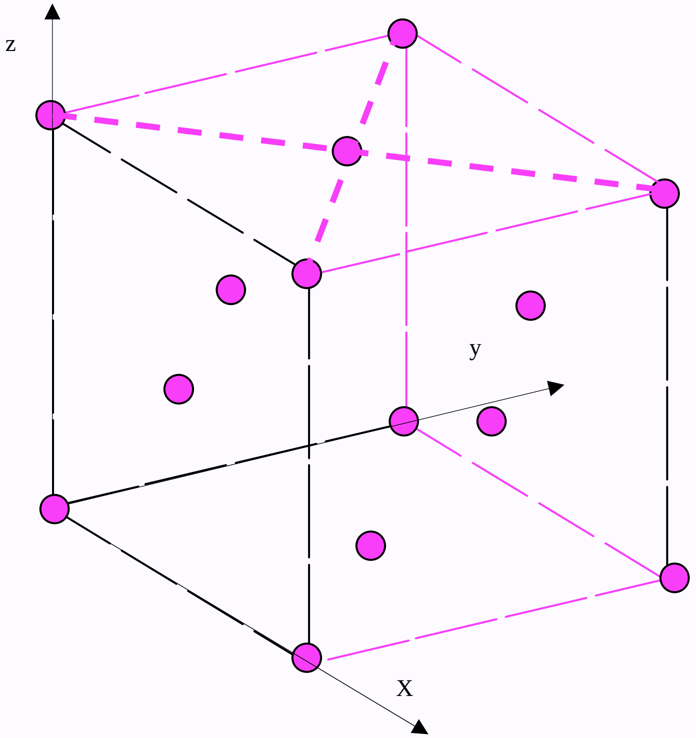
Face Centered Cubic
Two views - Conventional Cubic Cell

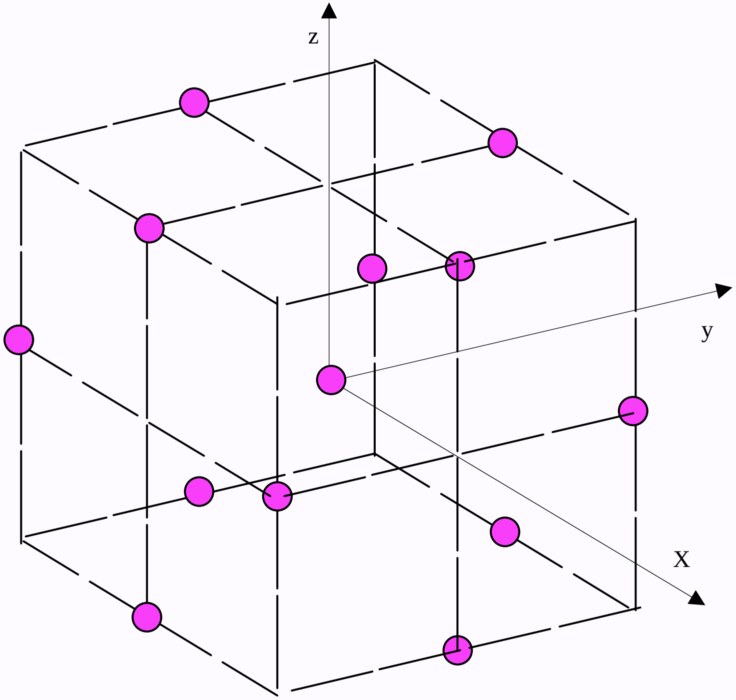




Conventional Cell of Face Centered Cubic Lattice
4 times the volume of a primitive cell

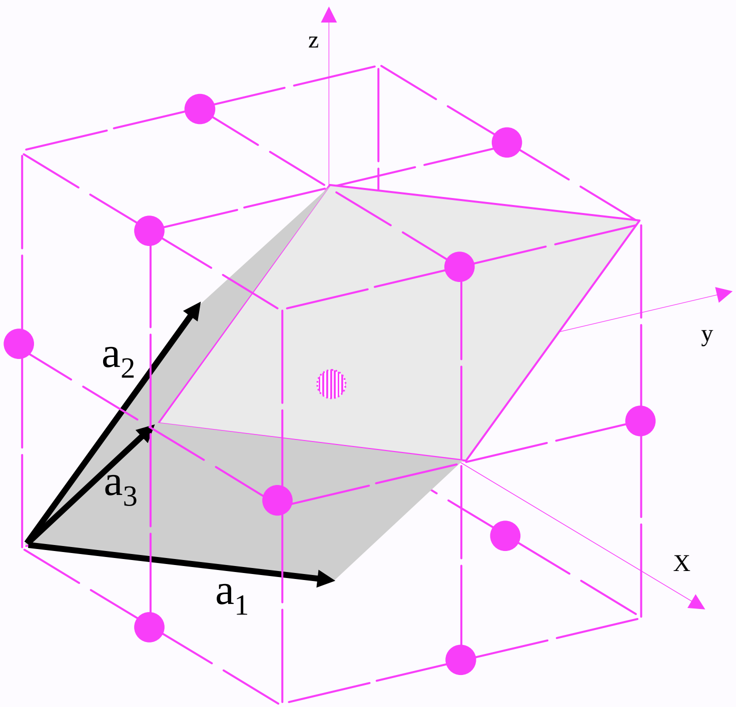
Face Centered Cubic (fcc)
Also called cubic closed packed (ccp)

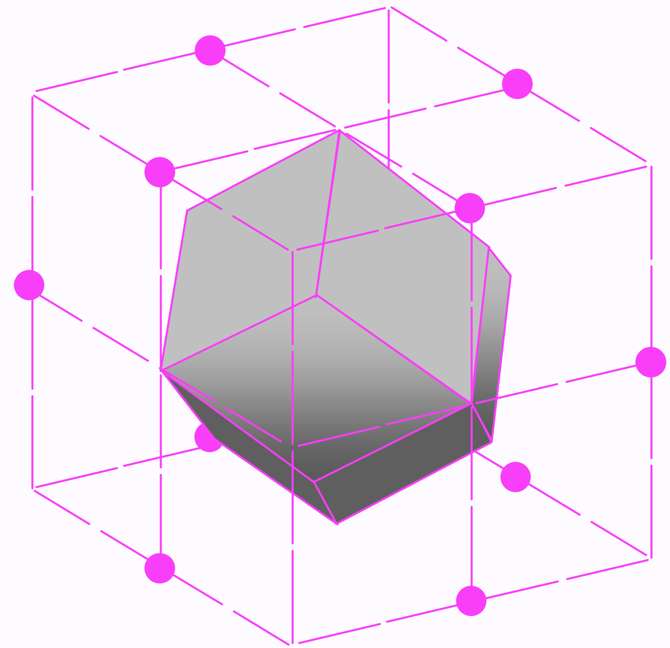




Each atom has 12 equal neighbors
We will see later that this is a “close packed” lattice

Face Centered Cubic





One Primitive Cell

Wigner-Seitz Cell

Primitive lattice vectors

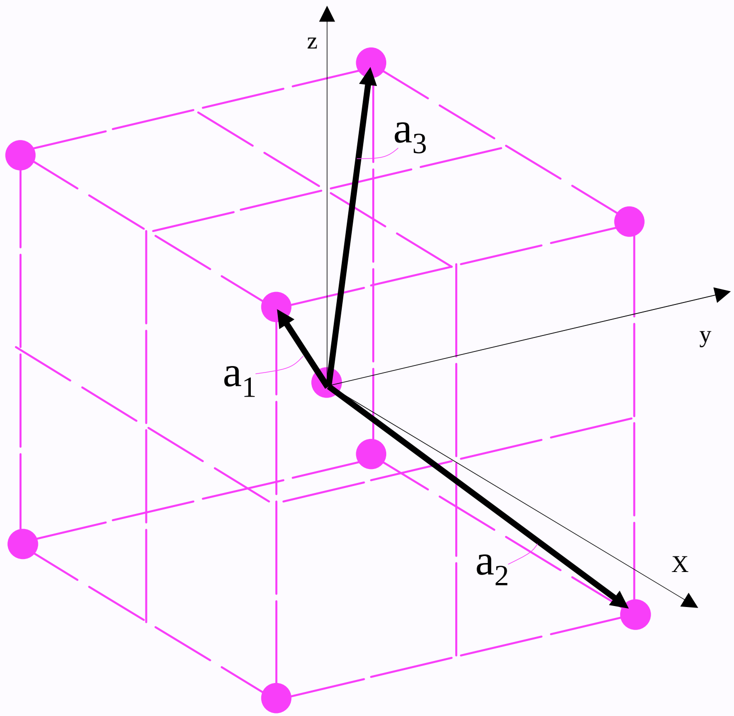
$\mathbf{a_1}$ = (1/2,1/2,0) a

$\mathbf{a_2}$ = (1/2,0,1/2) a

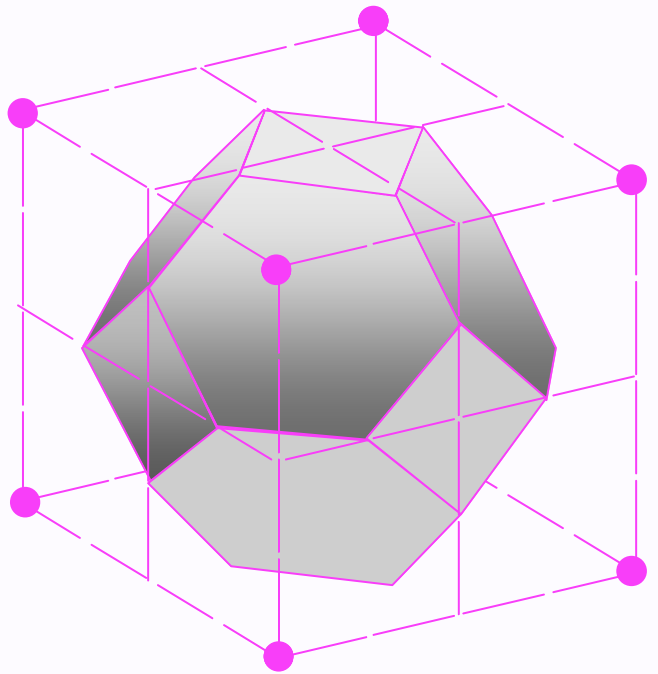
$\mathbf{a_3}$ = (0,1/2,1/2) a

One atom per cell at position (0,0,0)

