

Lecture 2: Crystal Structure and Periodic Atomic Arrangement

1. Introduction

In this lecture, we study how atoms are *arranged* in crystalline solids. The key concept that distinguishes crystalline solids from gases and amorphous materials is **the periodic arrangement of atomic positions**.

2. Special Features of Atomic Locations in Solids

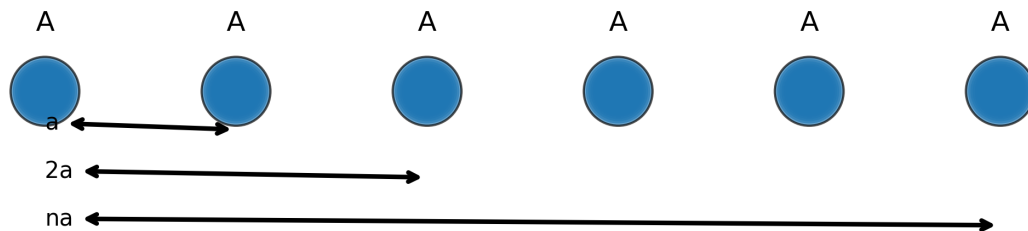
In gases, atoms are randomly distributed in space. In crystalline solids, atoms occupy well-defined equilibrium positions arranged in a regular and repeating pattern.

Consider an atom A at a given position.

If the atom is translated by the vector a , it ends up at the same atomic position.

Translating by $2a$, or in general by na (where n is an integer), also leads to the same atomic environment.

Translational Invariance in a One-Dimensional Crystal

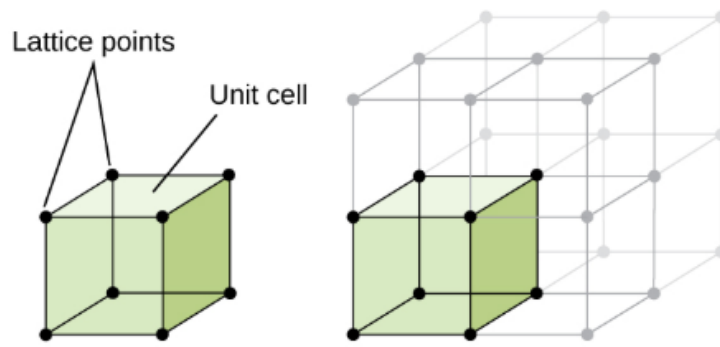


This translational invariance implies that atoms in crystalline solids form a **periodic array**.

3. Periodic Structure

A structure generated by the periodic repetition of a basic building block is called a **periodic structure**.

In crystalline solids, this building block is called a **cell**. The entire crystal structure can be obtained by repeating this cell in space.

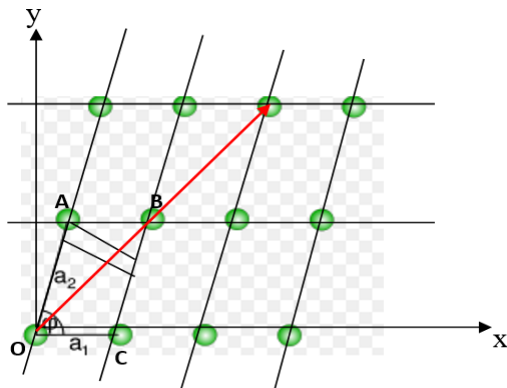


4. Two-Dimensional Periodic Structure

In two dimensions, we define two non-collinear vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, called primitive (or fundamental) vectors.

The position of any atom or lattice point in the crystal can be written as:

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2, \text{ where } n_1 \text{ and } n_2 \text{ are integers. } -\infty < n_1, n_2 < \infty$$



By connecting the points in each row and column, we find a number of identical cells, such as the cell (OABC). From this, we conclude that the overall structure is equivalent to a periodic repetition of the cell (OABC).

Hence, the entire structure is generated by the periodic repetition of a **single primitive cell**.

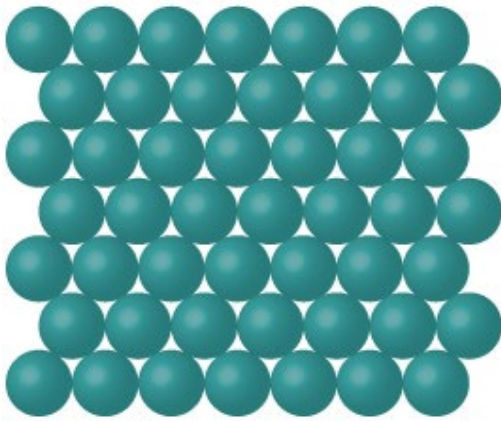
A structure formed by the periodic repetition of a cell is called a periodic structure.

