PHY 3107
Solid State Physics I

Elementary Materials Science Concepts

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An ideal crystal consists of atoms, ions, or molecules arranged in a perfectly periodic three-dimensional lattice. In a real crystal, this periodic arrangement is interrupted by missing atoms, extra atoms, impurities, dislocations, interfaces, and other irregularities. These irregularities are called **crystal imperfections or crystal defects**.

Why do crystal imperfections occur?

1. **Thermal vibrations:** Atoms vibrate around their equilibrium positions. At finite temperatures, some atoms acquire sufficient energy to leave their normal lattice sites.
2. **Crystal growth:** Rapid solidification and non-equilibrium growth can introduce vacancies, dislocations, and inclusions.
3. **Impurities:** Foreign atoms may enter the crystal during preparation or processing.
4. **Mechanical deformation:** Applied stress can generate and move dislocations.
5. **Radiation:** High-energy particles can displace atoms from their lattice sites.
6. **Heat treatment:** Heating and cooling can change defect concentrations, promote diffusion, and alter grain structures.

Why are defects important?

Crystal defects are not always undesirable. They can control or improve:

- Mechanical strength and hardness.
- Electrical and ionic conductivity.
- Diffusion and chemical reactions.
- Optical absorption and crystal color.
- Semiconductor behavior.
- Creep, fatigue, and fracture.

For example, dislocations allow metals to deform plastically, while deliberately introduced impurities enable the production of semiconductor devices.

Crystal imperfections

Four principal dimensional classes

0D — Point defects

Vacancies, interstitials, substitutional impurities, Frenkel and Schottky defects.

1D — Line defects

Edge dislocations, screw dislocations, and mixed dislocations.

2D — Planar defects

Grain boundaries, twin boundaries, stacking faults, and phase boundaries.

3D — Volume defects

Voids, pores, inclusions, precipitates, and cracks.

Type	Dimension	Examples
Point defects	Zero-dimensional (0D)	Vacancy, interstitial, impurity, Frenkel and Schottky defects
Line defects	One-dimensional (1D)	Edge, screw and mixed dislocations
Planar defects	Two-dimensional (2D)	Grain boundaries, twin boundaries, stacking faults, surfaces
Volume defects	Three-dimensional (3D)	Voids, pores, inclusions, precipitates and cracks

A. Intrinsic defects

These involve the host material itself, without requiring a foreign chemical species.

- Vacancy: a host atom is missing from its normal site.
- Self-interstitial: a host atom occupies an interstitial position.
- Frenkel defect: a host ion moves from a lattice site to an interstitial site.
- Schottky defect: a charge-balanced set of vacancies forms in an ionic crystal.

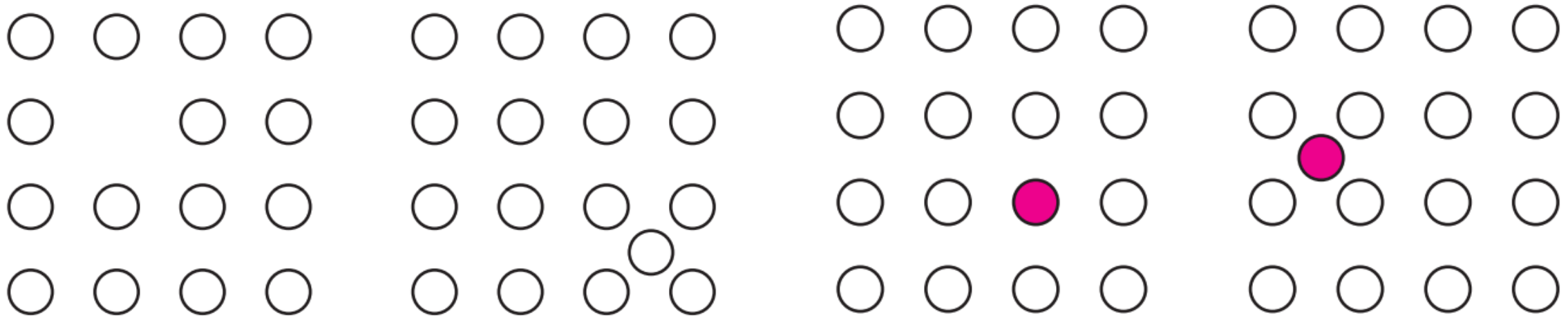
B. Extrinsic defects

These arise from foreign atoms or species introduced into the material.