Body Centered Cubic



One Primitive Cell



Wigner-Seitz Cell

Primitive lattice vectors

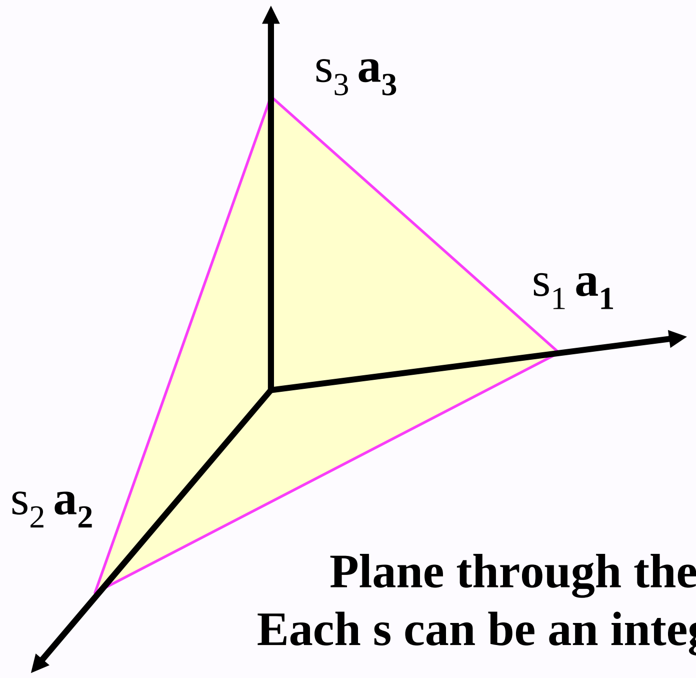
$\mathbf{a_1}$ = (1/2,1/2,-1/2) a

$\mathbf{a_2}$ = (1/2, -1/2,1/2) a

$\mathbf{a_3}$ = (-1/2,1/2,1/2) a

One atom per cell at position (0,0,0)

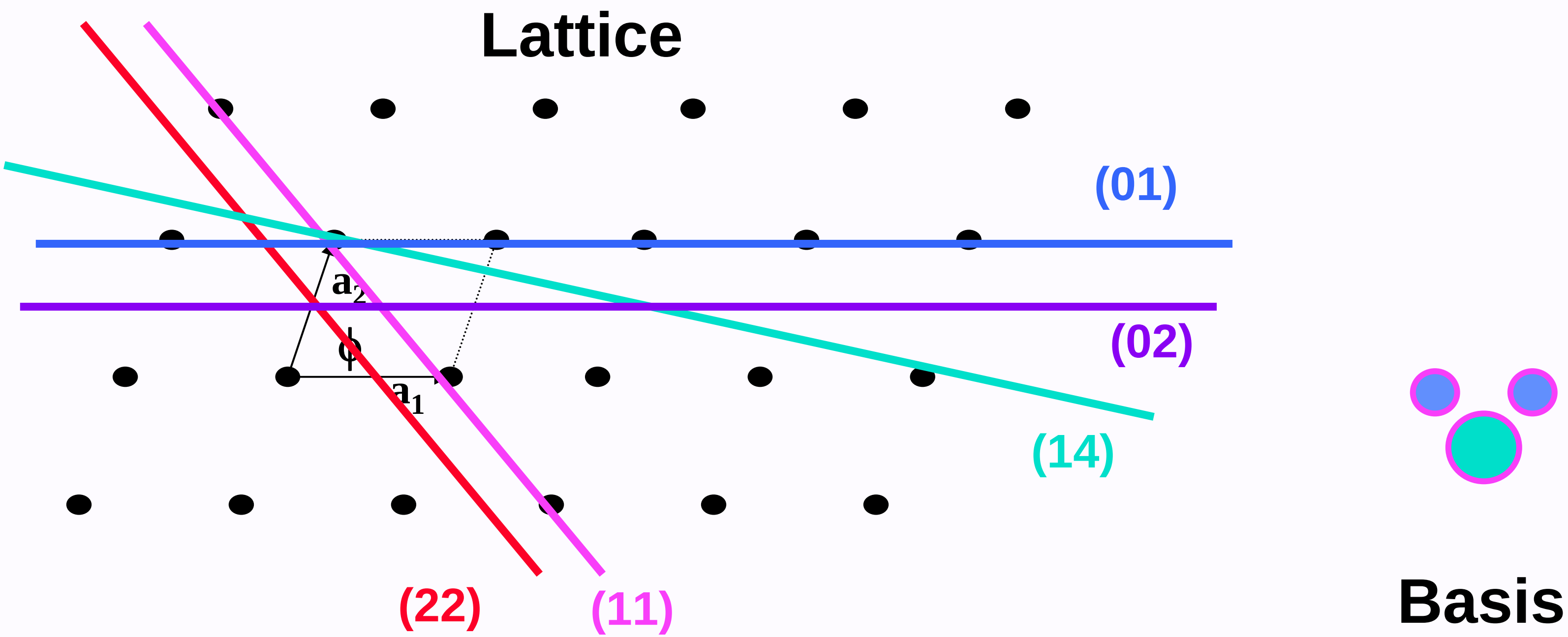
Lattice Planes - Index System



Plane through the points $s_1\,\mathbf{a_1}$, $s_2\,\mathbf{a_2}$, $s_3\mathbf{a_3}$
Each s can be an integer or a rational fractions

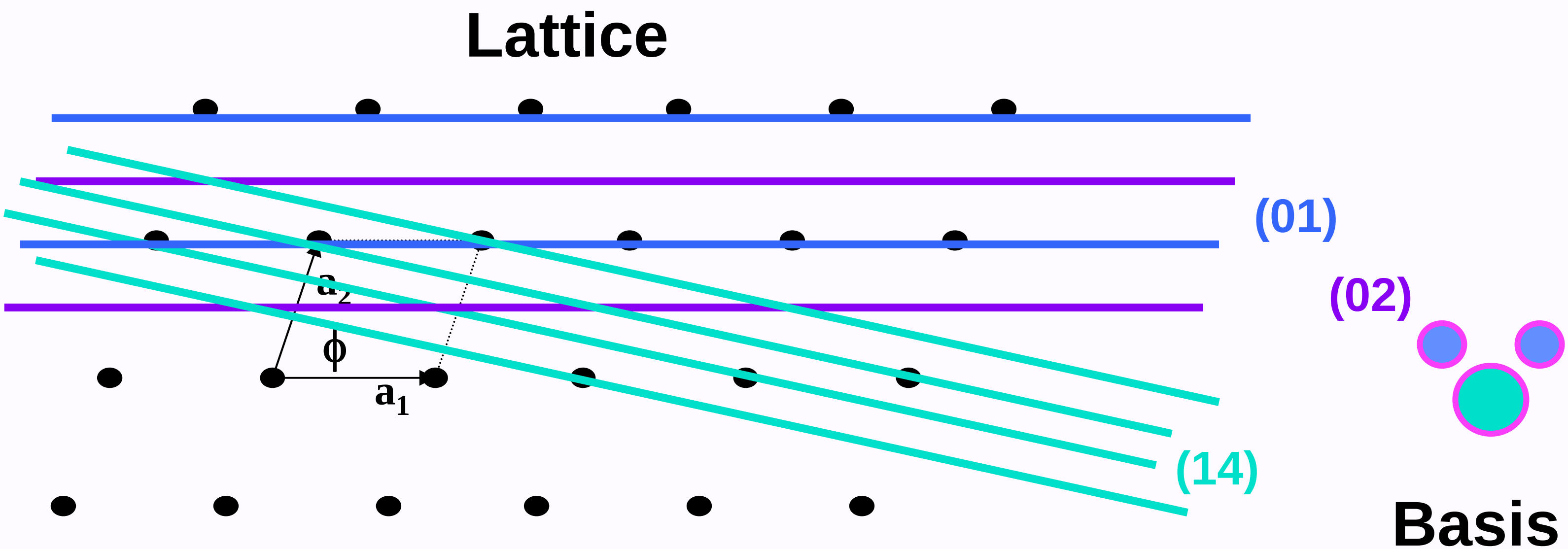
- **Define the plane by the reciprocals $1/s_1$, $1/s_2$, $1/s_3$**
- **Reduce to three integers with same ratio h,k,l**
- **Plane is defined by (h,k,l)**

