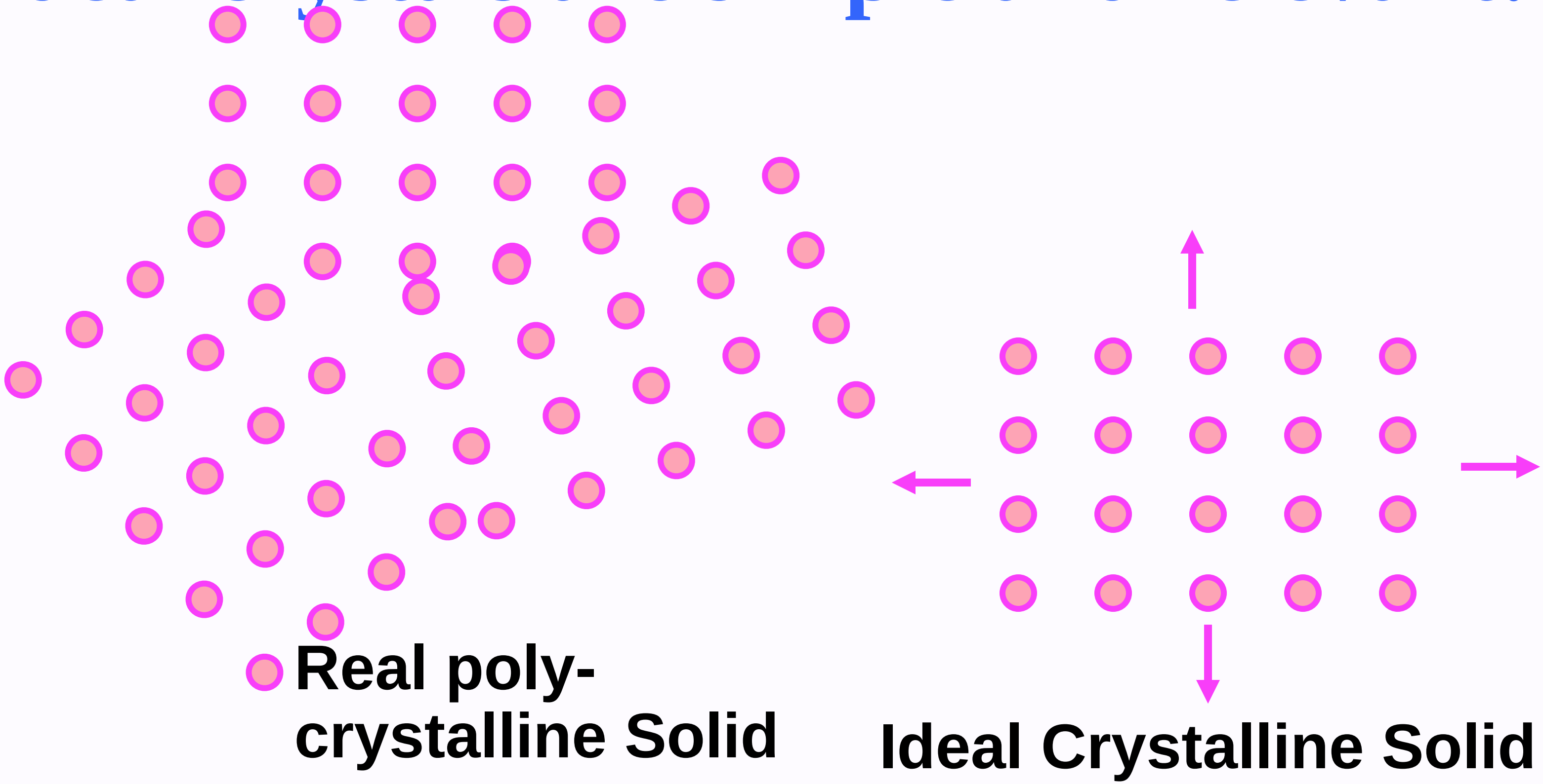
Solid State Physics 460- Lecture 2
Structure of Crystals
(Kittel Ch. 1)

See many great sites like "Bob's rock shop" with pictures and crystallography information on the web at

www.rockhounds.com/rockshop/xtal/index.html

Ideal crystals are simple and relevant!