5. Crystals and Crystal Lattices

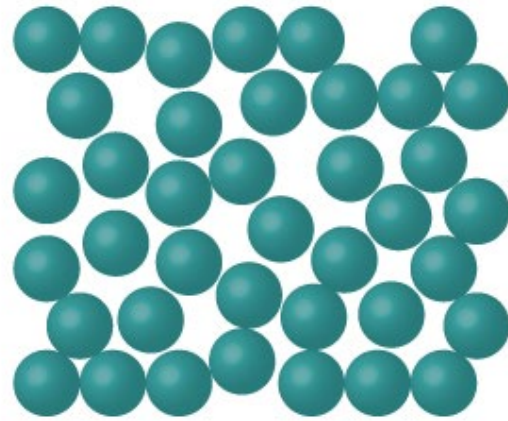
Not all solids possess a periodic structure. Solids that have a periodic atomic arrangement are called crystals.

Examples of crystalline solids include silicon (Si) and sodium chloride (NaCl). Materials such as glass, wood, and amorphous silicon do not have long-range periodicity.

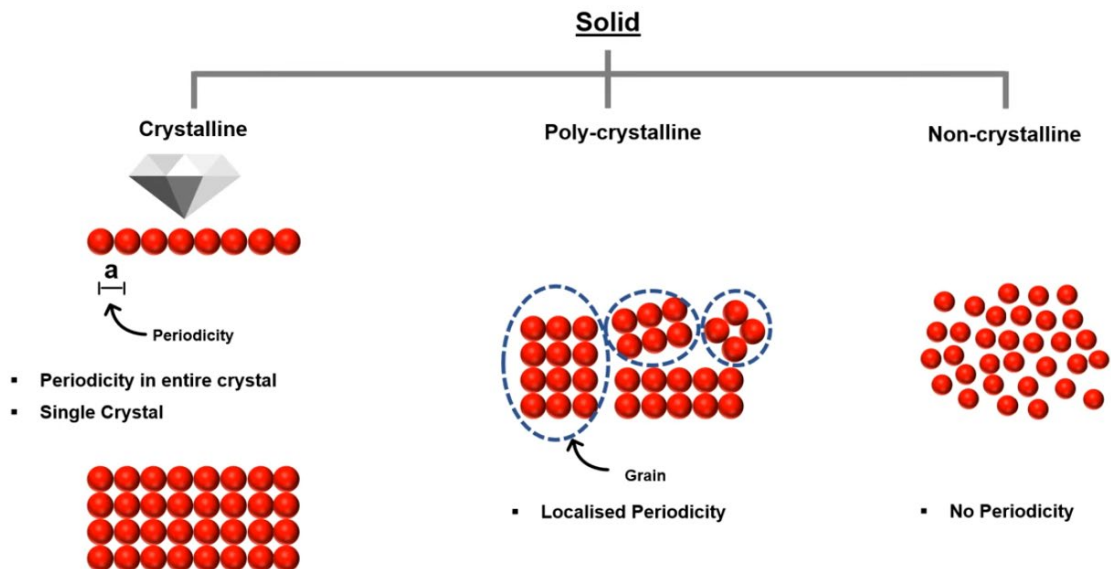
The crystal lattice is defined as an infinite periodic array of points in space that represents the translational symmetry of the crystal.



Crystalline



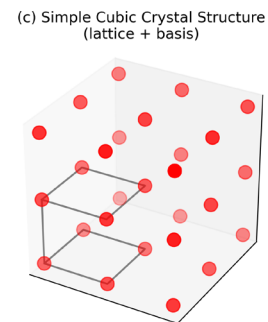
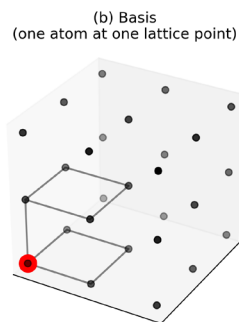
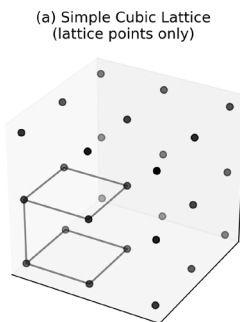
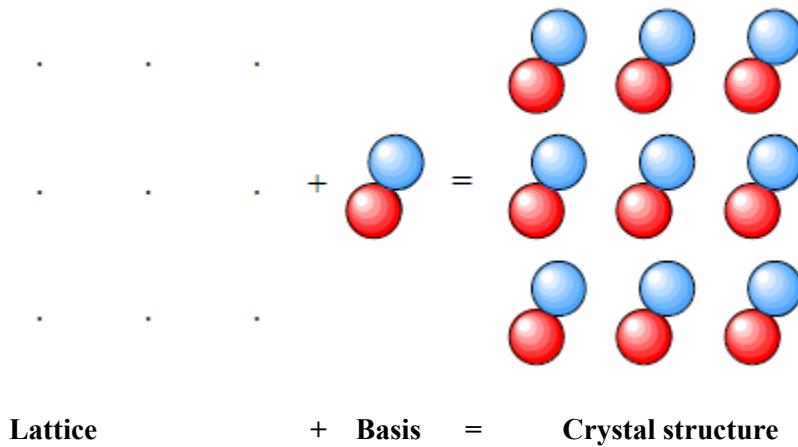
Amorphous