Schematic illustrations of lattice planes Lines in 2d crystals



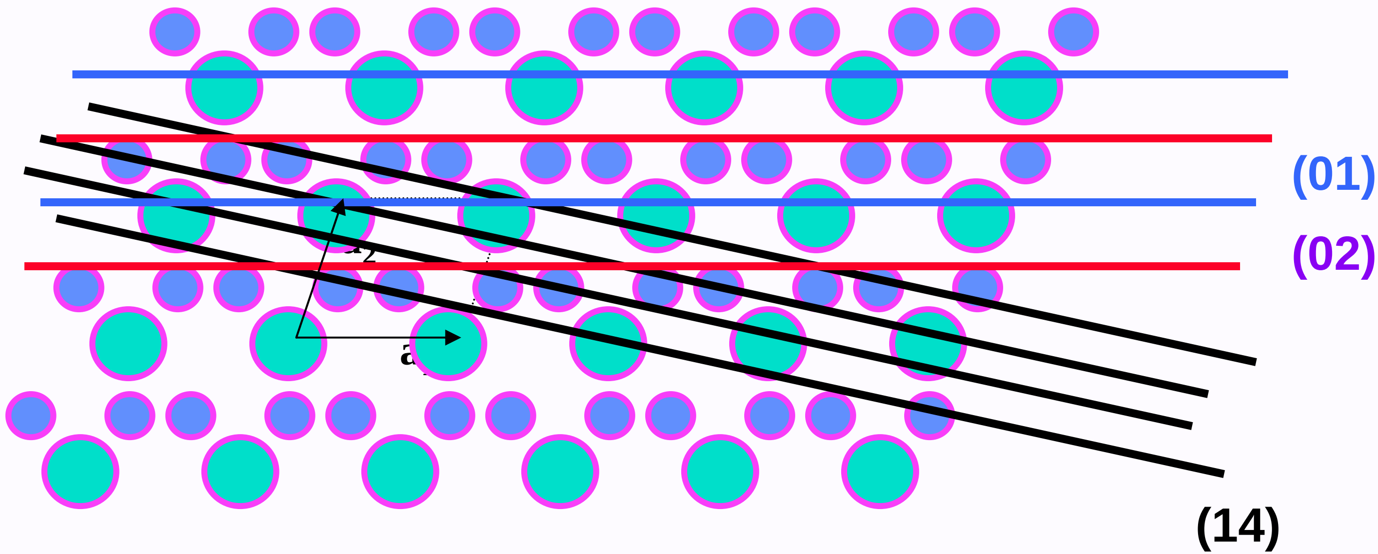
- Infinite number of possible planes
- Can be through lattice points or between lattice points

Schematic illustrations of lattice planes Lines in 2d crystals



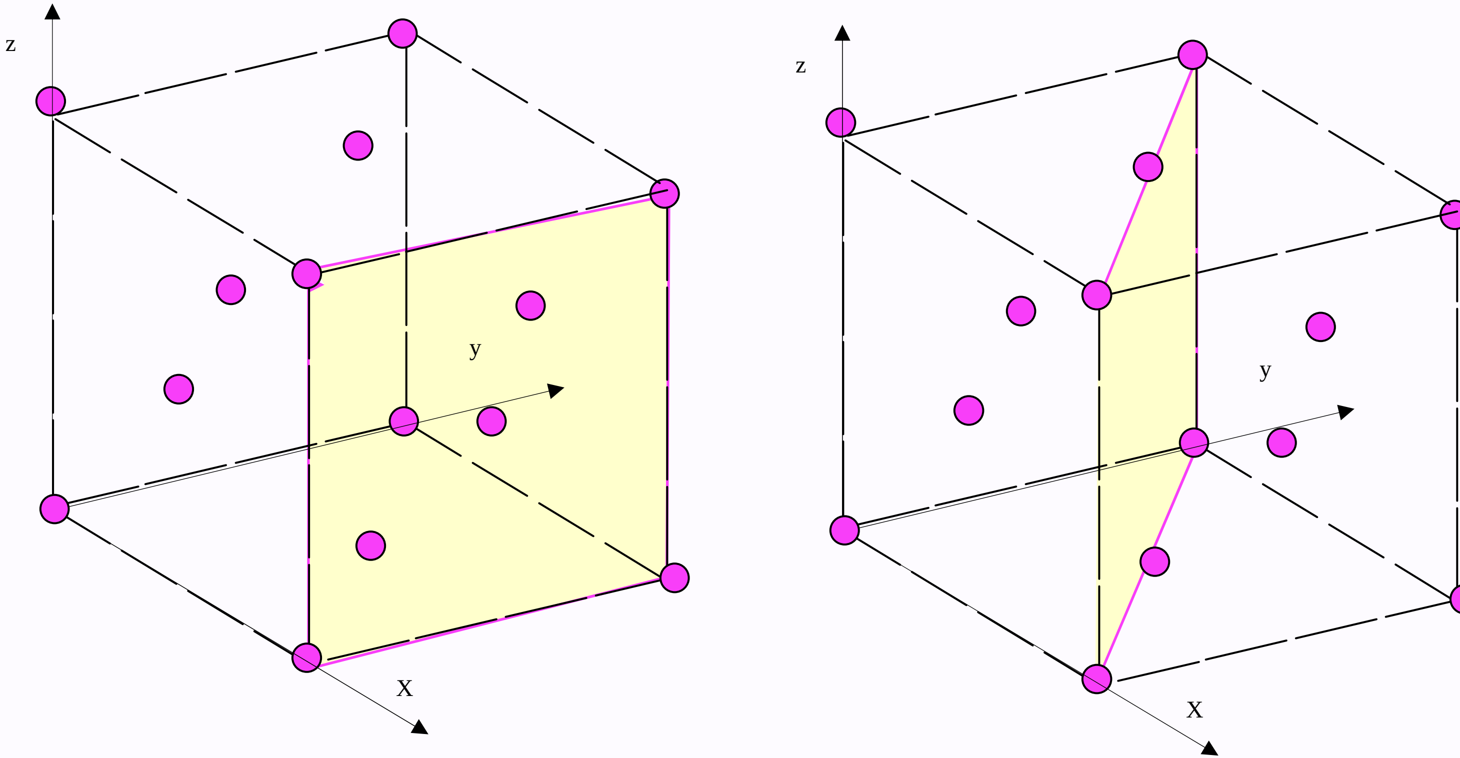
- Equivalent parallel planes
- Low index planes: more dense, more widely spaced
- High index planes: less dense, more closely spaced

Schematic illustrations of lattice planes
Lines in 2d crystals



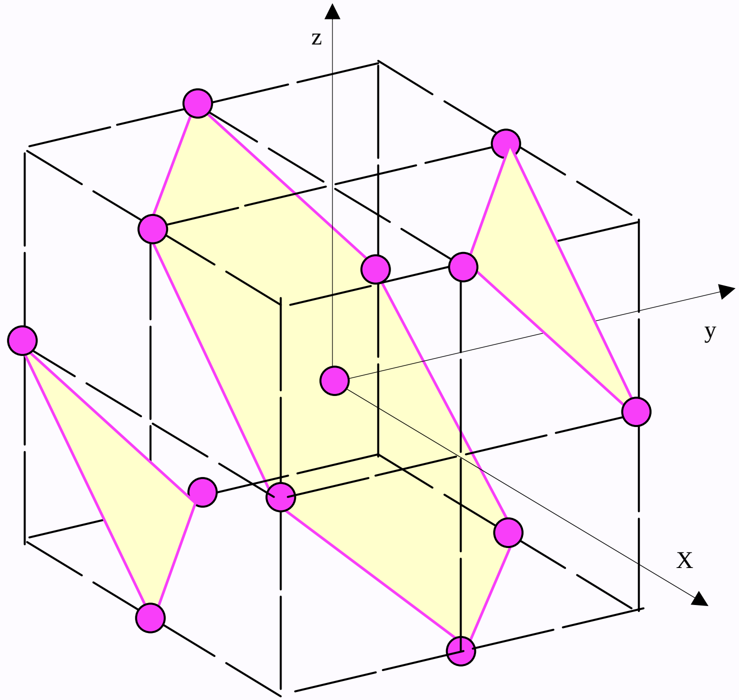
- **Planes “slice through” the basis of physical atoms**