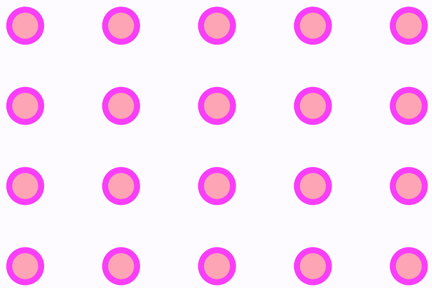


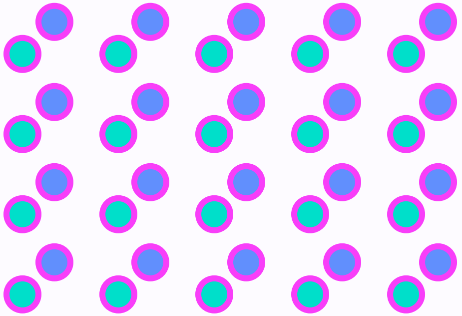
- **Many solids are made of crystallites that are microscopic - but contain ~ 10^{20} atoms!**

Crystals

- A crystal is a repeated array of atoms

- Examples

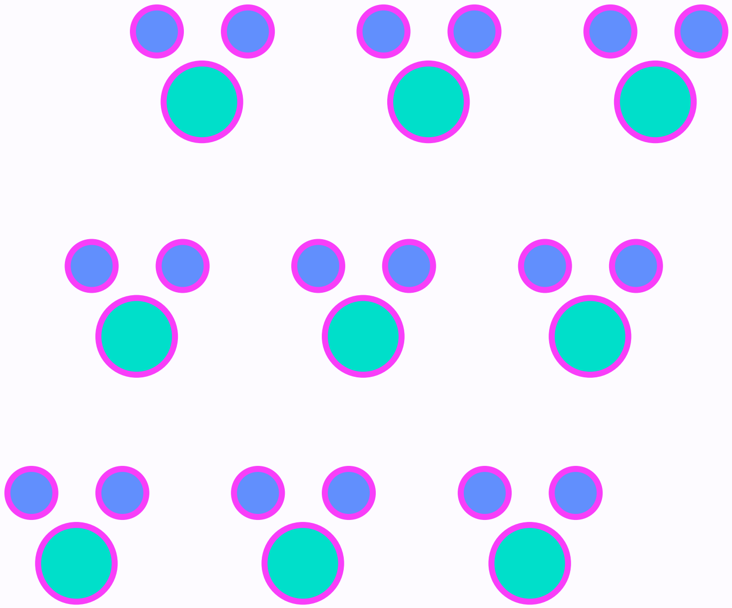




Array of atoms
Each atom is identical

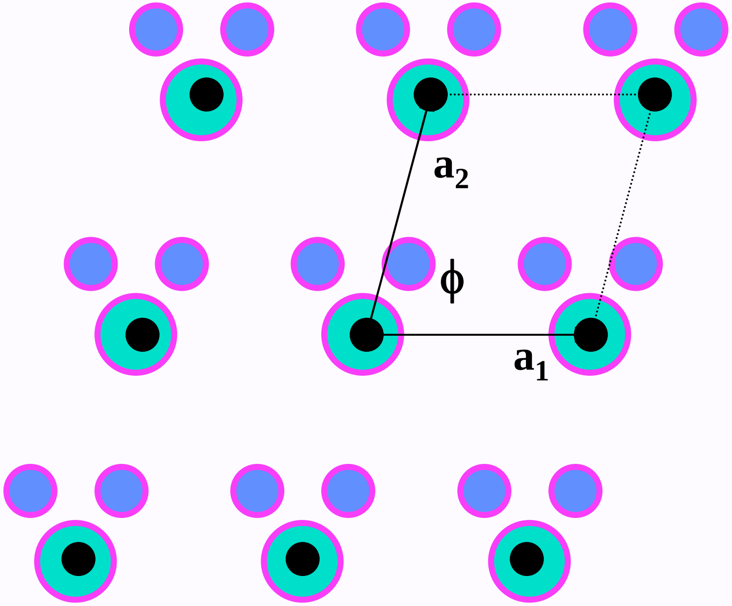
Array of atoms
Two types of atoms

Two Dimensional Crystals



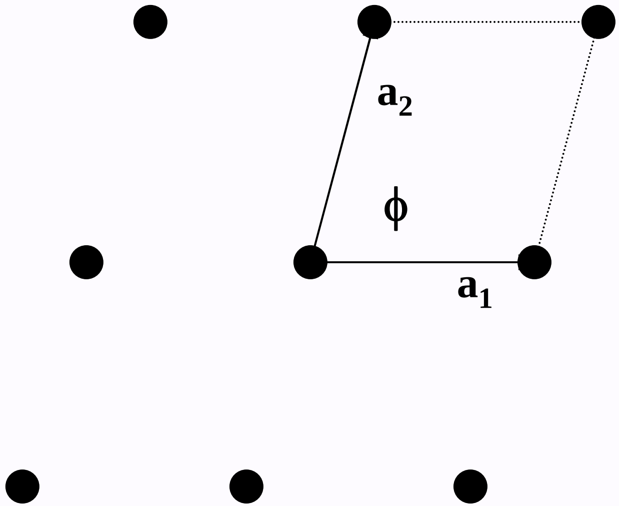
(Easier to draw in 2 dimensions – 3 dimensions later)

