Lecture 1

The major goal of the course is to understand the properties of materials starting from an atomistic view.

The first step is therefore is to understand how the atoms are arranged.

Some times the material can be found in a crystalline order. Why some materials occur in a crystalline order in the nature is a hard question to answer.

Simple answer could be, that is the lowest energy configuration.

Why the lowest energy arrangement is crystalline. It could be due to the fact that each atom in a crystalline arrangement has the same environment.

Some times however, equillibrium structure may be a function of temperature and pressure.

(Those are known as Allotropes)

Natural matter can be crystals | crystals with defects | or non crystals.

We will study:

- Atomic Structure
- Electronic Structure
- Mechanical Properties
- Electron transport
- Optical Properties
- Magnetism etc.

We will first study the idea of crystals using two-dimensional lattice structures.

We spend the rest of this lecture to talk about 2D crystal. It is important due to many reasons.

- Two dimensional lattices are easy to visualize, thus easy to understand

- We can develop the understanding of basic definitions related to crystallography using 2D structures.

  (Basically we can get familliar with the terminology)

- Finally you might think that 2D crystals are just some artificial creatures, But Not really....

  2-dimensional long range atomic arrangements are important to understand
  - surfaces
  - thin films and natural 2D materials such as graphene.

Any way let's continue our discussion with 2D crystal structures.

Two-Dimensional Crystal Structures

Crystal Structure:

This is a geometrical concept. Without thinking the details of the atomic structure, we look at the geometric pattern of the repeating structure. That repeating pattern is called a CRYSTAL LATTICE.

Basically it is a pattern of points.

Each point in thes pattern can be obtained by Lattice translation vectors.

If you consider the origin of the coordinate system on one of the lattice points, each point of the lattice can be explained by the vector

$$T = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$$

In 2D, we need only 2 vectors.

$$T = n_1 \bar{a}_1 + n_2 \bar{a}_2$$

where n_1, n_2 & n_3 are integers.

If you pick the set of vectors a_i such that there is no other cell of volume than that covered by a_i, which can serve as a building block of the lattice structure,

the set of vectors a_i are known as the primitive translation vectors

However in some cases, we pick non-primitive translation vectors.

The primitive translation vectors cover a volume that contain only one lattice point.

Non-primitive translation vectors cover a volume with more than one lattice point.

Both primitive and non-primitive vectors define a volume that can act as a Building Block of the lattice.

Basis and the Crystal Structure.

By now we know crystal lattice is a geometrical concept.

There are different types of Crystal types, those are explained by Bravais Lattices.
(We will talk about the Crystal lattice types in detail later)

In order to make a Crystal lattice, we put atoms on to each lattice point.

In order to make a certain lattice, if you have to put only a single atom on each lattice point,
that Lattice is called a BRAVAIS Lattice.

If you have to put more than a single atom on each Lattice point,
that Lattice is called a non-Bravais Lattice.

And that set of atoms you put on a single lattice point is called a Basis.

Now we will discuss two-dimensional lattice types to better understand the terminology.