Physics 0551

Lecture 1

Course Topics: (In order of appearance)

1. Crystal Structure: lattice types; crystal symmetries

2. Diffraction Theory: x-ray, neutron, electron diffraction; experimental techniques; reciprocal lattice; single particle diffraction; diffraction by crystals (static)

3. Crystal Binding: bonding types; lattice energies; thermodynamic properties, defects

4. Lattice Vibrations: phonon dispersion relationships; inelastic neutron scattering; Debye-Waller factor; density of states, heat capacity; phonon statistics; thermal transport

5. Electrons in a Solid: classical Drude' theory; Hall effect; Sommerfeld free electron gas; electron dispersion relationships

6. Electrons in a Crystal (i.e.-Band Theory): band gaps; transport properties; semiconductors; Bloch theorem; tight-binding approximation; Fermi surfaces

7. Magnetism: paramagnetism, diamagnetism, and ferromagnetism; exchange forces

8. Superconductivity: Meissner effect, London equation; BCS pairing

Question: What are the characteristics of a crystalline solid?
A crystalline solid is characterized by long-range order in which there is a *periodic arrangement* of the atoms. Central to this concept of periodicity is the BRAVAIS LATTICE or Space Lattice.

Definition: a) A Bravais lattice is an infinite array of discrete points such that the surroundings, when viewed from any discrete point, appears to be invariant.

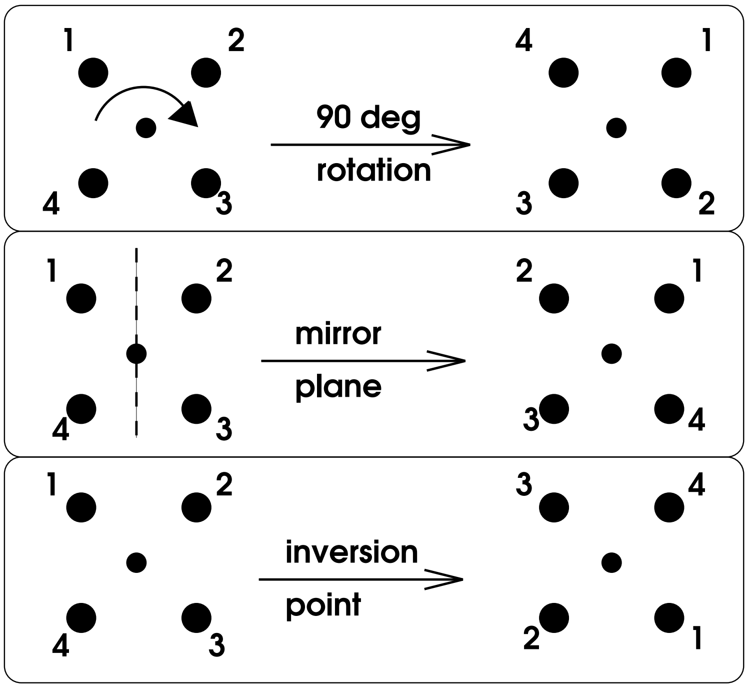
or b) the set of all points formed by three *non*-coplanar vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ where $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ and n_1, n_2, n_3 are integers; $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are called primitive vectors and span the lattice.

There are **5** Bravais lattice types in 2-D and **14** Bravais lattice types in 3-D
These various lattices can be distinguished by the different point group operations which can be performed. **Point group operations:** rotation, reflection, and inversion.
These operations bring a lattice onto itself.

ROTATION

REFLECTION

INVERSION



Note: There are an infinite number of point groups, but a finite number of crystal point groups.

Dimension	Number of crystal point groups	
1	2	Unity, Mirror
2	9	Unity, 4 Mirror, 4 Rotation
3	18	
4	118	

In addition to point group operations, we can define a new operation; T $\equiv$ translation.

$$T(\vec{r}) = \vec{r} + \vec{R}\ ;\ \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

There are also symmetry operations which consist of

non-primitive T's + rotation $\rightarrow$ Screw axis

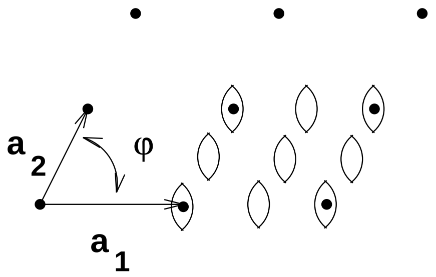
non-primitive T's + mirror plane $\rightarrow$ Glide plane

Note: These symmetry operations require a lattice with a non-trivial basis. In 3-D the total set of distinguishable crystal types has 230 possibilities. Of these, not all have been seen in nature.

