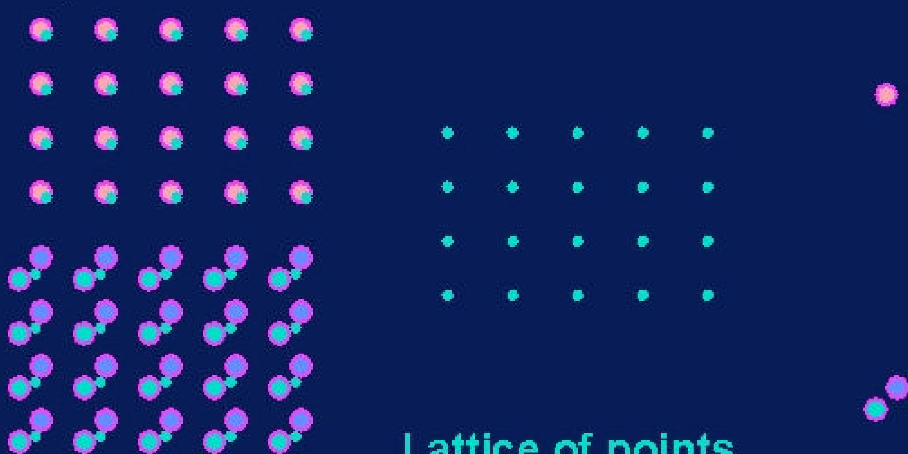
Crystals

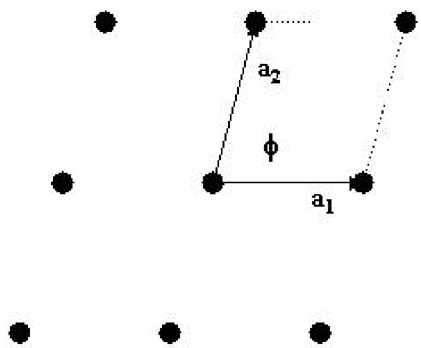
- A crystal is a repeated array of atoms
- Crystal = Lattice + Basis

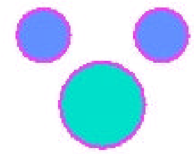


Classification of Crystal Structures

- Crystal structures classified by:
- Translation symmetry
  - Only the Bravais lattice
  - Limited number of possible crystal translation types
- Rotation, Inversion, reflection symmetry
  - Depends upon basis
  - Limited number of possible crystal types
- Examples in 2 dimensions, 3 dimensions
- See Kittel for lists of possible translation types, other crystallography references for all possible crystal types

Two Dimensional Crystals



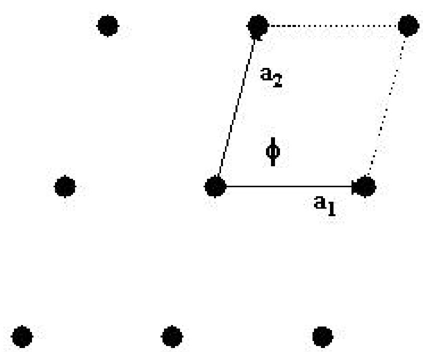


Basis

Lattice

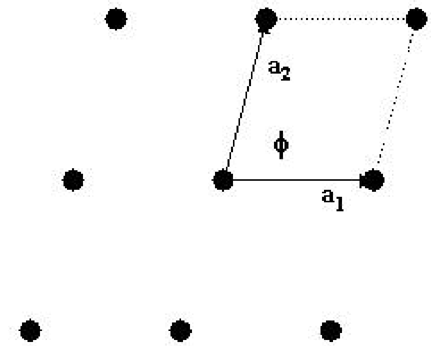
- Infinite number of possible crystals
- Finite number of possible crystal types

Lattices and Translations



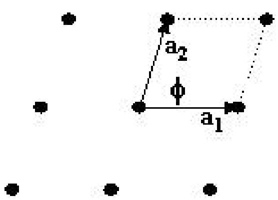
- The entire infinite lattice is specified by the primitive vectors a_1 and a_2 (also a_3 in 3-d)
- $T(n_1, n_2, \ldots) = n_1 a_1 + n_2 a_2$ ($+ n_3 a_3$ in 3-d), where the n's are integers

Possible Two Dimensional Lattices

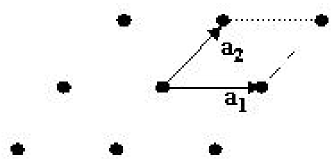


- Special angles ϕ = 90 and 60 degrees lead to special crystal types
- In addition to translations, the lattice is invariant under rotations and/or reflections

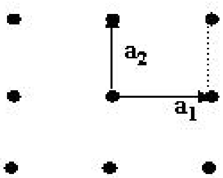
Possible Two Dimensional Lattices



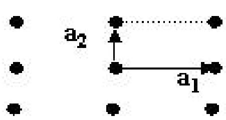
General oblique



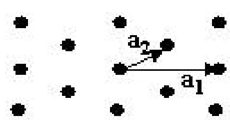
Hexagonal $\Phi = 60$, $a_1 = a_2$
6-fold rotation , reflections



Square
4-fold rot., reflect.