Two Dimensional Crystals

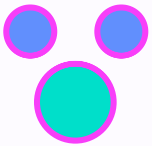


Lattice

Two Dimensional Crystals



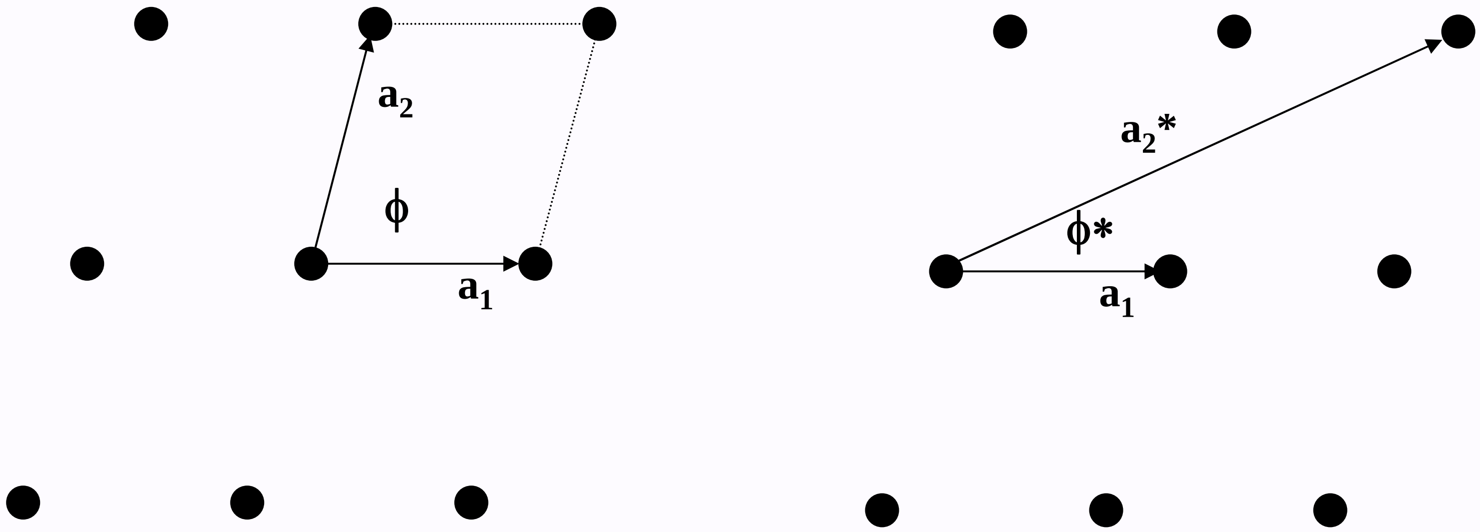
Lattice



Basis

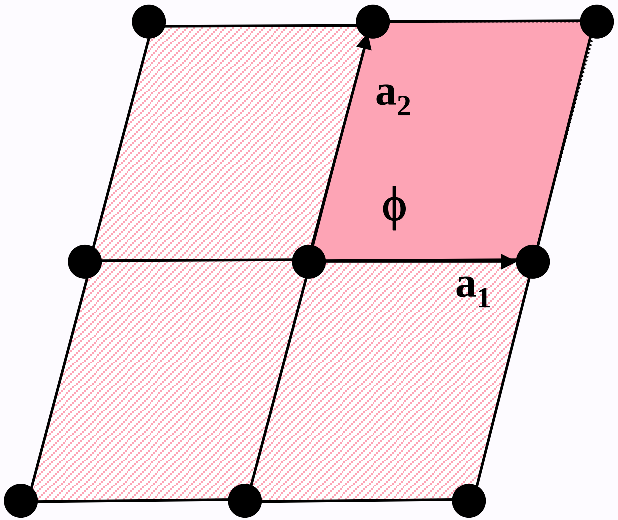
- Infinite number of possible crystals
- Finite number of possible crystal types