Back to (2-D) Bravais lattices

Point Group Symmetry Operations

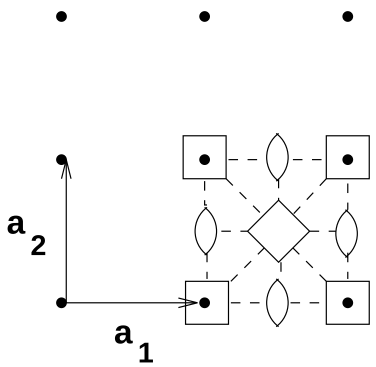
1. Oblique
   $\phi \neq 90°$
   $|a_1| \neq |a_2|$



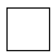
Inversion
1-fold, 2-fold rotations

 = Diads; 2-fold rotations

2. Square
   $|\vec{a}_1| = |\vec{a}_2|$
   $\phi \ = \ 90°$

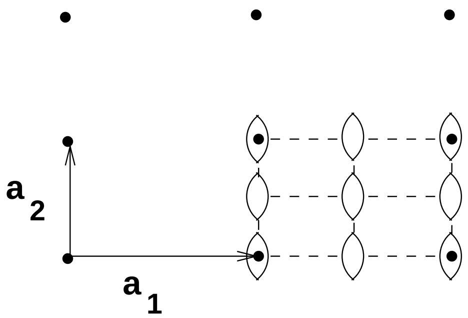


Inversion, Mirror Planes
1-fold, and 4-fold rotations

 = Tetrads; 4-fold rotation

- - - - - = Mirror planes

3. Rectangular
   $|\vec{a}_1 \neq |\vec{a}_2|$
   $\phi = 90°$



Inversion, Mirror Planes
1-fold, 2-fold rotations

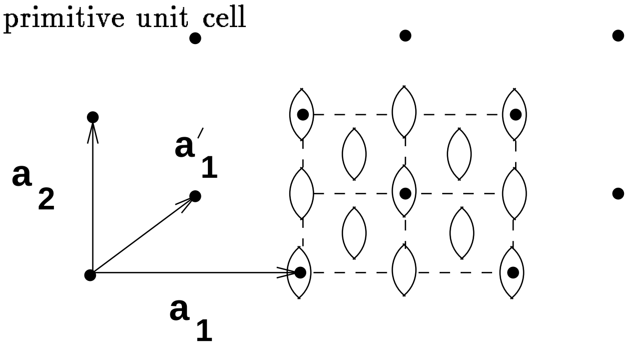
4. Centered Rectangular

$\vec{a}_1$, $\vec{a}_1$ conventional unit cell

$\vec{a}_1'$, $\vec{a}_2$ primitive unit cell

Inversion, Mirror Planes

1-fold, 2-fold rotations



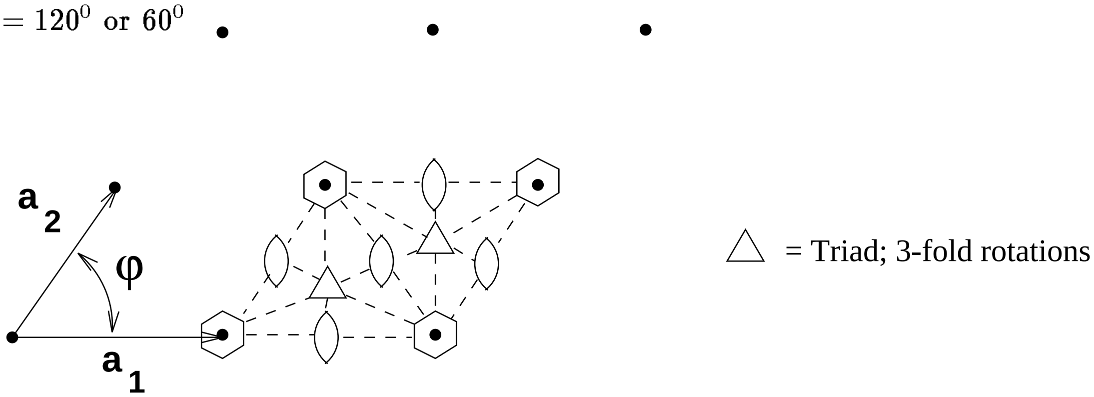
5. Hexagonal

$|\vec{a}_1| = |\vec{a}_2|$

$\phi = 120^0$ or 60^0

Inversion, Mirror Planes

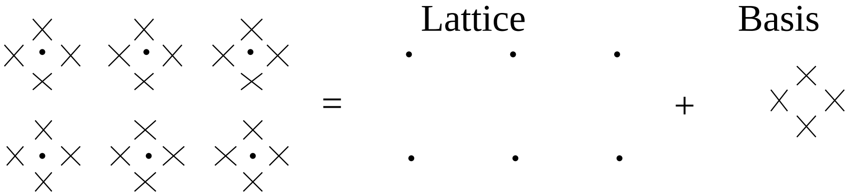
1,2,3 and 6-fold rotations



(Note: you should know all the 2-D and 3-D Bravais lattice types.)

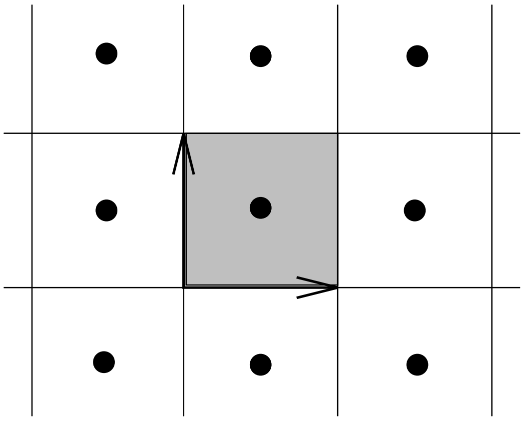
We have yet to define a real crystal. In order to do this we need to define a basis. A *basis* is the internal arrangement of atoms within a unit cell. Thus a crystal consists of a primitive lattice and its basis.

crystal = lattice + basis

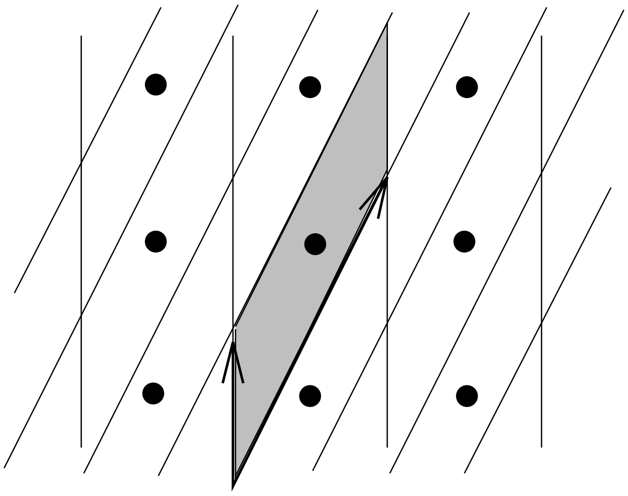


Note: All centrosymmetric bases have inversion symmetry.

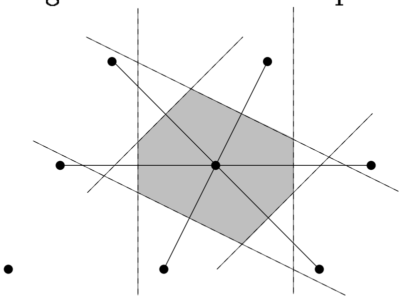
Definition: PRIMITIVE UNIT CELL $\equiv$ The parallelepiped represented by the primitive lattice vectors or any volume of space, that when translated through all translation vectors of the Bravais lattice, just fills all of space.



or



Wigner-Seitz cell $\rightarrow$ A special kind of primitive unit cell.



Smallest volume contained by the perpendicular bisectors. The utility of this construction will become apparent later.

In 3-D, 14 Bravais lattices (7 crystal classes)

*CUBIC: simple, face-centered, body-centered

*TETRAGONAL: simple, body centered

*ORTHORHOMBIC: simple, body-centered, face-centered, base-centered

*MONOCLINIC: simple, body-centered

*TRICLINIC

*HEXAGONAL

*TRIGONAL (Rhombohedral)

*These form the seven crystal classes