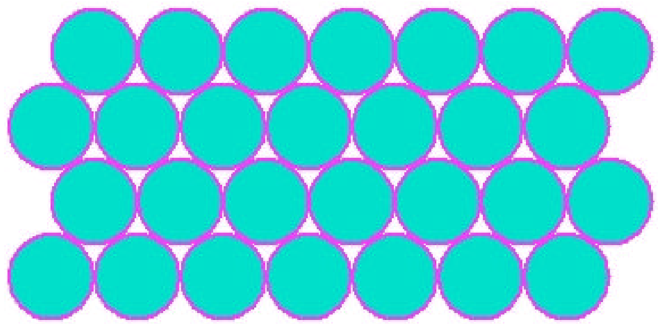
Rectangular
2-fold rot., reflect.



Centered Rectangular
2-fold rot., reflect.

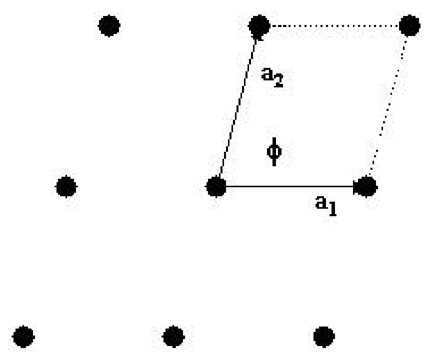
- These are the only possible special crystal types in two dimensions

Close packing of spheres in a 2-d crystal



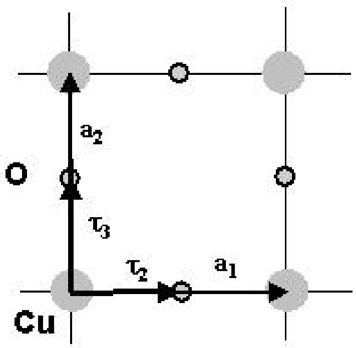
- Each sphere has 6 equal neighbors
- Close packing for spheres
- Hexagonal symmetry (rotation by 60 degrees)

More on Two Dimensional Lattices

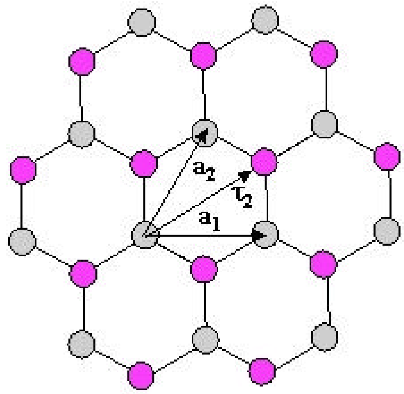


- Why cannot there be a five-fold rotation in a crystal lattice?
- Why is the centered square not a special type?

Crystalline layers with >1 atom basis



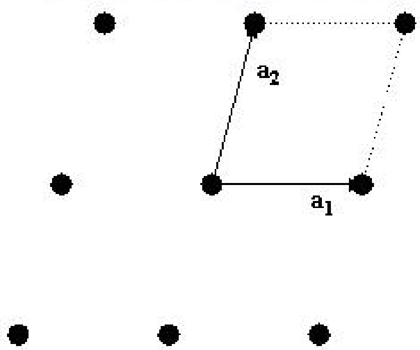
CuO_2 Square Lattice



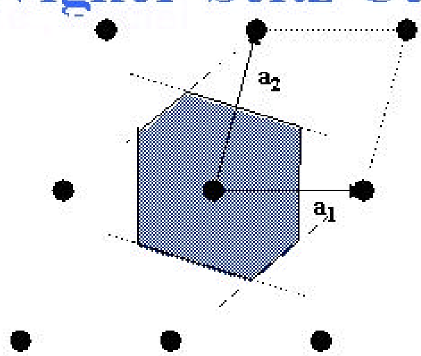
Honeycomb Lattice
(Graphite or BN layer)

- Left - layers in the High Tc superconductors
- Right - single layer of carbon graphite or hexagonal BN (the two atoms are chemically different in BN, not in C)

Two Dimensional Lattices
Primitive Cell and Wigner-Seitz Cell



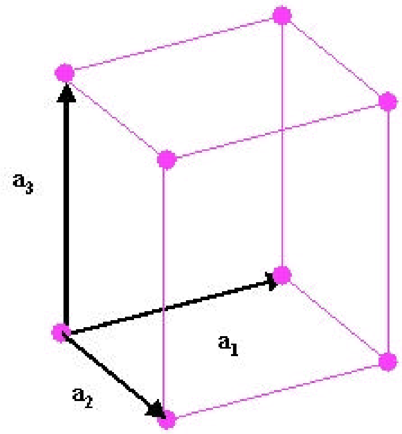
One possible Primitive Cell



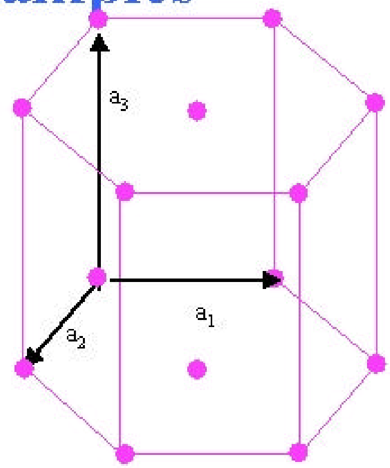
Wigner-Seitz Cell -- Unique

- All primitive cells have same area (volume)
- Wigner Seitz Cell is most compact, highest symmetry cell possible
- Also same rules in 3 dimensions

Three Dimensional Lattices
Simplest examples



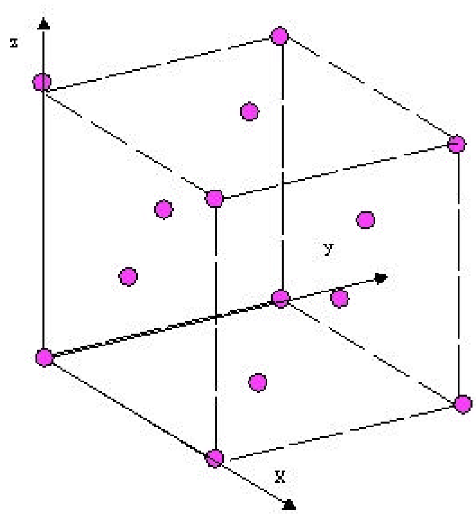
Simple Orthorhombic Bravais Lattice

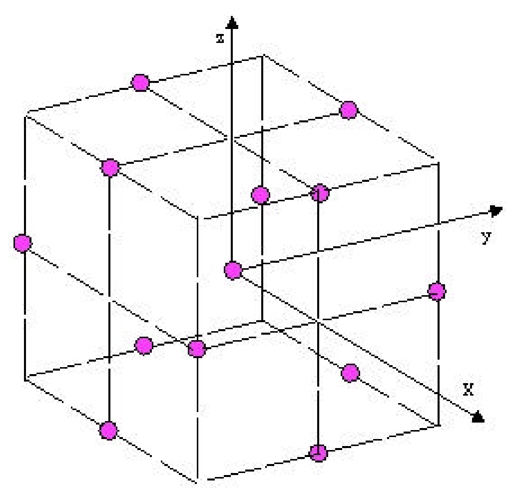


Hexagonal Bravais Lattice

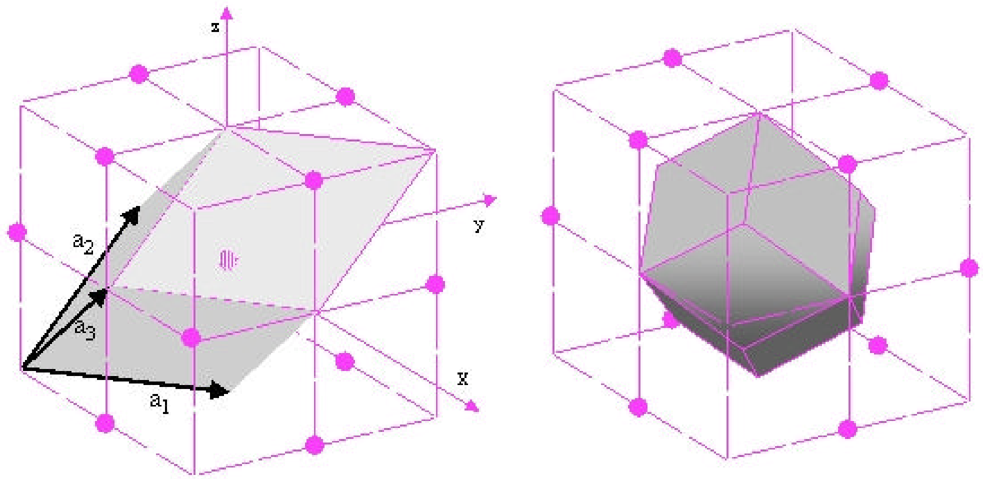
- **Orthorhombic: angles 90 degrees, 3 lengths different**
  Tetragonal: 2 lengths same; Cubic: 3 lengths same
- **Hexagonal: a_3 different from a_1, a_2 by symmetry**