6. Crystal Lattice and Basis

The actual crystal structure is obtained by associating a basis (one atom or a group of atoms) with each lattice point.

The basis (or motif) is the atom or group of atoms located at each lattice point that, when repeated, builds the actual crystal structure



In simple crystal structures, there is one atom per lattice point, as in copper, gold, and silver. In more complex crystals, the basis may consist of several atoms, provided they are identical in composition and orientation.

- A **unit cell** is a repeating unit of the space lattice which can be used to reproduce the entire cell.
- **Lattice:** How do we repeat?
- **Motif / Basis:** What do we repeat?
- **Crystal:** Lattice + Motif (Basis)

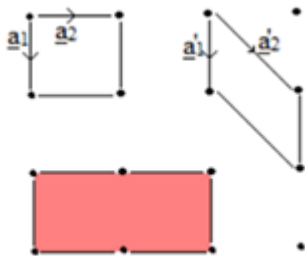
7. Primitive Cell

The smallest cell whose periodic repetition reproduces the entire structure is called the **primitive cell (or unit cell)**.

The primitive cell is **not unique**. Different choices of primitive vectors may lead to different primitive cells with the **same area**.

In the last figure, the smallest cell, such as (OABC), is called the primitive cell or unit cell. It is a parallelogram whose repeated translation using the fundamental vectors generates the entire crystal lattice.

Knowing the two vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ determines the two-dimensional periodic order. Therefore, knowledge of $\mathbf{a}_1$ and $\mathbf{a}_2$ defines the primitive cell.



You can note that there are two choices of primitive vectors for a 2D lattice. The shaded region is a non-primitive cell with twice the area of a primitive cell.

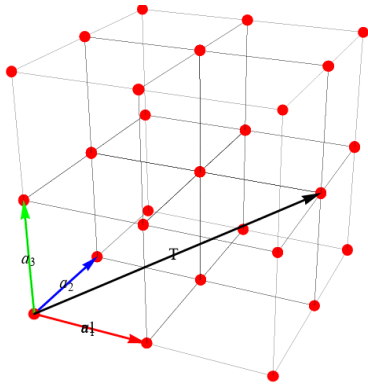
The concepts introduced in two dimensions can be extended naturally to three-dimensional crystals.

8. Three-Dimensional Periodic Structure

In three dimensions, three non-coplanar vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are required to describe the periodic arrangement of atoms.

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Knowing these vectors uniquely defines the three-dimensional periodic array and the corresponding primitive cell.



3D lattice

a_1 , a_2 , and a_3 are primitive lattice vectors. Lattice points (red circles). T is the translation vector; $T = 2a_1 + a_2 + a_3$. The lattice is defined by three primitive translation vectors, a_1 , a_2 , and a_3 .

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

Where: n_1 , n_2 , and n_3 are integers.

9. Specification of Atomic Positions in Crystals

Since all unit cells in a crystal are identical, it is sufficient to specify the atomic positions inside a **single unit cell**.

Once the atomic positions in one unit cell are known, the positions of all atoms in the crystal are automatically determined.

Summary

The crystal structure of a solid is completely determined by:

- The primitive vectors a_1 , a_2 , and a_3
- The atomic positions within one unit cell

Exercise-1:

For a three-dimensional crystal, let:

$$\mathbf{a}_1 = (1, 0, 0), \mathbf{a}_2 = (0, 1, 0), \mathbf{a}_3 = (0, 0, 2).$$

- Draw schematically the primitive cell formed by these vectors.

- Explain why specifying atomic positions inside one unit cell is sufficient to describe the entire crystal.

Exercise-2:

Is it possible for two different crystals to share the same lattice but have different bases?

Exercise-3:

