

## MSE 205 Lecture 5

### Lattice, basis and unit cell

A lattice is a collection of points, called lattice points, which are arranged in periodic pattern so that the surroundings of each point in the lattice are identical. A lattice may be one, two or three dimensional. The arrangement of ions and atoms is called lattice.

CRYSTAL: Translationally periodic arrangement of ATOMS in space.

LATTICE: Translationally periodic arrangement of POINTS in space.

BASIS (or MOTIF): An atom or a group of atoms associated with each lattice point in crystal.

CRYSTAL=LATTICE+BASIS

LATTICE of a crystal tells how to repeat (the periodicity of the crystal).

BASIS tells what to repeat according to the lattice to get the crystal.

LATTICE TRANSLATION: A vector from one lattice point to another.

UNIT CELL: A finite region of space which when translated by all lattice translations, or a subset of lattice translations, can fill the entire space without gaps or overlaps (i.e., it tiles the space).

#### SPACE LATTICE - DEFINITION

A space lattice is an array of points showing how particles (atoms, ions or molecules) are arranged at different sites in three dimensional spaces.

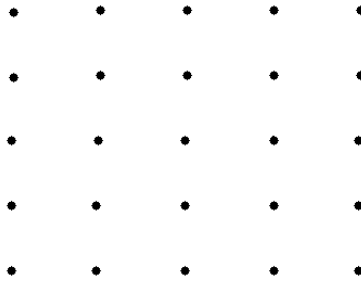
Thus all the information about a crystal can be deduced if its unit cell is given.

A given crystal or the associated lattice can have infinitely many differently shaped and sized unit cells.

#### Lattice and basis

What is a lattice?

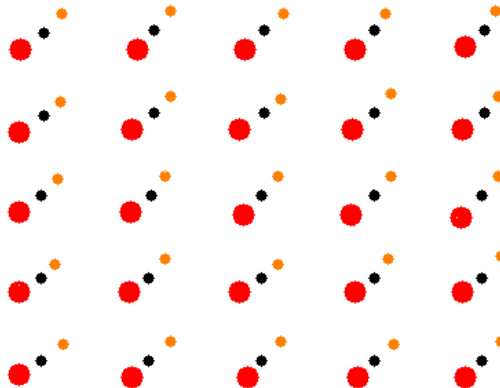
A lattice is a hypothetical regular and periodic arrangement of points in space. It is used to describe the structure of a crystal. Lets see how a two-dimensional lattice may look.



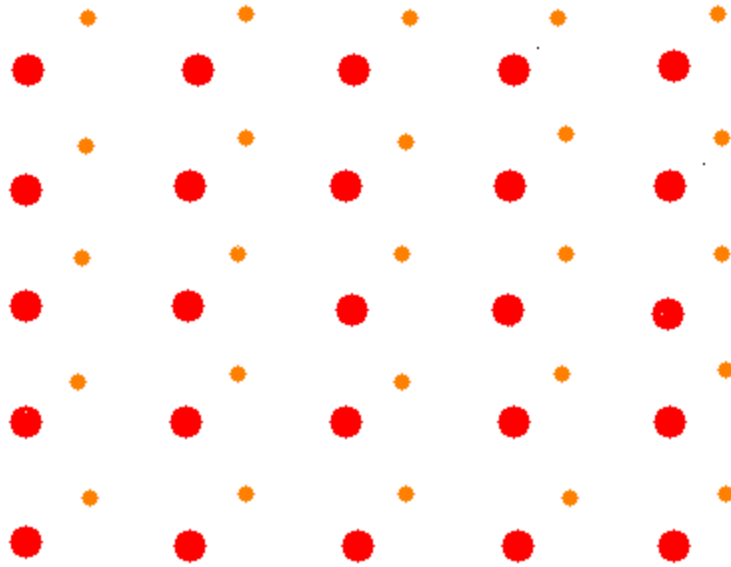
A basis is a collection of atoms in particular fixed arrangement in space. We could have a basis of a single atom as well as a basis of a complicated but fixed arrangement of hundreds of atoms. Below we see a basis of two atoms inclined at a fixed angle in a plane.