Lattice planes in cubic crystals



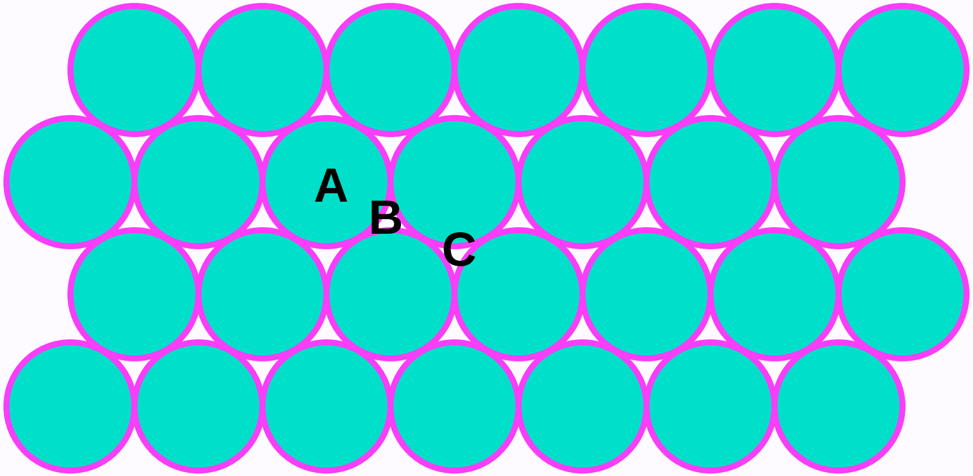
(100) and (110) planes in a cubic lattice
(illustrated for the fcc lattice)

(111) lattice planes in cubic crystals



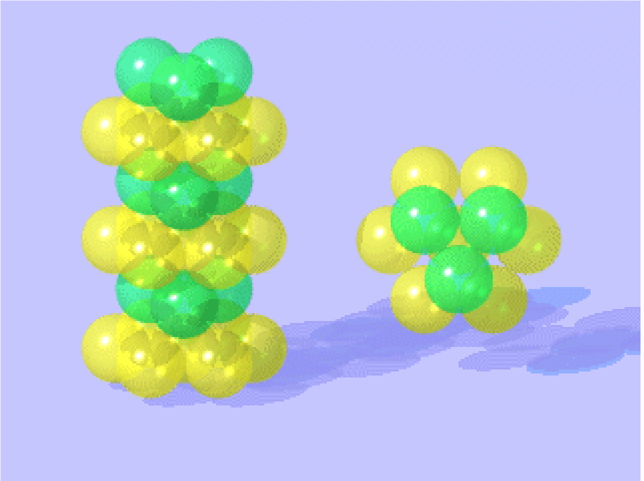
Face Centered Cubic Lattice
Lattice planes perpendicular to [111] direction
Each plane is hexagonal close packed array of points

Stacking hexagonal 2d layers to make close packed 3-d crystal



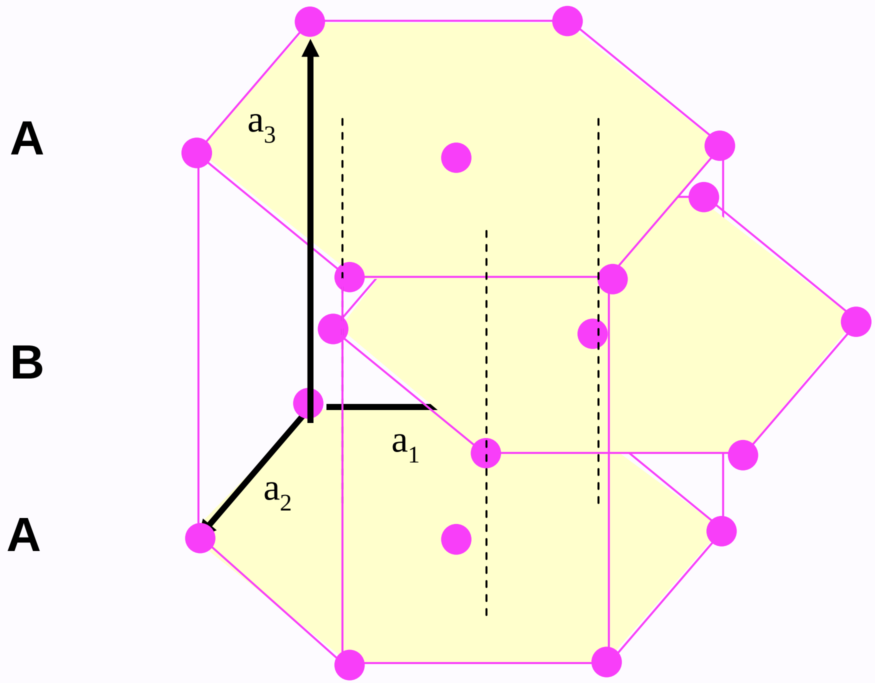
- Each sphere has 12 equal neighbors
- 6 in plane, 3 above, 3 below
- Close packing for spheres
- Can stack each layer in one of two ways, B or C above A
- Also see figure in Kittel

Stacking hexagonal 2d layers to make hexagonal close packed (hcp) 3-d crystal



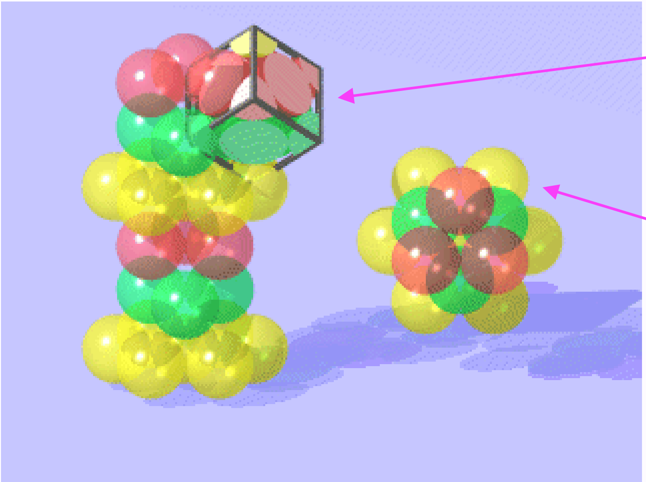
- Each sphere has 12 equal neighbors
- Close packing for spheres
- See figure in Kittel for stacking sequence
- HCP is ABABAB….. Stacking
- Basis of 2 atoms

Hexagonal close packed



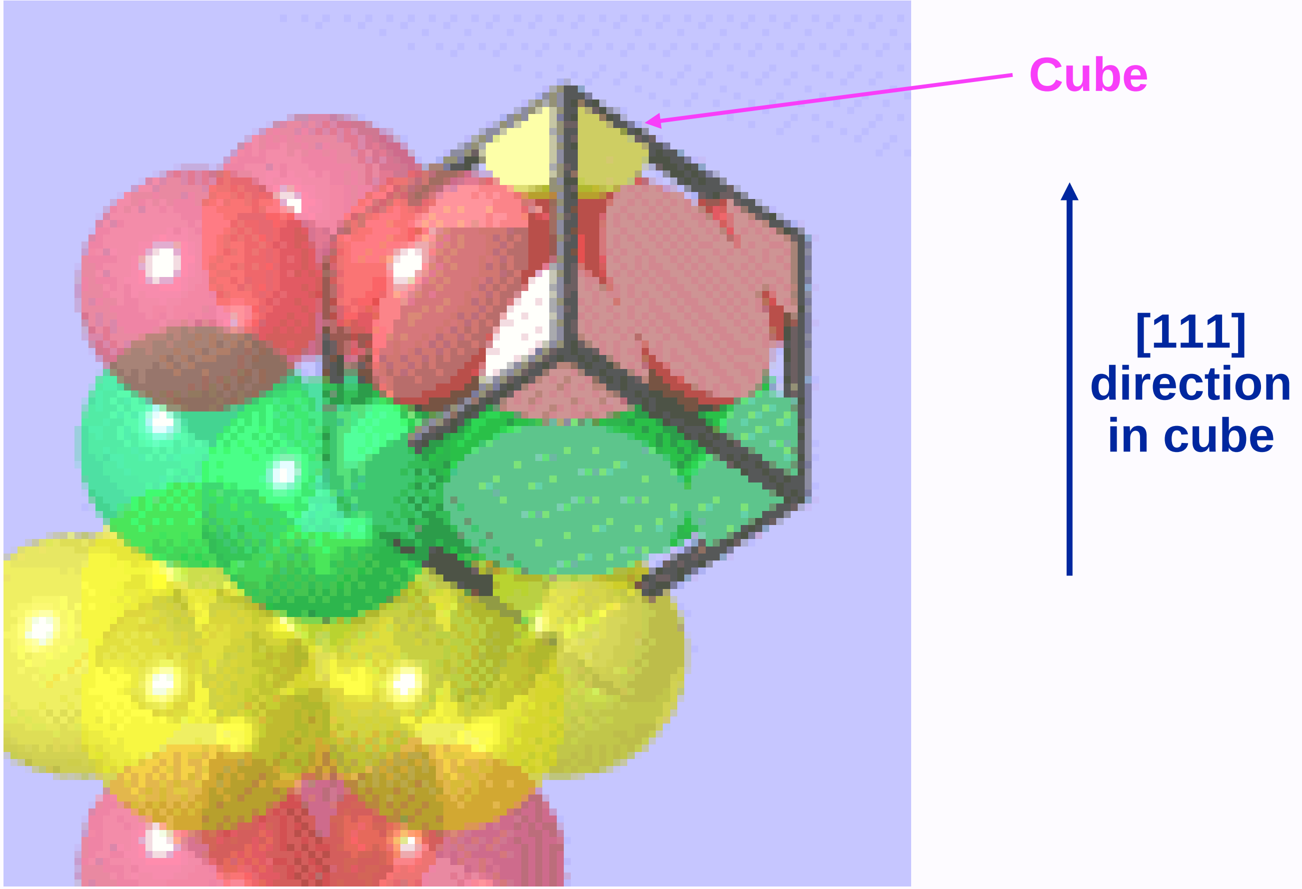
Hexagonal Bravais Lattice
Two atoms per cell