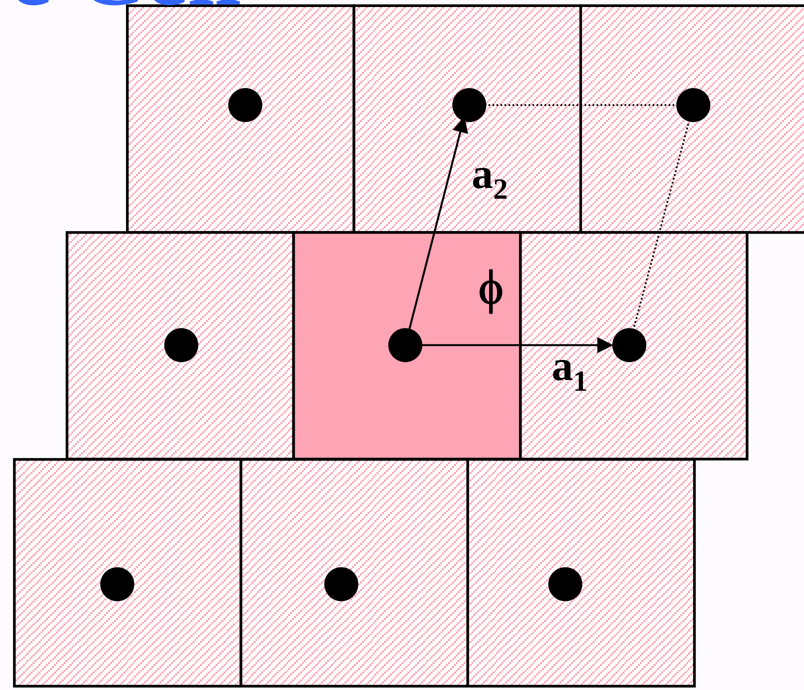
Lattices and Translations



- The entire infinite lattice is specified by 2 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
- Note: the primitive vectors are not unique different vectors a_1 and a_2 can define the same lattice

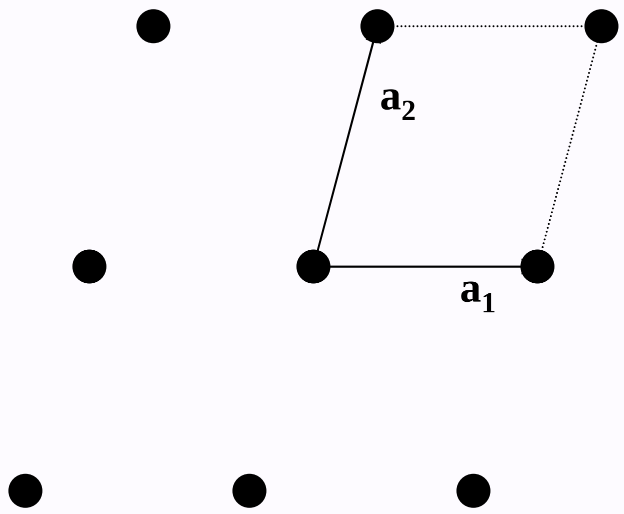
Primitive Cell



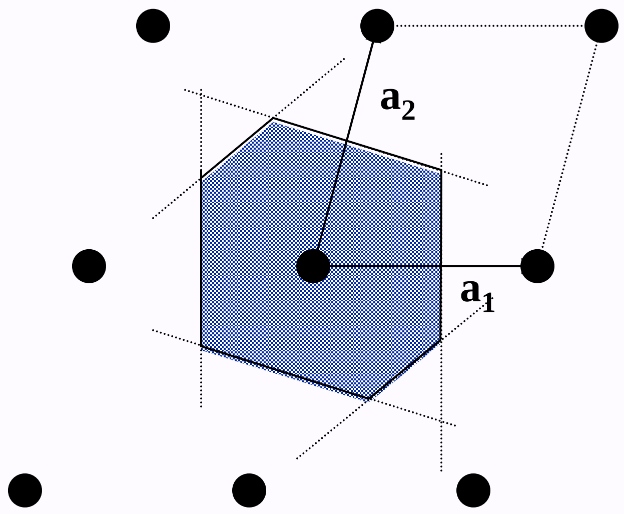


- A representative cell
- Translation of a primitive cell fills space
- $T(n_1,n_2,\ldots) = n_1\, a_1 + n_2\, a_2$ where the n's are integers
- Note: the primitive cells are not unique different cells can fill all space
- All primitive cells have the same are (volume)

Two Dimensional Lattices
Primitive Cell and Wigner-Seitz Cell



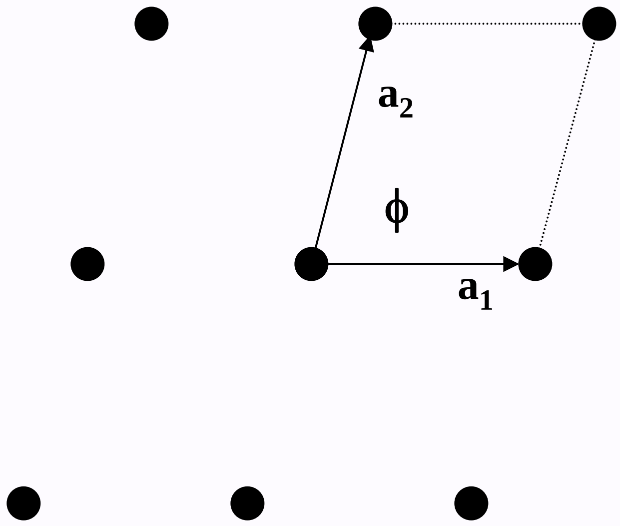
One possible Primitive Cell



Wigner-Seitz Cell -- Unique

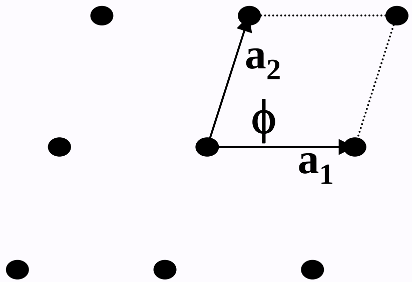
- **All primitive cells have same area (volume)**
- **Wigner Seitz Cell is most compact, highest symmetry cell possible**
- **Also same rules in 3 dimensions**