- Substitutional impurity: a foreign atom replaces a host atom.
- Interstitial impurity: a foreign atom occupies an interstitial position.
- Dopants in semiconductors: impurities intentionally added to control electrical conductivity.

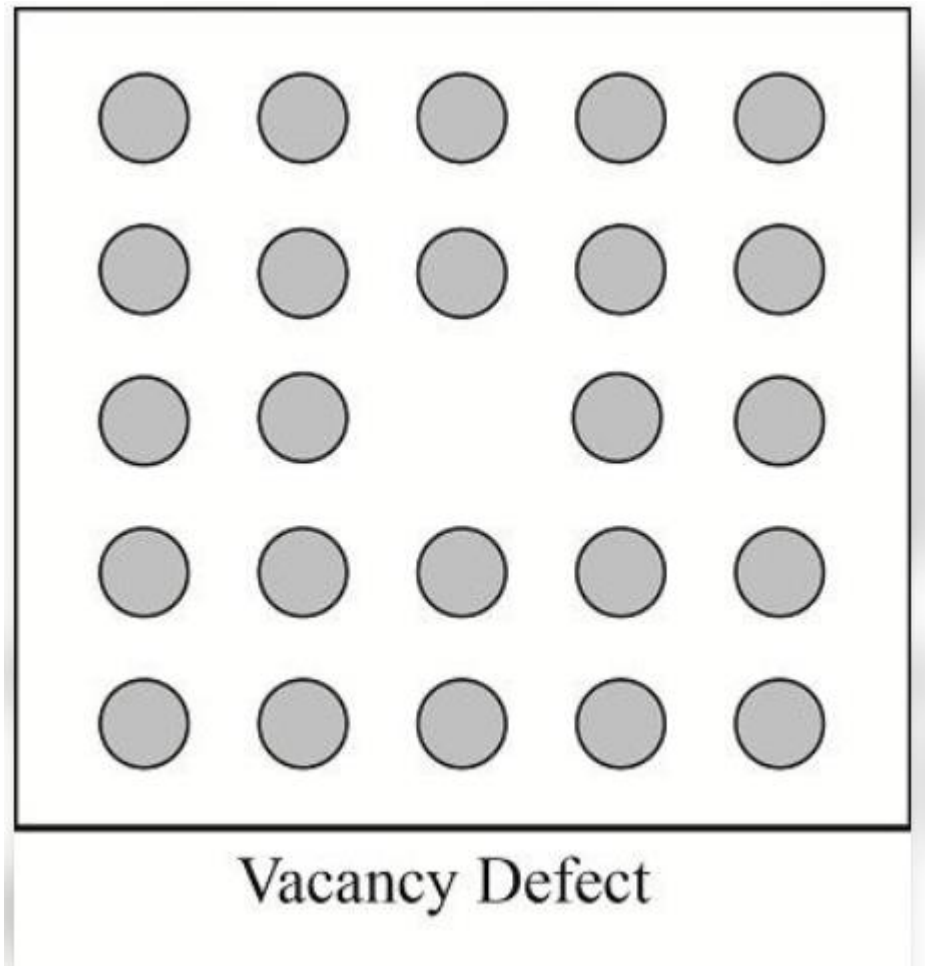
Important distinction: Frenkel and Schottky defects are commonly discussed as intrinsic point defects in ionic crystals. However, impurity atoms can also produce charge-compensating defects, so real materials may contain both intrinsic and extrinsic defects.

