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.

![Diagram of Bravais lattice operations](image)

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

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Number of crystal point groups</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2 Unity, Mirror</td>
</tr>
<tr>
<td>2</td>
<td>9 Unity, 4 Mirror, 4 Rotation</td>
</tr>
<tr>
<td>3</td>
<td>18</td>
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<tr>
<td>4</td>
<td>118</td>
</tr>
</tbody>
</table>

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

\[
T(\vec{r}) = \vec{r} + \vec{R} ; \quad \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3
\]
There are also symmetry operations which consist of
non-primitive T's + rotation → Screw axis
non-primitive T's + mirror plane → 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

1. Oblique
   $\phi \neq 90^\circ$
   $|a_1| \neq |a_2|$

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

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

Point Group Symmetry Operations

- Inversion
- 1-fold, 2-fold rotations

- Tetrads; 4-fold rotation
- Mirror planes

Back to (2-D) Bravais lattices
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
\[ |\vec{a}_1| = |\vec{a}_2| \]
\[ \phi = 120^\circ \text{ or } 60^\circ \]

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.

\[ \text{crystal} = \text{lattice} + \text{basis} \]

\[ \begin{array}{cccc}
  \times & \times & \times & \times \\
  \times & \times & \times & \times \\
\end{array} \quad \begin{array}{c}
  \cdot \\
  \cdot \\
\end{array} \quad \begin{array}{c}
  \text{Lattice} \\
  \text{Basis} \\
\end{array} \]

Note: All centrosymmetric bases have inversion symmetry.
Definition: PRIMITIVE UNIT CELL ≡ 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.

Wigner-Seitz cell → 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