Let us now attach the above basis to each lattice point (in black) as follows.



Next remove the lattice points in black (remember that the lattice is an abstract entity). Lets see what we have got?



We have got the actual two-dimensional crystal in real space. So we may write:

lattice + basis = crystal

So the crystal structure is formed by associating every lattice point with an assembly of atoms or molecules or ions, which are identical in composition, arrangement and orientation, is called as the basis. The atomic arrangement in a crystal is called crystal structure. If the basis is substituted for the lattice points, then the resulting structure is called crystal structure

How do we define a lattice mathematically?

If  $\mathbf{r}$  be the coordinates of a lattice point from any origin, then if we apply a lattice translation through the lattice translation vector

$$\mathbf{T} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

then we would arrive at any other lattice point  $\mathbf{r}'$  around which the environment would look exactly the same as around  $\mathbf{r}$ .

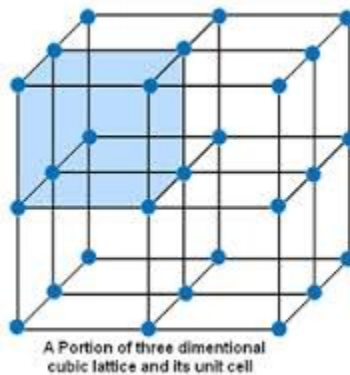
$$\begin{aligned}\mathbf{r}' &= \mathbf{r} + \mathbf{T} \\ &= \mathbf{r} + u\mathbf{a} + v\mathbf{b} + w\mathbf{c}\end{aligned}$$

**a**, **b** and **c** are the primitive translation vectors or basis vectors which form the primitive cell of the lattice and  $u$ ,  $v$ ,  $w$  are integers.

### CHARACTERISTICS OF A CRYSTAL LATTICE

1. In a crystal lattice there is the parallelepiped constructed from vectors which correspond to translational periods called unit cells.
2. A crystal is an array of atoms packed together in a regular pattern. A unit cell of a pattern is a piece of the pattern which, when repeated through space without rotation and without gaps or overlaps, reconstructs the pattern to infinity. For filling space without holes, a unit cell must be either a parallelogram (in 2D) or a parallelepiped (in 3D).
3. These can be chosen in different ways. Commonly, unit cells are chosen so that its vertex coincides with one of the atoms of the crystal. Then lattice sites are occupied by atoms, and of the atoms of the crystal. Thus, the lattice sites are occupied by atoms, and vectors that connect the nearest equivalent atoms.
4. The unit cell contains at least one atom of each of the types that make up the crystal. Providing that the unit cell is made up of only one type of atom, it is called monatomic, anymore than that and it is polyatomic. Correspondingly a monatomic lattice is often identified as a simple lattice and a polyatomic one, a composite lattice.

The constituent particles of a crystalline solid are arranged in a definite fashion in 3-D space.



## Primitive and Non-Primitive Unit Cell

The most common unit cell shape is parallelepiped. It is also common, though not necessary, to take the corners of the unit cell at the lattice points. If these are the only lattice points, the unit cell is **PRIMITIVE**. If there are lattice points other than those at the corners, it is **NONPRIMITIVE**. Primitive unit cell will have effectively one lattice point per cell. A non primitive one will have more than one lattice point per cell.

A primitive cell is a unit cell that contains exactly one lattice point which is made up from the lattice points at each of the corners. It is the smallest possible cell. If there is a lattice point at the edge of a cell and thus shared with another cell, it is only counted half. Non-primitive unit cells contain additional lattice points, either on a face of the unit cell or within the unit cell, and so have more than one lattice point per unit cell. Or Primitive unit cell has atoms present at corners and in non primitive unit cell atoms are present in corners as well as other positions in a crystal.