Possible Two Dimensional Lattices

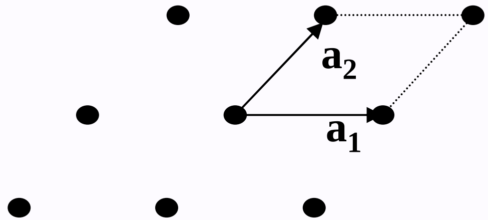


- Special angles ϕ = 90 and 60 degrees lead to special crystal types
- In addition to translations, the lattice is invariant under rotations and/or reflections

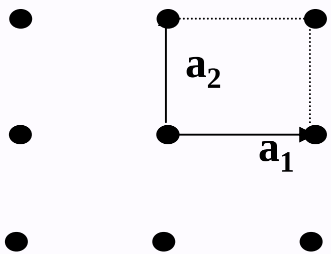
Possible Two Dimensional Lattices



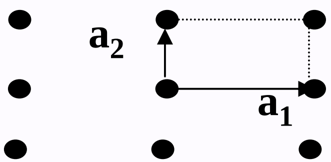
General oblique



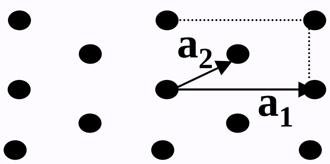
Hexagonal $\Phi = 60$, $a_1 = a_2$
6-fold rotation , reflections



Square
4-fold rot., reflect.



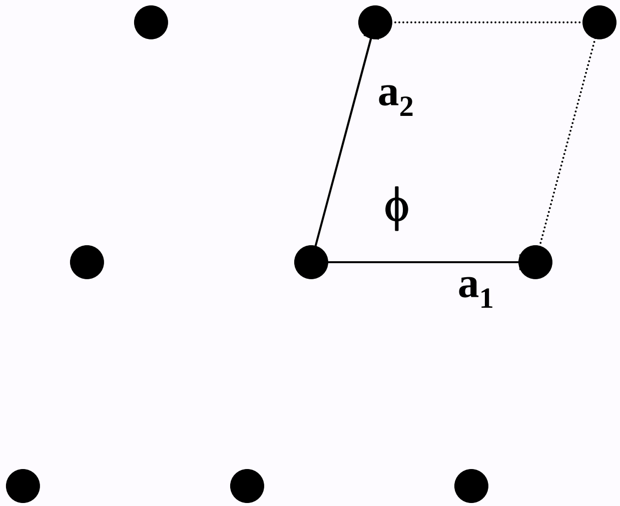
Rectangular
2-fold rot., reflect.



Centered Rectangular
2-fold rot., reflect.

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

More on Two Dimensional Lattices



- Why is it imposible to have a crystal with a five-fold rotation symmetry?
- Why is the centered square not a special type?