Stacking hexagonal 2d layers to make cubic close packed (ccp) 3-d crystal

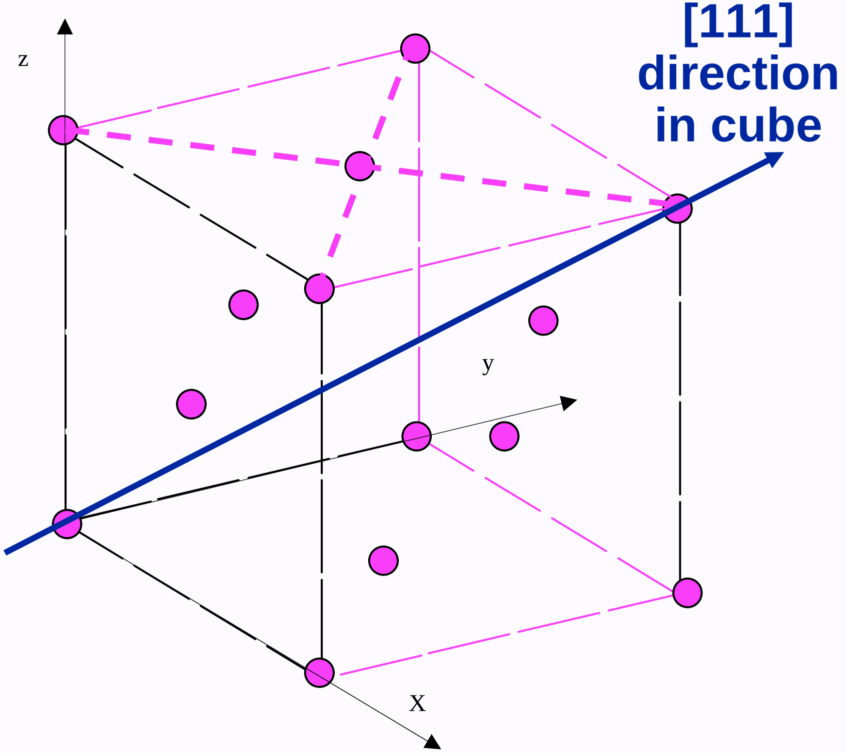


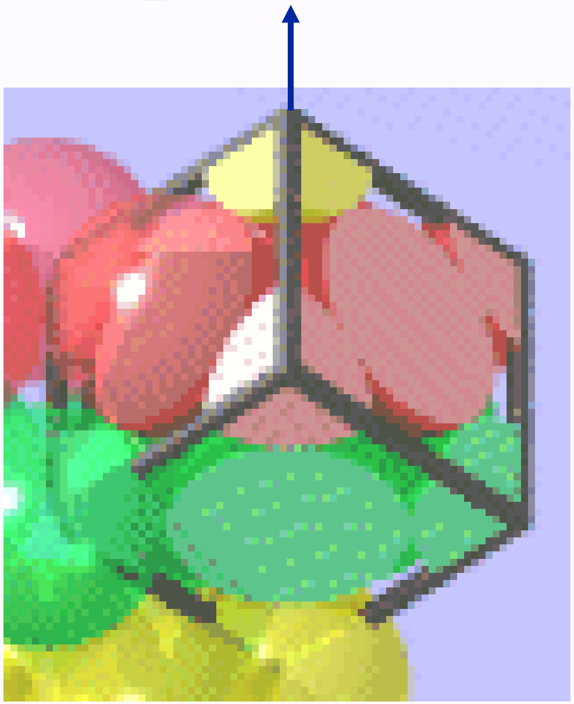
- Each sphere has 12 equal neighbors
- Close packing for spheres
- See figure in Kittel for stacking sequence
- CCP is ABCABCABC….. Stacking
- Basis of 1 atom

Stacking hexagonal 2d layers to make cubic close packed (ccp) 3-d crystal



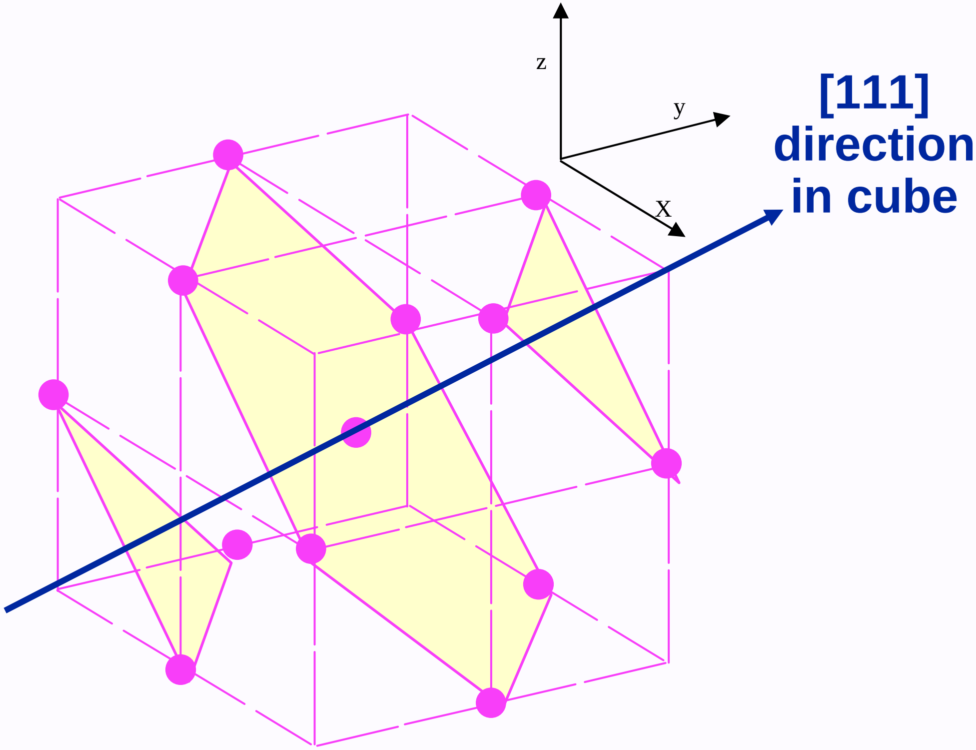
Face Centered Cubic (fcc)
Also called cubic closed packed (ccp)

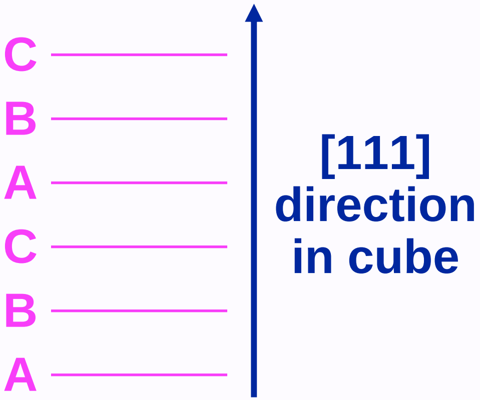




Each atom has 12 equal neighbors
The figure at the right shows the face centered character

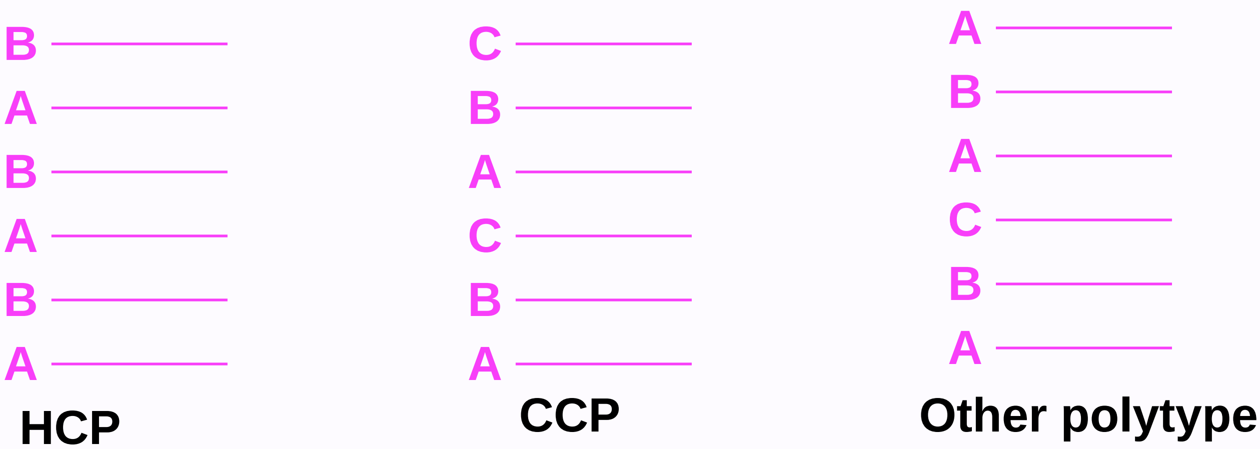
(111) planes in an fcc crystal





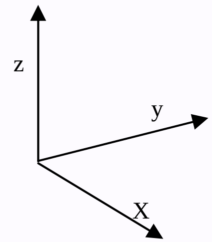
ABCABC... stacking of hexagonal planes ⇒ fcc crystal
fcc is a close packed crtsal – cubic close packed - ccp

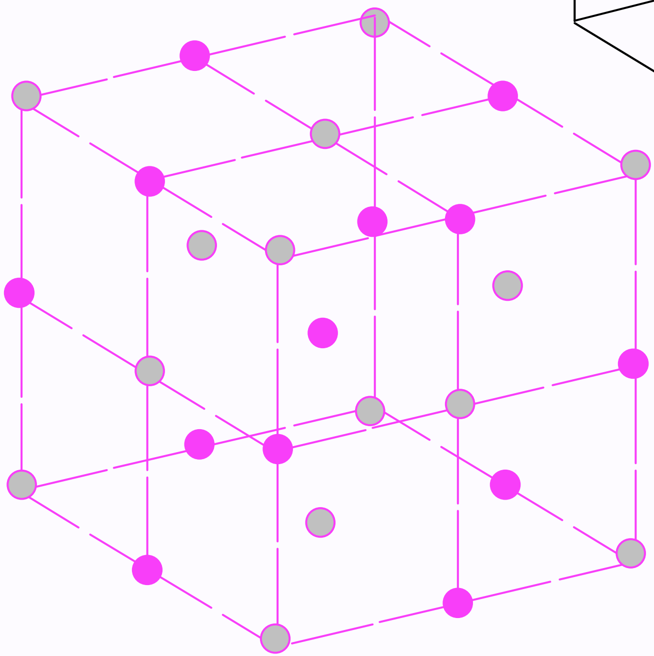
More on stacking hexagonal 2d layers



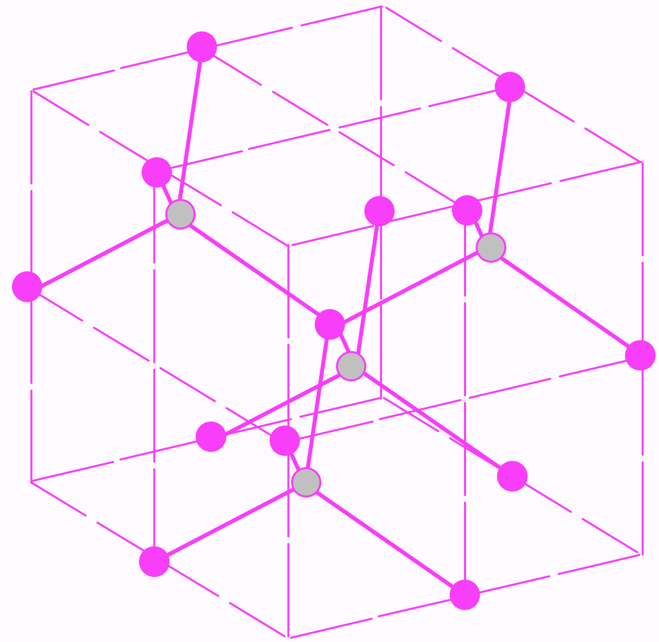
- Infinite number of ways to stack planes
- Polytypes occur in some metals, some compounds like silicon carbide (SiC)

Cubic crystals with a basis



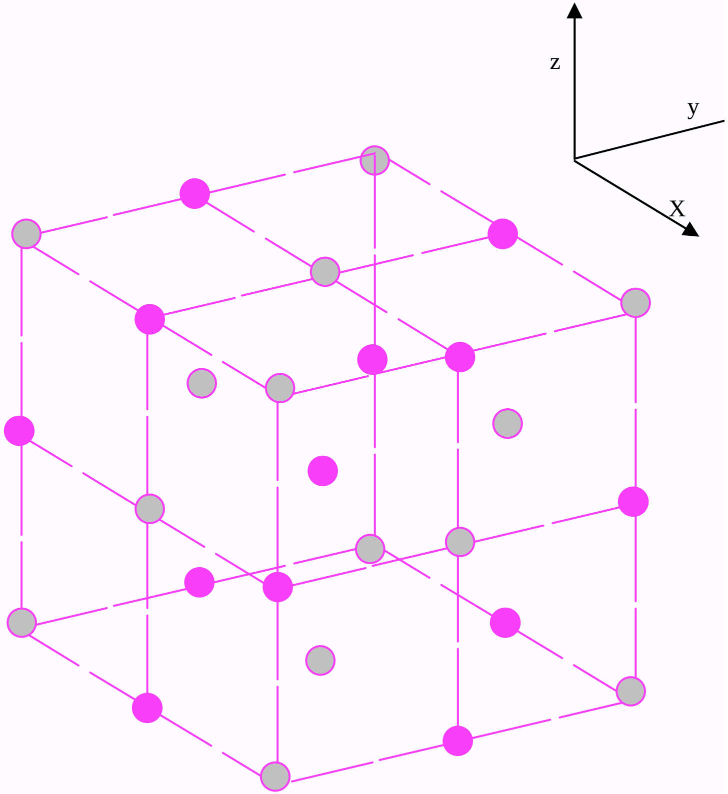


NaCl Structure with
Face Centered Cubic Bravais Lattice

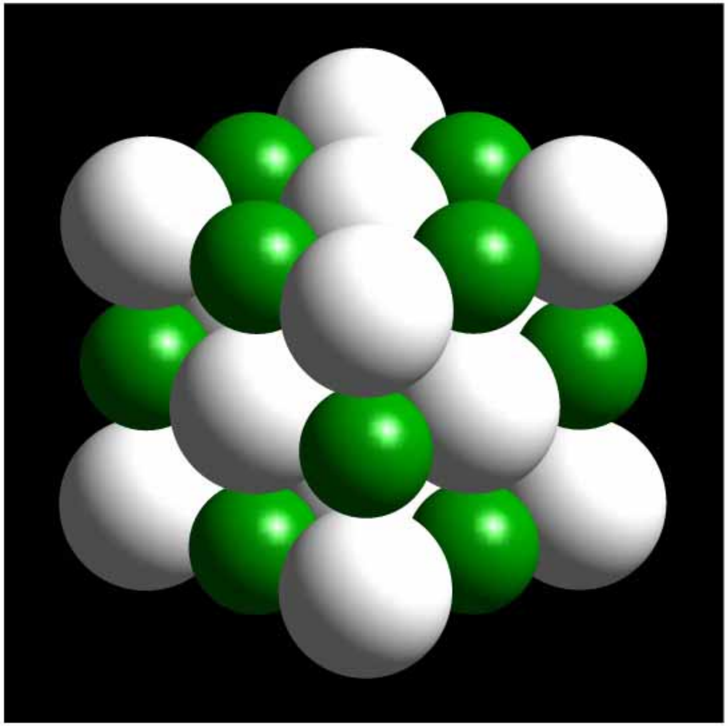


ZnS Structure with
Face Centered Cubic Bravais Lattice
C, Si, Ge form diamond structure with
only one type of atom

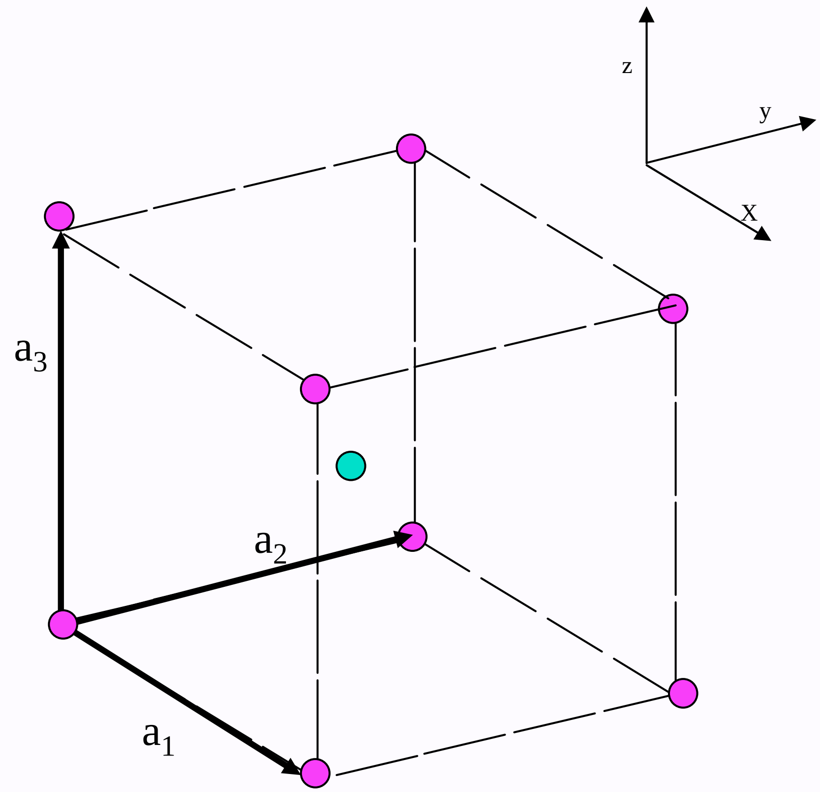
NaCl Structure



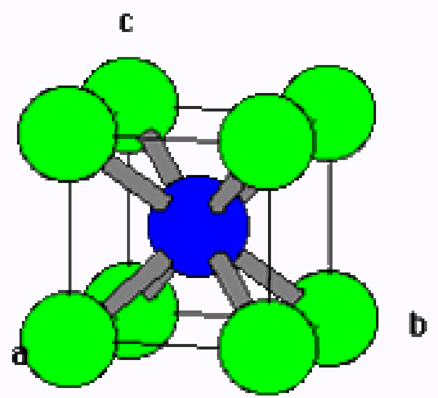
NaCl Structure with
Face Centered Cubic Bravais Lattice

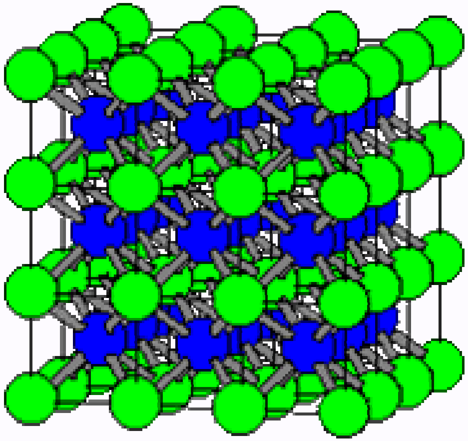


CsCl Structure



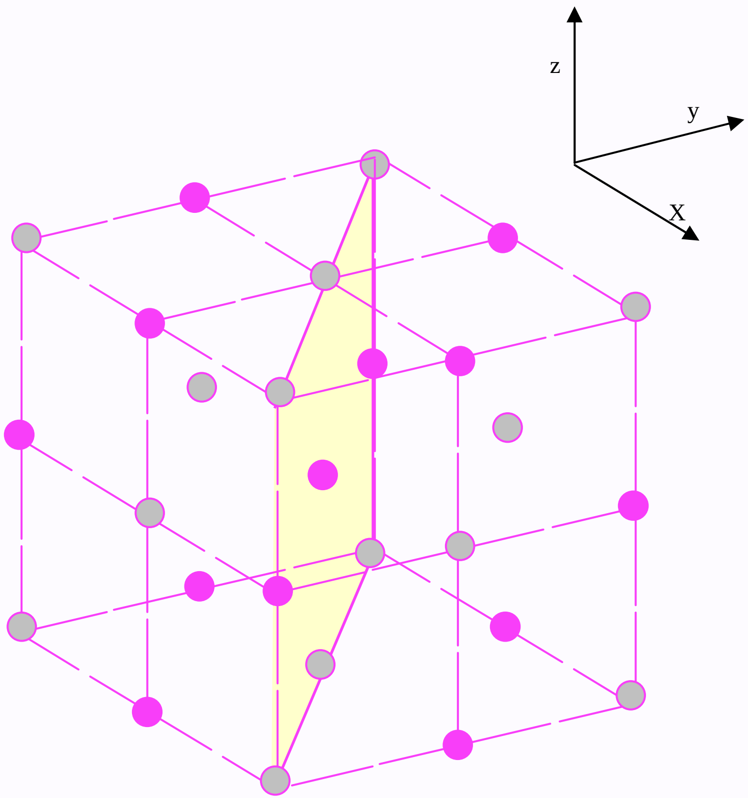
CsCl Structure
Simple Cubic Bravais Lattice