Face Centered Cubic
Two views - Conventional Cubic Cell





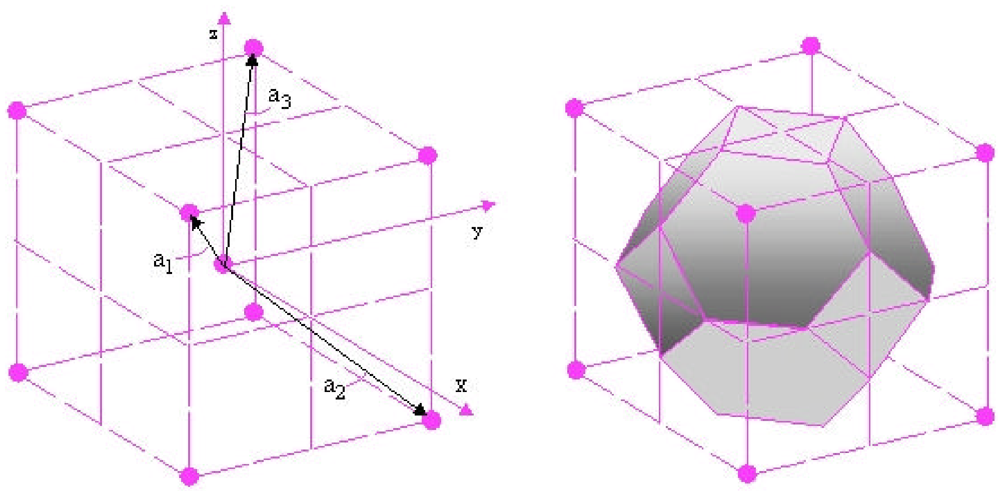
Conventional Cell of Face Centered Cubic Lattice
4 times the volume of a primitive cell



One Primitive Cell

Wigner-Seitz Cell

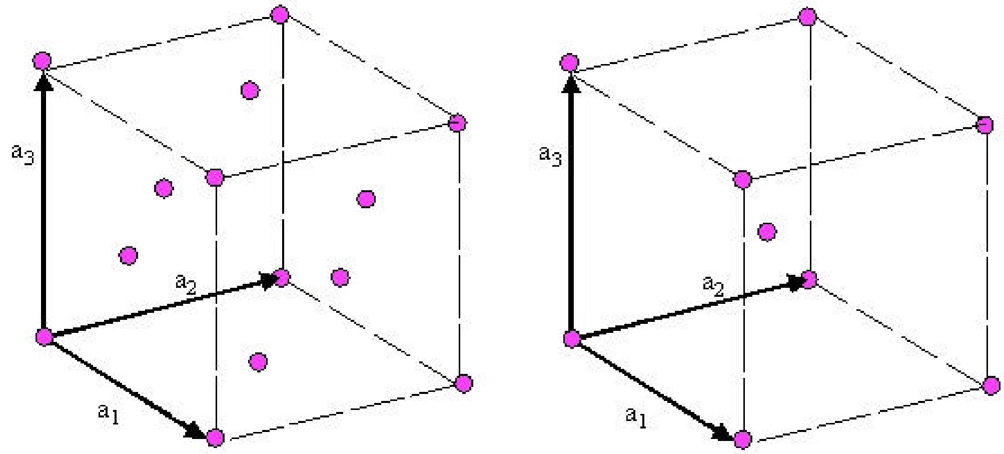
Face Centered Cubic Lattice



Body Centered Cubic Lattice

Wigner-Seitz Cell for
Body Centered Cubic Lattice

Conventional Cell
Face Centered and Body Centered

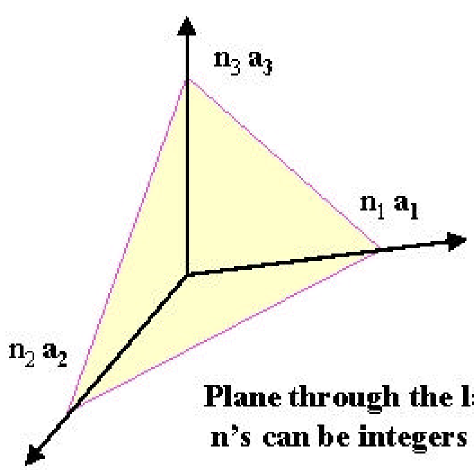


Conventional Cells

BCC: atoms at (000), (1/2,1/2,1/2)

FCC: atoms at (000), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0)

