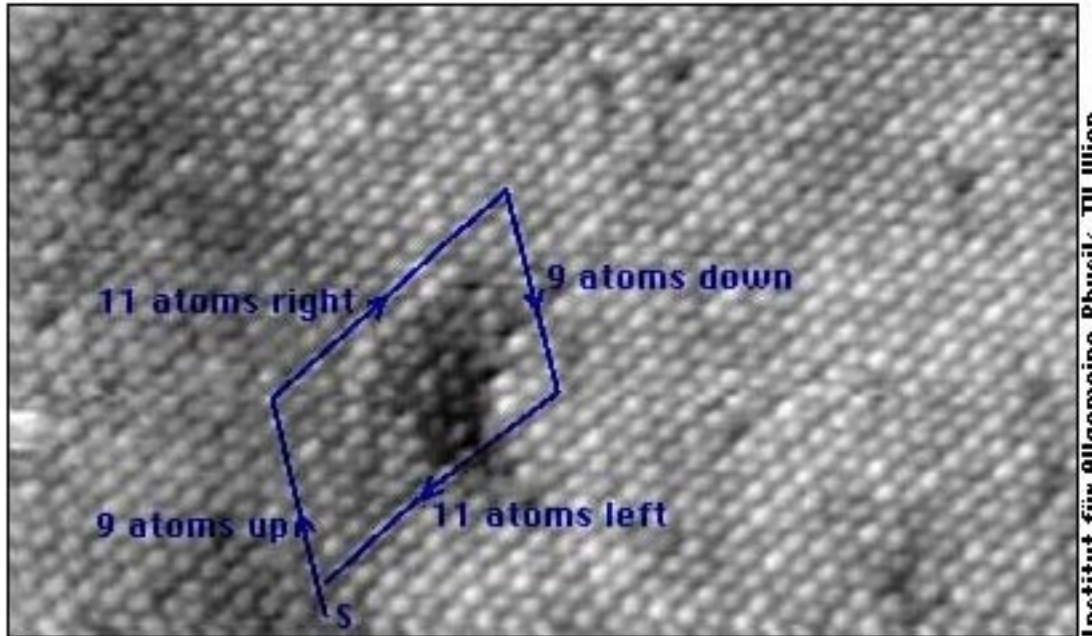


Lecture 10: Defects in Crystals



1- What are crystal defects?

An ideal crystal has atoms arranged periodically and without any deviations from the ideal crystal structure. Real crystals, however, contain imperfections or deviations from this ideal arrangement. These imperfections are called crystal defects.

Defects may involve missing atoms, extra atoms, impurity atoms, or distortions of the crystal lattice.

Defects can exist because, although their formation requires energy, they also increase the entropy of the crystal. At finite temperature, the balance between energy and entropy allows defects to exist in equilibrium.

$$F = E - TS.$$

At finite temperature, thermally activated defects can exist in crystals. Therefore, real crystals are generally not perfectly periodic.

2- Classification of Crystal Defects

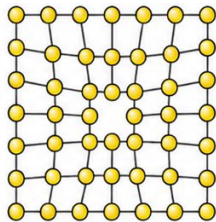
Based on “dimensionality”:

Defects are classified based on their dimensionality

- Point Defects 0-D
- Line Defects 1-D
- Surface Defects 2-D
- Bulk Defects 3-D

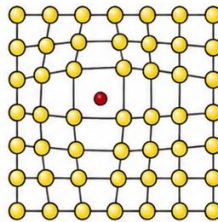
Dimensionality	Defect type	Example
0-D	Point defect	Vacancy
1-D	Line defect	Dislocation
2-D	Surface defect	Grain boundary
3-D	Bulk defect	Void / inclusion

Point Defects:



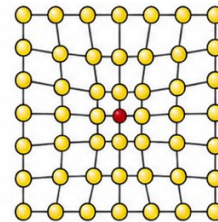
(a) **Vacancy**

A lattice site that should be occupied by an atom is empty.



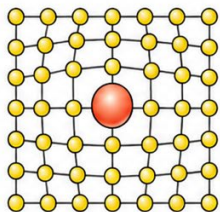
(b) **Interstitial atom**

An extra atom occupies an interstitial site (a position that is not a lattice site).



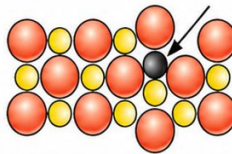
(c) **Small substitutional atom**

A smaller impurity atom replaces a host atom at a normal lattice site.



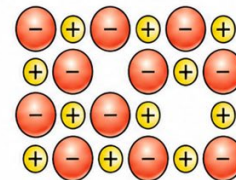
(d) **Large substitutional atom**

A larger impurity atom replaces a host atom at a normal lattice site, causing significant local distortion.



(e) **Frenkel defect**

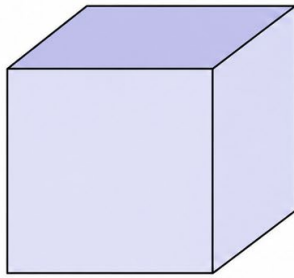
A vacancy and an interstitial atom formed when a host atom moves from a lattice site to an interstitial site. The total number of atoms remains unchanged.



(f) **Schottky defect**

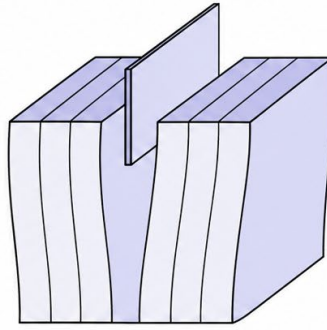
Paired cation and anion vacancies in an ionic crystal, maintaining overall charge neutrality and stoichiometry.

Line Defects



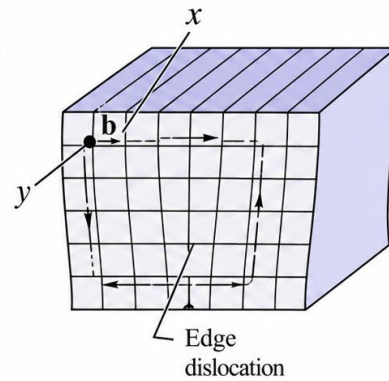
(a) Perfect crystal

A perfect crystal with a regular and continuous arrangement of atomic planes.



(b) Insertion of an extra plane

An extra half-plane of atoms is inserted into the crystal, causing a distortion of the surrounding atomic planes.



(c) Edge dislocation and Burgers vector

The bottom edge of the extra half-plane is an edge dislocation. A Burgers vector $\mathbf{b}$ is required to close a circuit around the dislocation, indicating the lattice distortion.