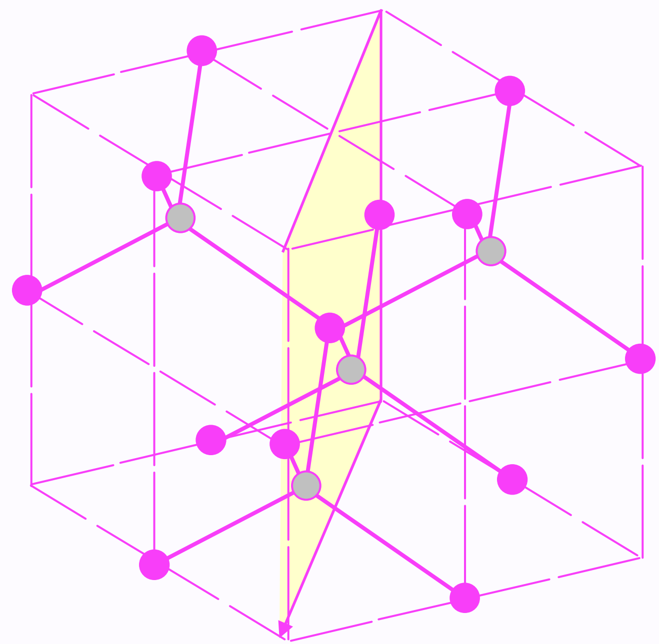


From http://www.ilpi.com/inorganic/structures/cscl/index.html

Atomic planes in NaCl and ZnS crystals

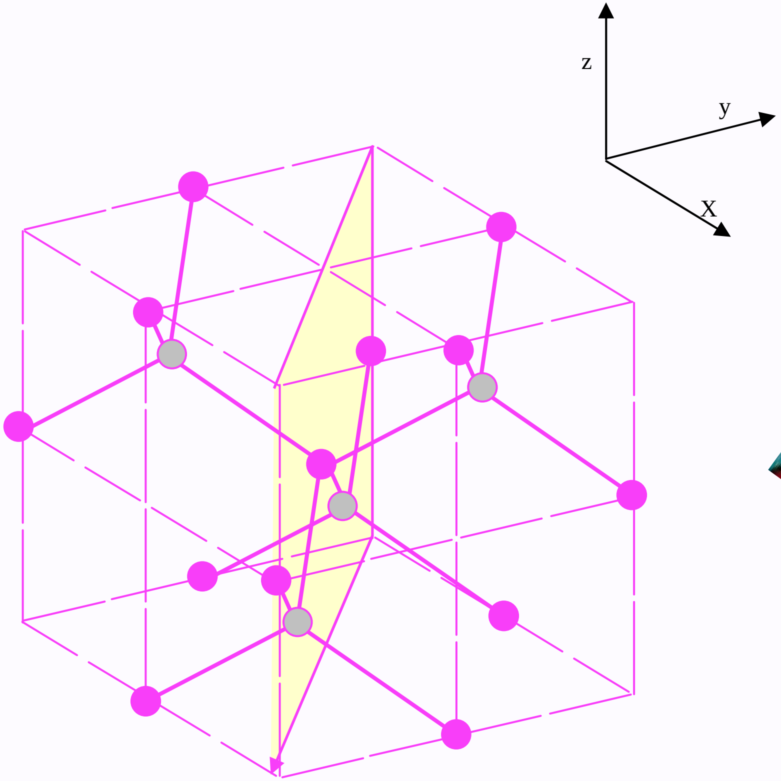


(110) planes in NaCl crystal
rows of the Na and Cl atoms

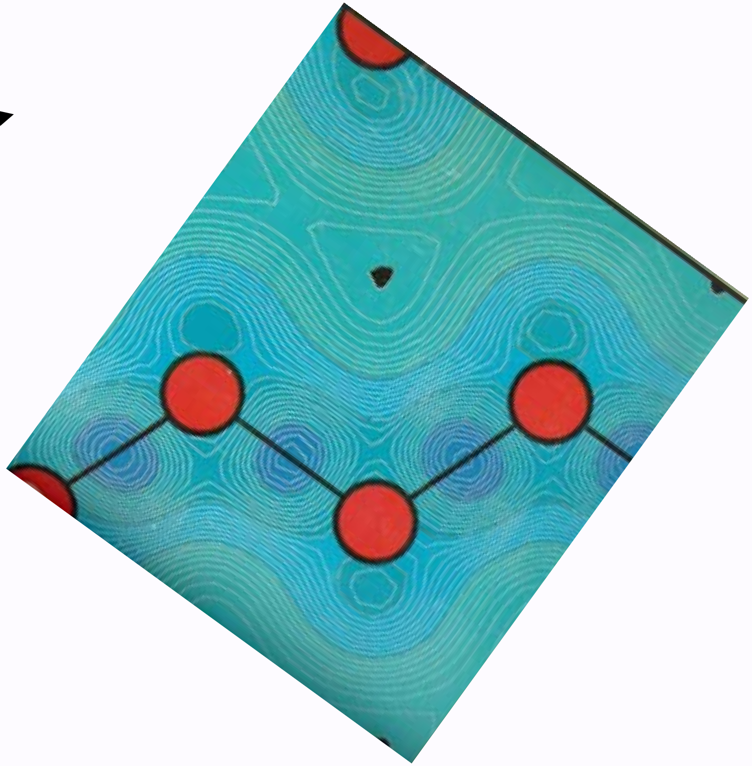


(110) plane in ZnS crystal
zig-zag Zn-S chains of atoms

(110) plane in diamond structure crystal

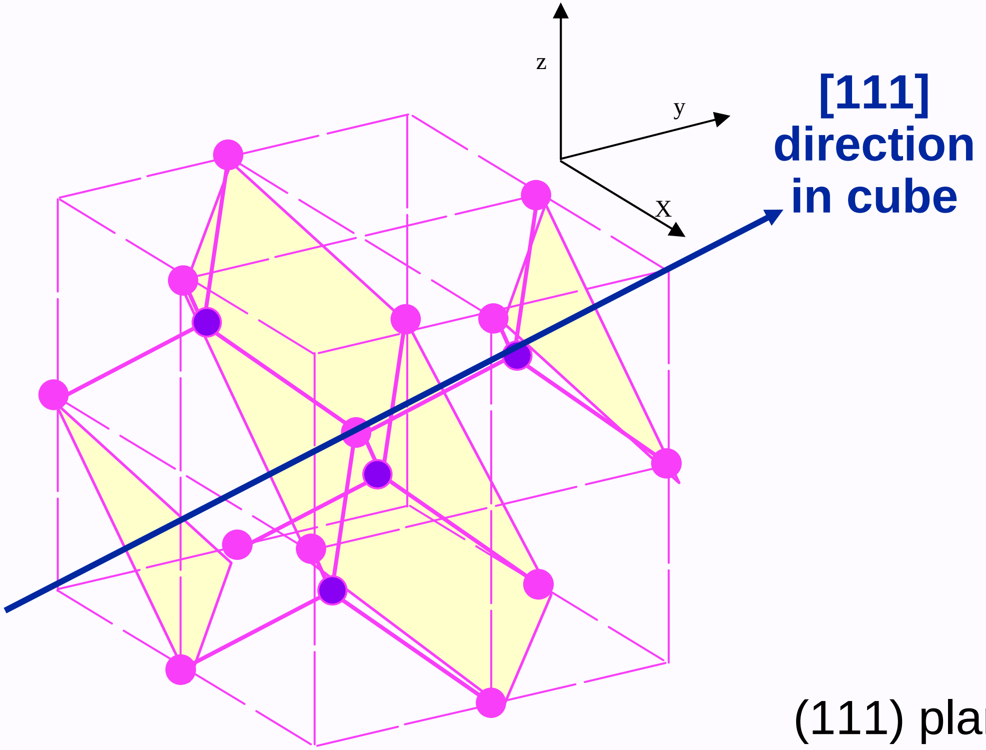


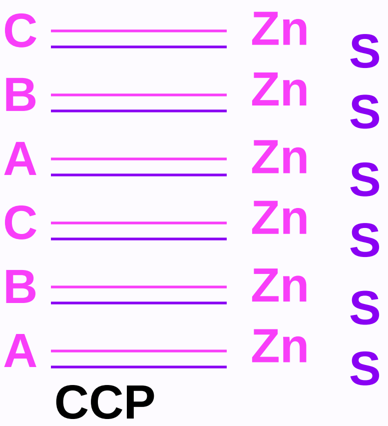
(100) plane in ZnS crystal
zig-zag Zn-S chains of atoms
(diamond if the two atoms are the same)



Calculated valence electron density
in a (110) plane in a Si crystal
(Cover of Physics Today, 1970)

(111) planes in ZnS crystals

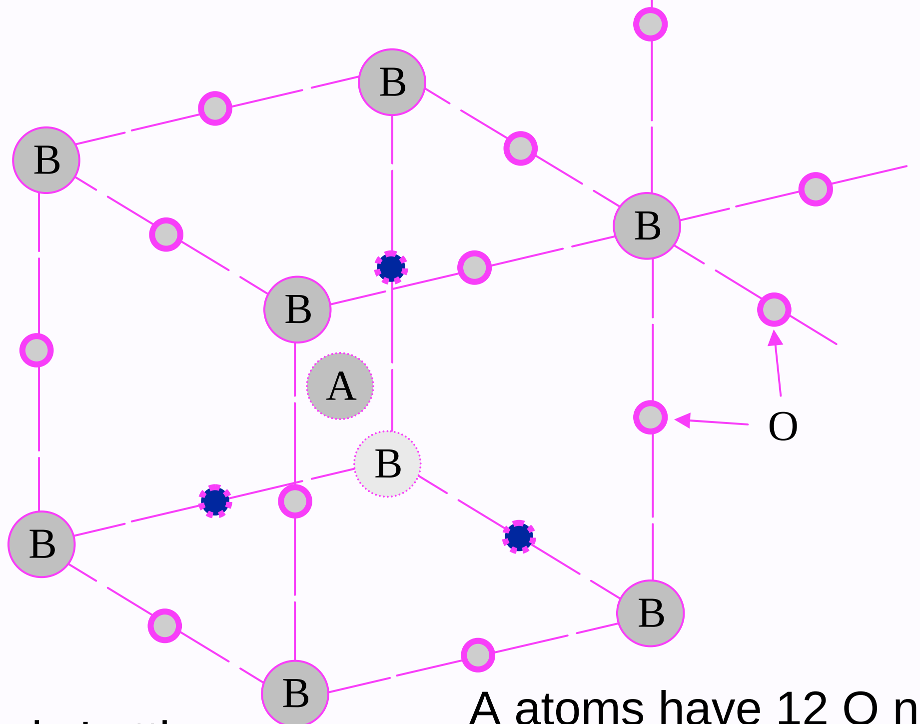




(111) planes in cubic ZnS crystal

Note: ABAB... stacking gives hexagonal ZnS

Perovskite Structure ABO_3



Simple Cubic Bravais Lattice

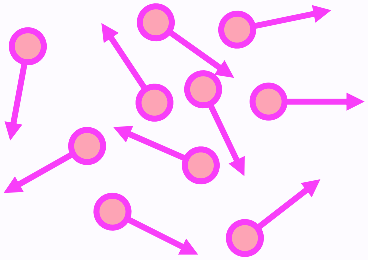
A atoms have 12 O neighbors
B atoms have 6 closer O neighbors

Many compounds form the perovskite structure,
$SrTiO_3$, $BaTiO_3$, $LaMnO_3$, . . .

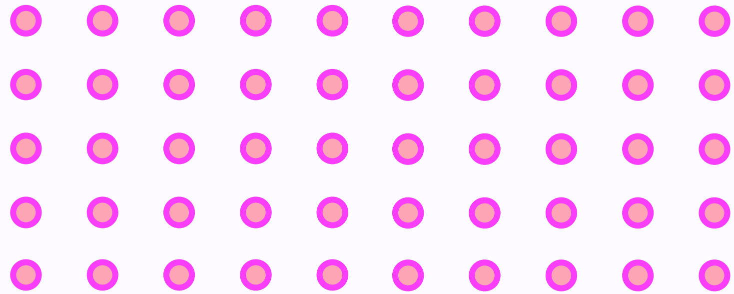
Symmetries of crystals in 3 dimensions

- **All Crystals can be classified by:**
- **7 Crystal systems (triclinic, monoclinic, orthorhombic, tetragonal, cubic, hexagonal, trigonal)**
- **14 Bravais Lattices (primitive, face-centered or body-centered for each system – 14 of the 7x3 possibilities describe all Bravais lattices)**
- **32 Points groups (rotations, inversion, reflection)**
- **See references in Kittel Ch 1,   G. Burns, "Solid State Physics"**

Is a crystal really different from a liquid?



Liquid



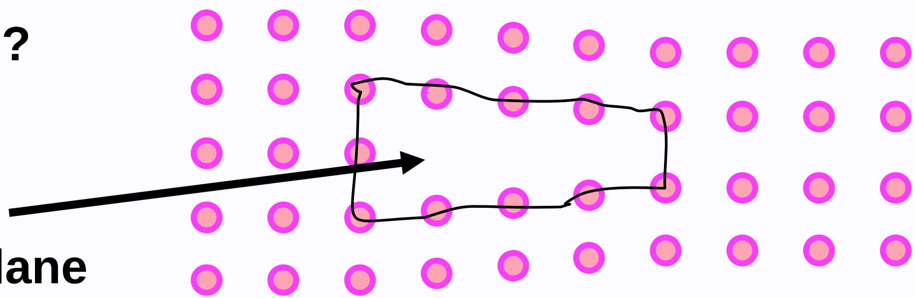
Crystal

Yes – the crystal has "order" – different directions are different

Other crucial differences?

Yes – dislocations

Example of a dislocation
-a crystal with an extra plane
of atoms on the left
- The dislocation can move but
it cannot disappear!



Crystal with a "dislocation"

Important for deformations, … See Kittel Ch. 20

Next Time

- Diffraction from crystals
- Reciprocal lattice
- Read Kittel Ch 2