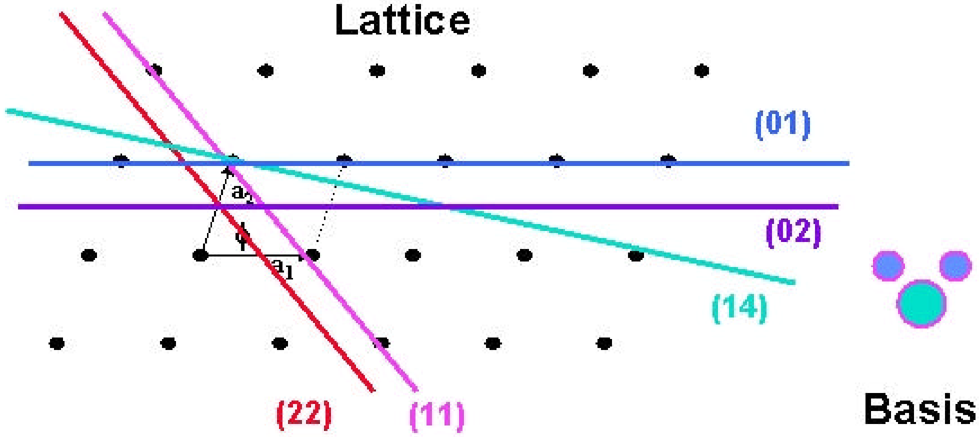
Lattice Planes - Index System



Plane through the lattice n_1 $\mathbf{a}_1$, n_2 $\mathbf{a}_2$, $n_3\mathbf{a}_3$
n's can be integers or rational fractions

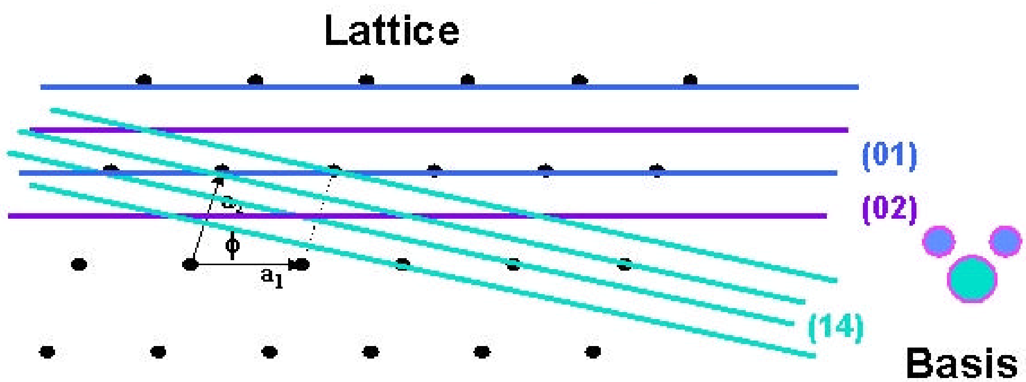
- **Define the plane by the reciprocals $1/n_1$, $1/n_2$, $1/n_3$**
- **Reduce to three integers with same ratio h,k,l**
- **Plane is defined by h,k,l**

Schematic illustrations of lattice planes Lines in 2d crystals



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

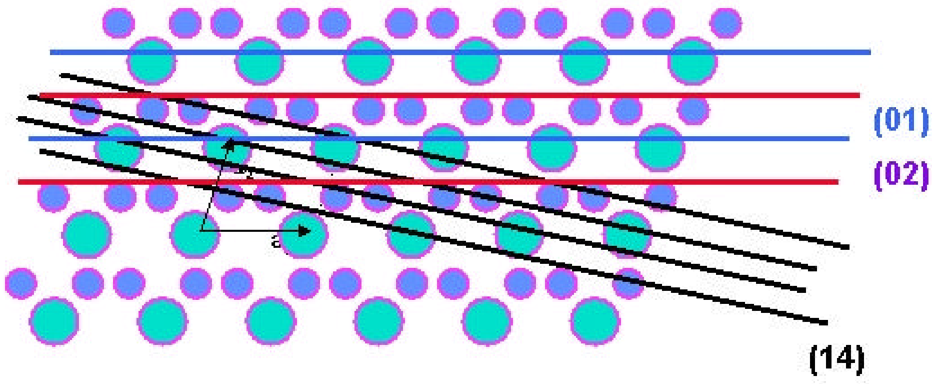
Schematic illustrations of lattice planes Lines in 2d crystals



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

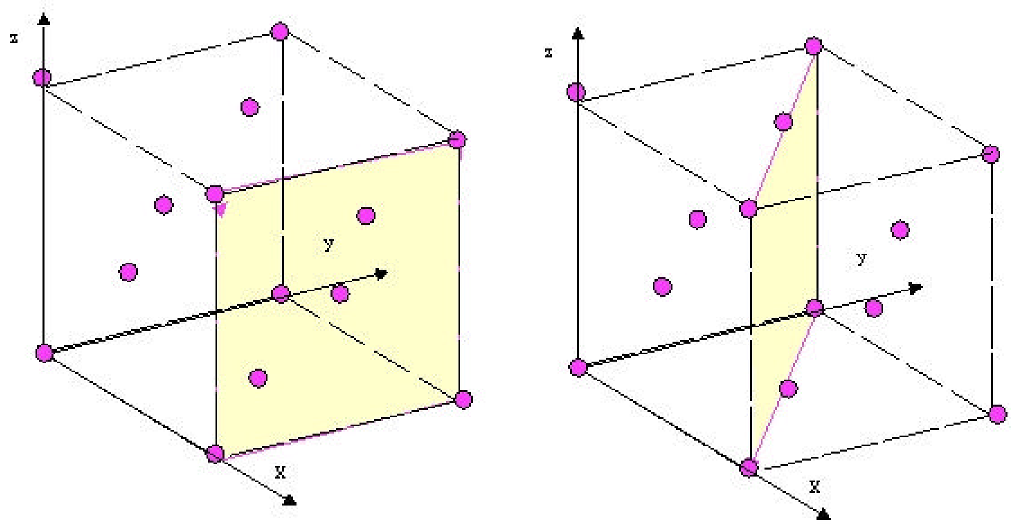
Obtenido del curso de Richard Martin: http://www.physics.uiuc.edu/research/electronicstructure/389/

Schematic illustrations of lattice planes
Lines in 2d crystals



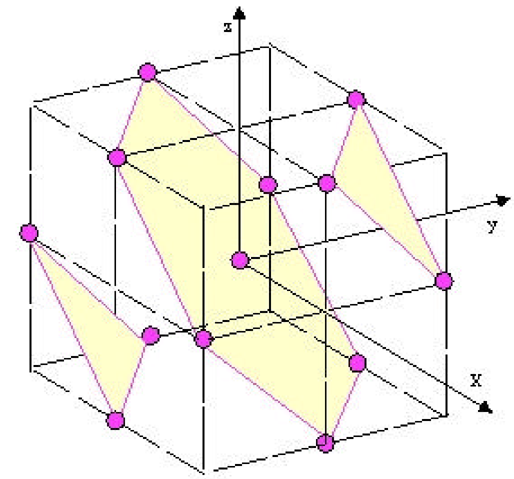
- Planes "slice through" the basis of physical atoms

Lattice planes in cubic crystals



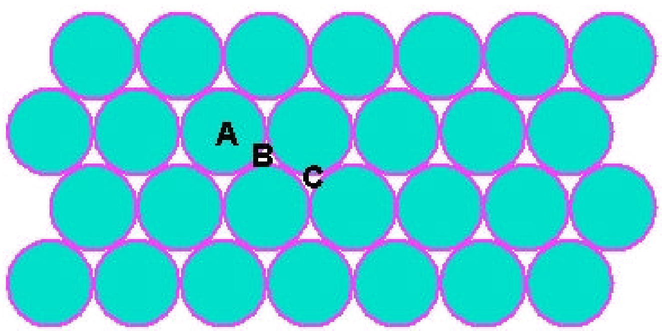
(100) and (110) planes in a cubic lattice
(illustrated for the fcc lattice)

(111) lattice planes in cubic crystals



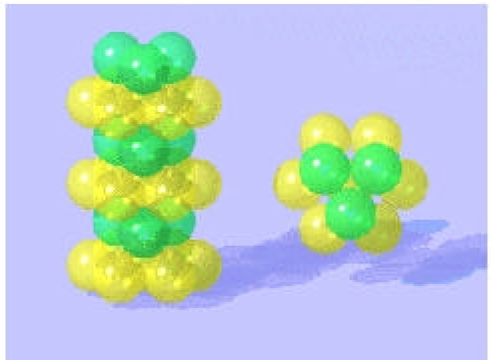
Face Centered Cubic Lattice
Lattice planes perpendicular to [111] direction
Each plane is hexagonal close packed array of points

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



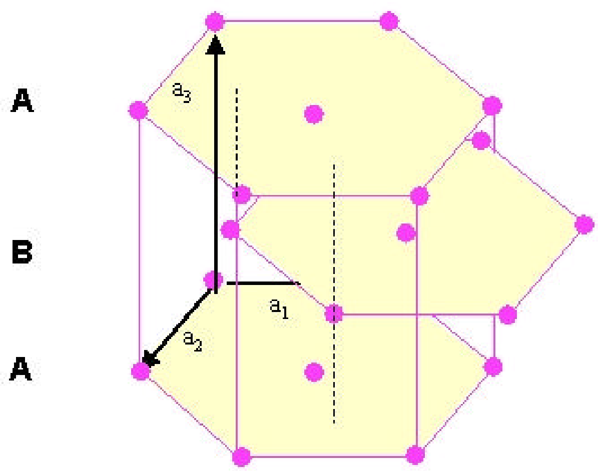
- Each sphere has 12 equal neighbors
- 6 in plane, 3 above, 3 below
- Close packing for spheres
- Can stack each layer in one of two ways, B or C above A
- Also see figure in Kittel