Classification of Crystal Structures

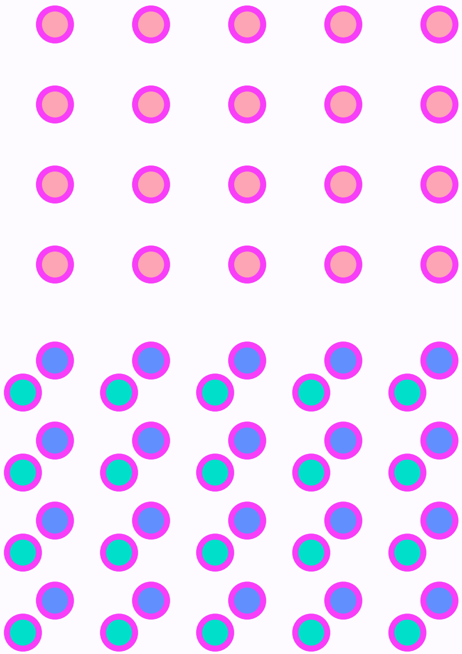
- Crystal structures classified by:
- Translation symmetry
  - Only the Bravais lattice
  - Limited number of possible Bravais lattice types
- Rotation, Inversion, reflection symmetry
  - Depends upon basis
  - Limited number of possible crystal types

- Examples in 2 dimensions
  - (3 dimensions later)

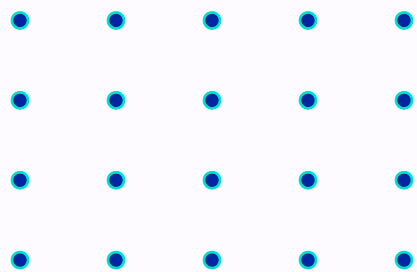
- See Kittel for lists of possible translation types.
  - See other crystallography references for lists of all possible crystal types

Summary at this point

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



Crystal

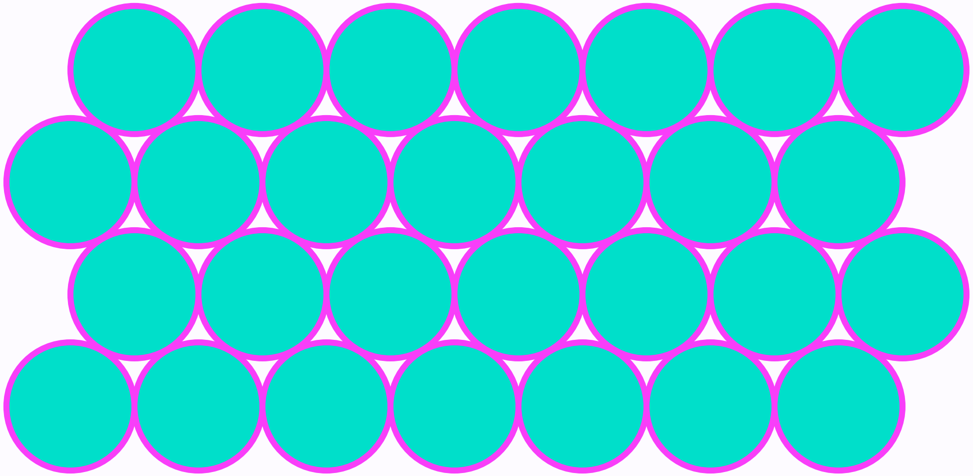


Lattice of points (Bravais Lattice)

Basis of atoms

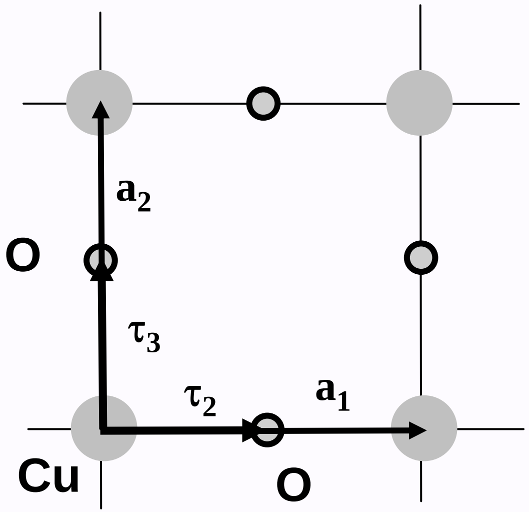
- Crystals can be classified into a small number of types – See text for more details

Examples of Crystals
Close packing of spheres in a 2-d crystal

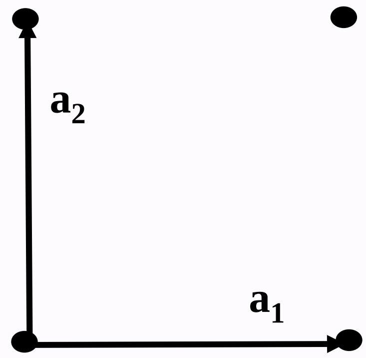


- Each sphere has 6 equal neighbors
- Close packing for spheres
- Hexagonal symmetry (rotation by 60 degrees)
- Actually occurs for rare gas atoms (spherical) on a flat surface

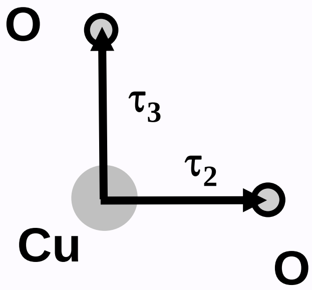
Crystalline layers with >1 atom basis



CuO_2 Square Lattice



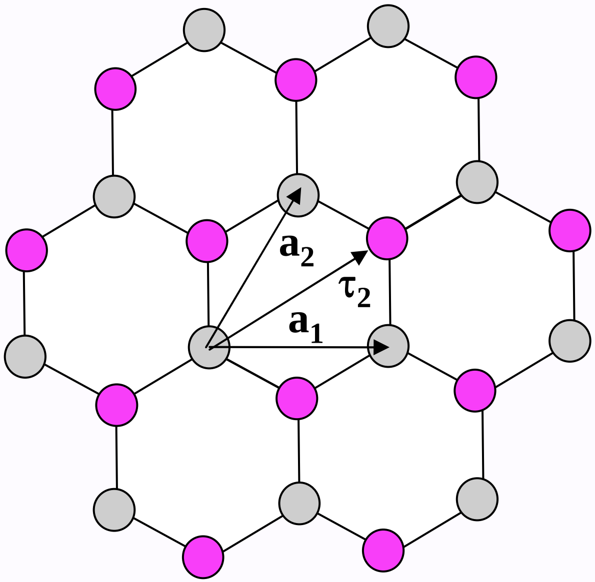
Square Lattice



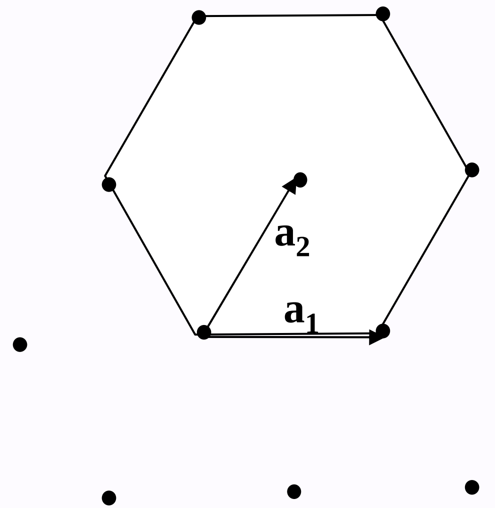
CuO_2 Basis

- **One CuO_2 layer in the High Tc superconductors**
- **Square lattice**
- **One basis unit on each site**

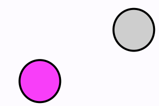
Crystalline layers with >1 atom basis



Honeycomb Lattice
(graphene or BN layer)



Hexagonal Lattice



Basis
2 C atoms
or BN pair

- **A single layer of graphitic carbon (graphene)**
  - **The two atoms in the cell are both Carbon**
- **A single layer of hexagonal boron nitride (BN)**
  - **The two atoms in the cell are B and N**

Next Time

- More on Crystal Lattices - Continue Kittel, Ch. 1
- 3 Dimensions
- Lattice planes
- Examples of crystals