Stacking hexagonal 2d layers to mak hexagonal close packed (hcp) 3-d crys



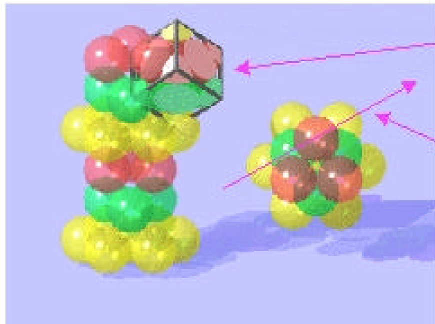
- Each sphere has 12 equal neighbors
- Close packing for spheres
- See figure in Kittel for stacking sequence
- HCP is ABABAB….. Stacking
- Basis of 2 atoms

Hexagonal close packed



Hexagonal Bravais Lattice
Two atoms per cell

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



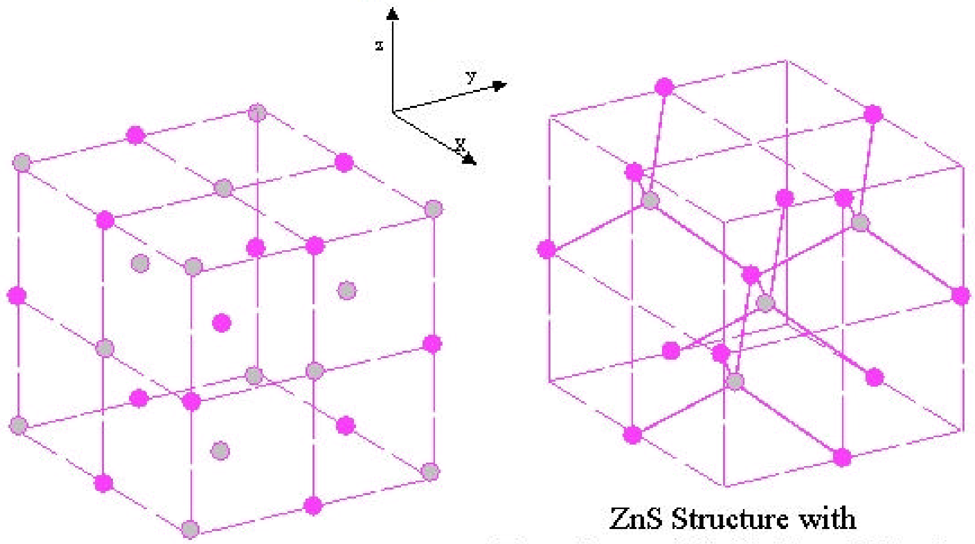
- Each sphere has 12 equal neighbors
- Close packing for spheres
- See figure in Kittel for stacking sequence
- CCP is ABCABCABC….. Stacking
- Basis of 1 atom

More on stacking hexagonal 2d layers

HCP	CCP	Other polytype
B	C	A
A	B	B
B	A	A
A	C	C
B	B	B
A	A	A

- Infinite number of ways to stack planes
- Polytypes occur in some metals, materials like SiC

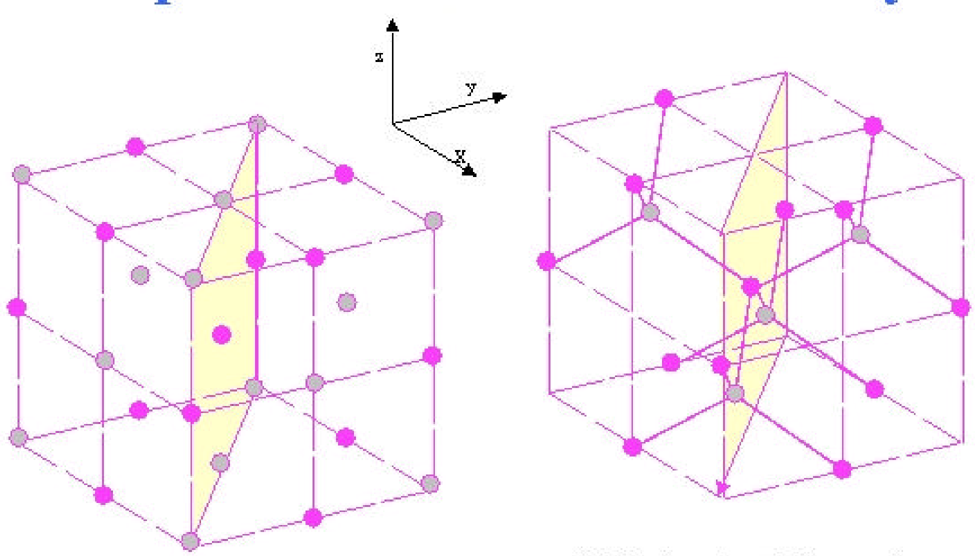
Cubic crystals with a basis



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

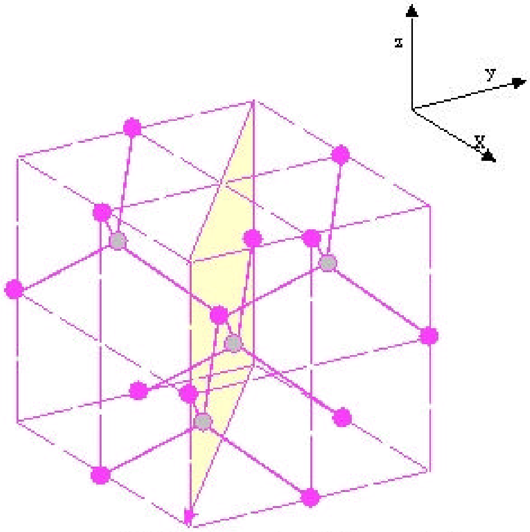
Atomic planes in NaCl and ZnS crystals



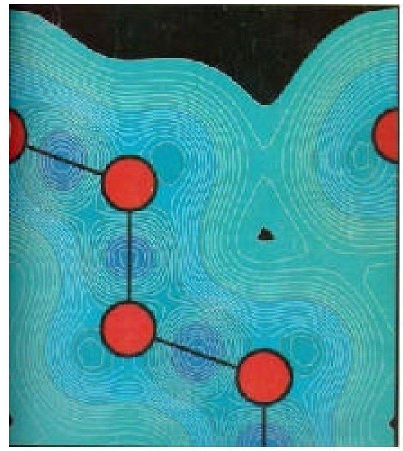
(110) planes in NaCl crystal
rows of the Na and Cl atoms

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

(110) plane in diamond structure crystal

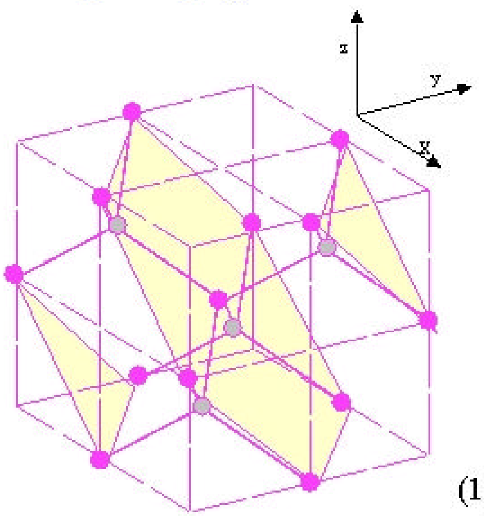


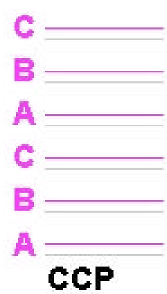
(100) plane in ZnS crystal
zig-zag Zn-S chains of atoms
(diamond if the two atoms are the same)



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

(111) planes in ZnS crystals

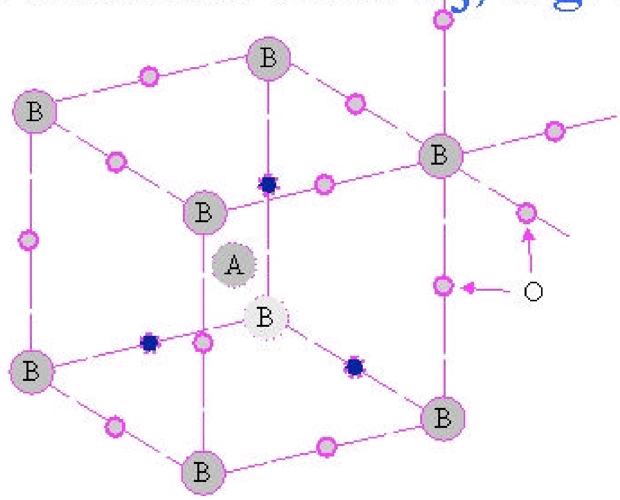




(111) plane in cubic ZnS crystal
unequal spaced planes of Zn and S atoms

ABAB... stacking gives hexagonal ZnS crystal

Perovskite Structure ABO_3, e.g. $BaTiO_3$



Simple Cubic Bravais Lattice

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

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 of the 7 systems)
- 32 Points groups (rotations, inversion, reflection)
- See references in Kittel Ch 1, G. Burns, "Solid State Physics"