Crystal Defects

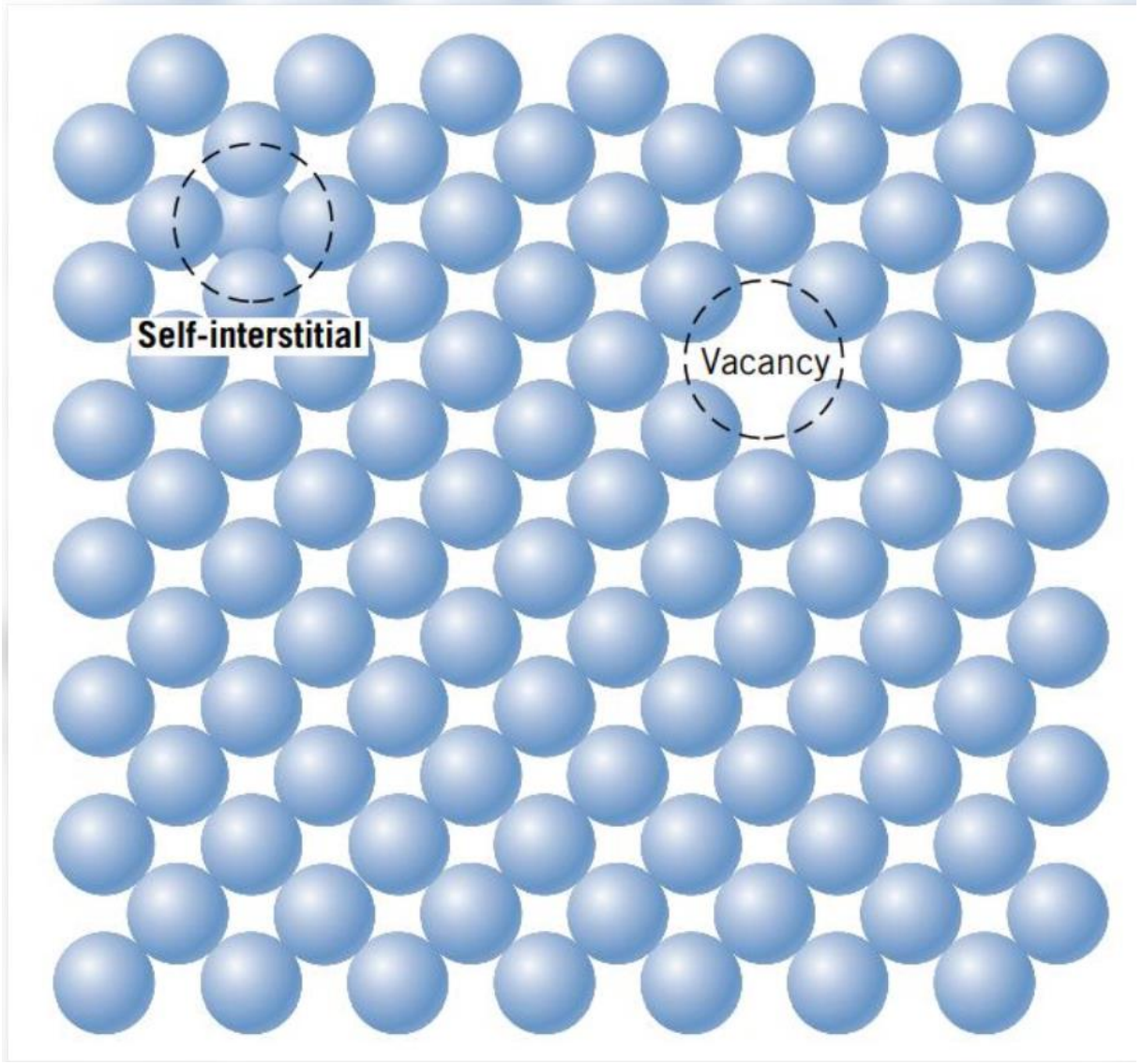


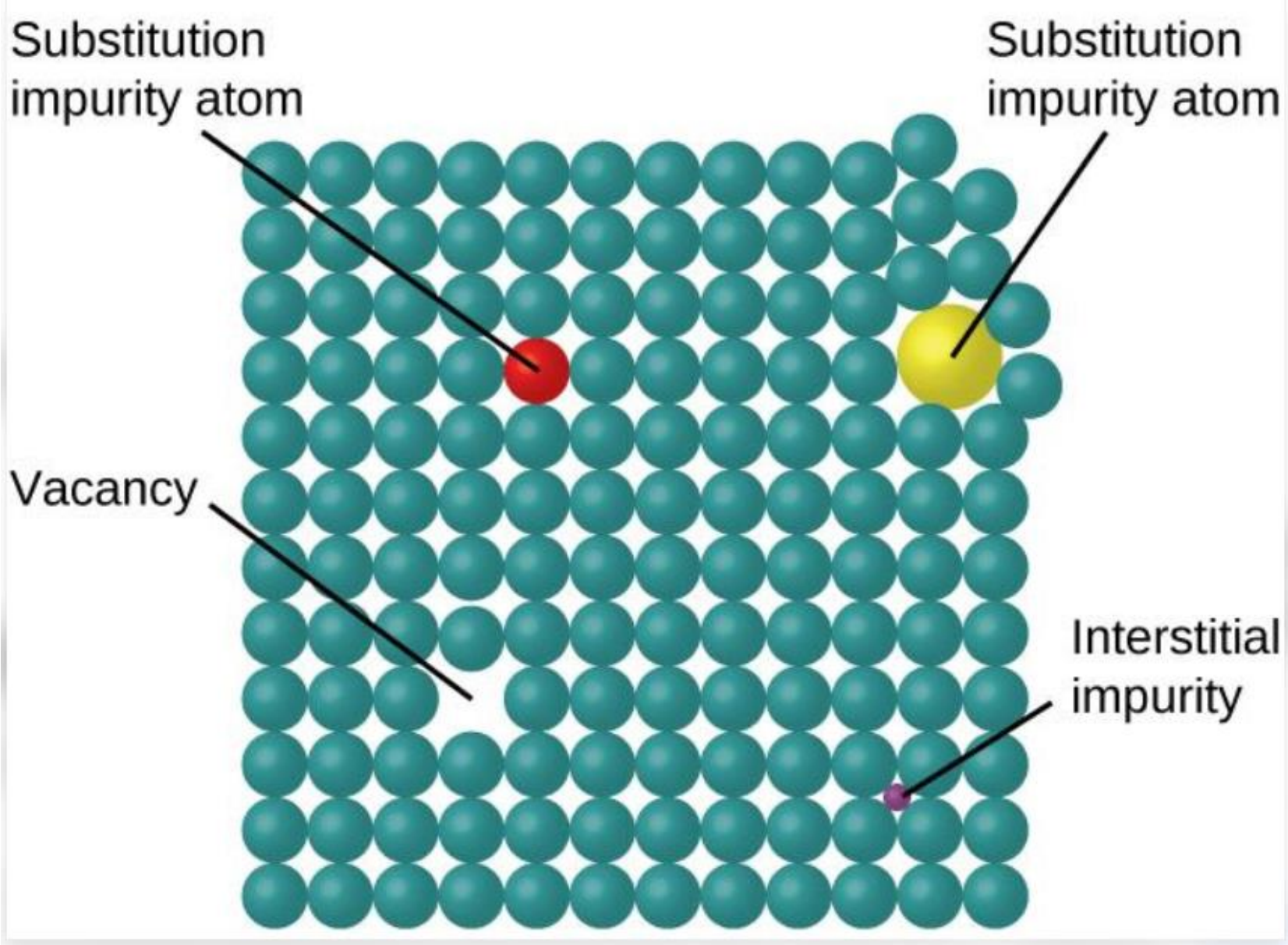
Point defects in a crystal. (*a*) Vacancy. (*b*) Interstitial. (*c*) Substitutional impurity. (*d*) Interstitial impurity.

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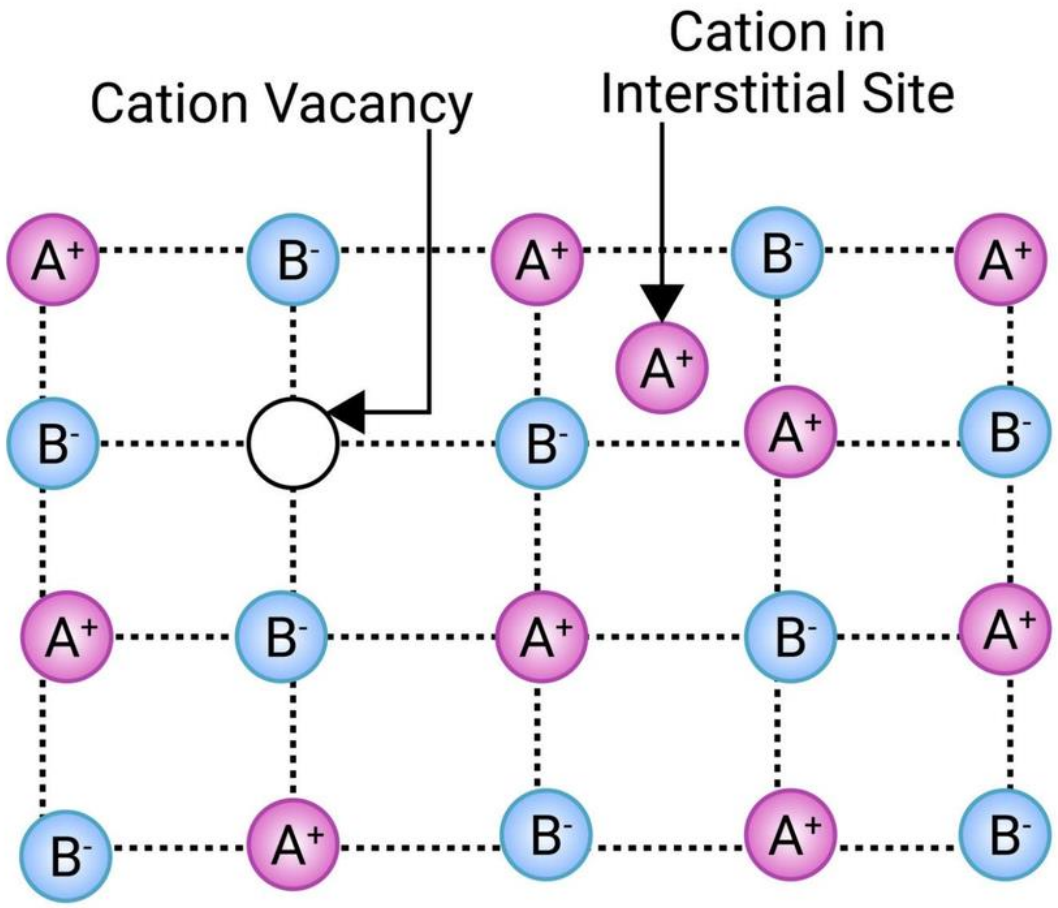


Vacancy Defect

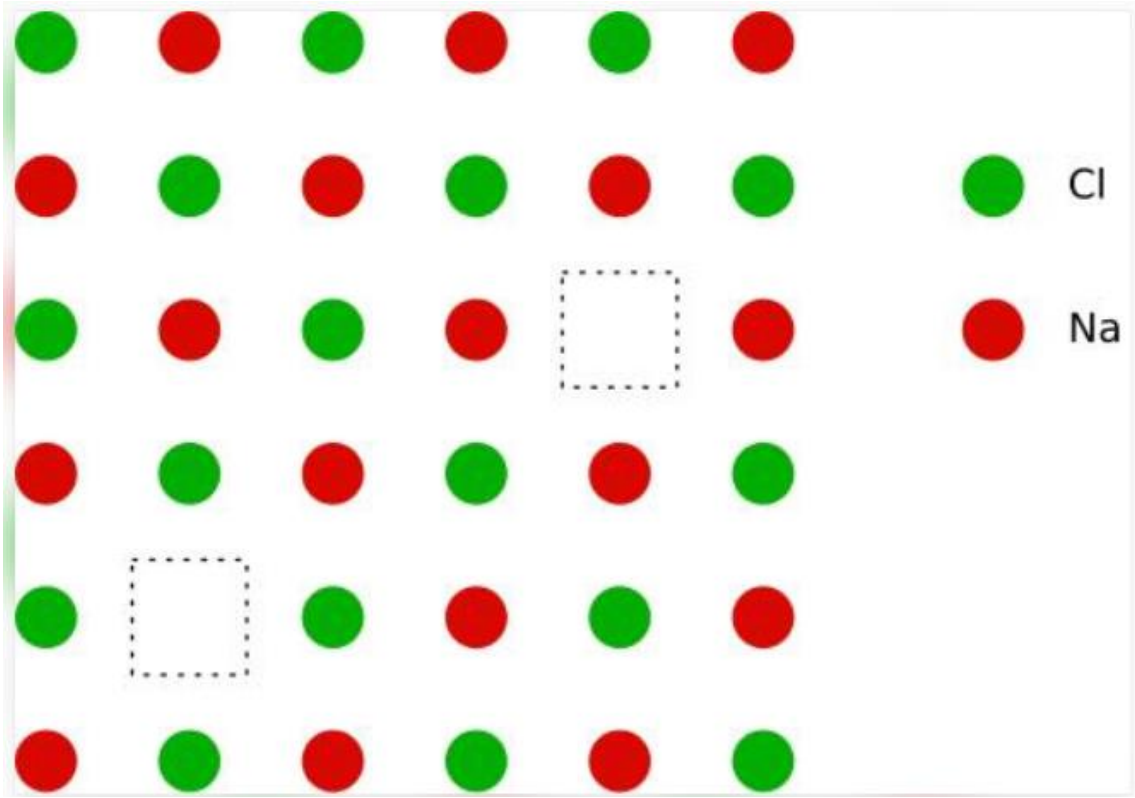



Substitution
impurity atom
Substitution
impurity atom
Vacancy
Interstitial
impurity

Frenkel defect

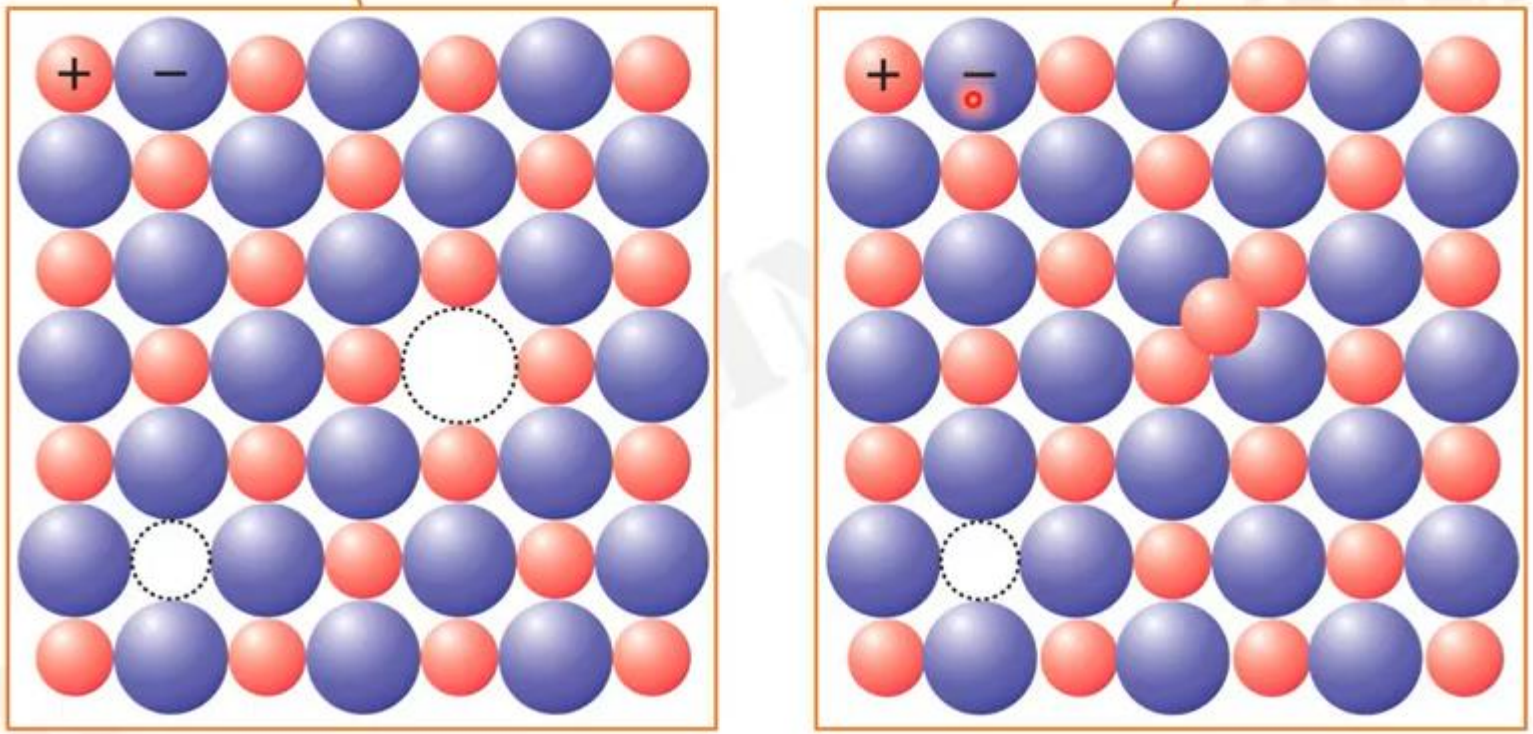


Schottky defect

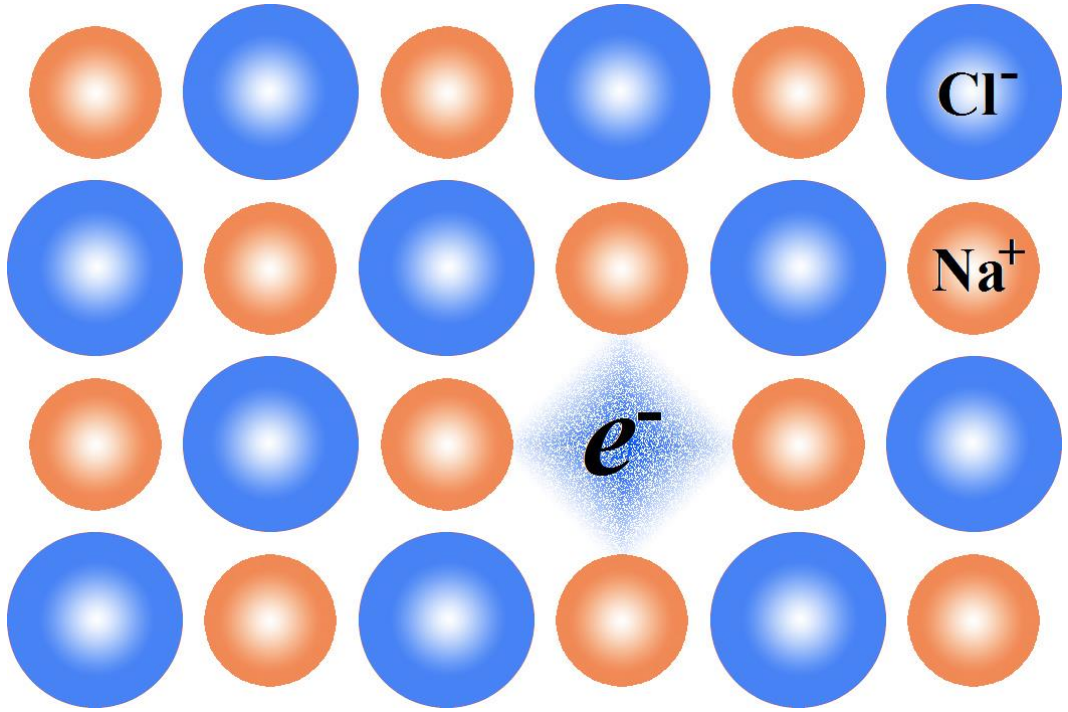


These *specific* point defects (Schottky and Frenkel) occur primarily in ionic crystals.

Schottky Defect & Frenkel Defect



Schottky Defect	Frenkel Defect
Schottky defect occurs in those ionic crystals where difference in size between cation and anion is small.	Frenkel defect usually occurs in those ionic crystals where size of anion is quite large as compared to that of the cation.
In Schottky defect, both cation and anion leave the solid crystal.	In Frenkel defect, only the smaller ion (cation) leaves its original lattice site; whereas, the anion remains in original lattice sites.
The atoms permanently leave the crystal.	Here, atoms leave the original lattice site and occupy interstitial position. So atoms reside within the solid crystal.
One Schottky defect leads to the formation of two vacancies.	One Frenkel defect creates one vacancy and one self-interstitial defect.
Two atoms reduce from the crystal for each Schottky defect.	The number of atoms present in the crystal before and after Frenkel defect remains same.
Due to vacancy formation, Schottky defect reduces density of the solid.	Density of the solid crystal before and after Frenkel defect remains same as no atom leaves the solid.



F-center in an NaCl crystal

An F-center or color center or Farbe center is a type of crystallographic defect in which an anionic vacancy in a crystal lattice is occupied by one or more unpaired electrons. Electrons in such a vacancy in a crystal lattice tend to absorb light in the visible spectrum such that a material that is usually transparent becomes colored. The greater the number of F centers, the more intense the color of the compound. F centers are a type of color center.

3.6 Antisite defects

In an ordered compound containing more than one atomic species, an antisite defect occurs when an atom occupies a lattice site normally assigned to another species.

For example, in a compound AB, an A atom may occupy a B site.

Antisite defects are important in semiconductors, intermetallic compounds, and ordered alloys. They can affect electronic properties, magnetic behavior, and phase stability.

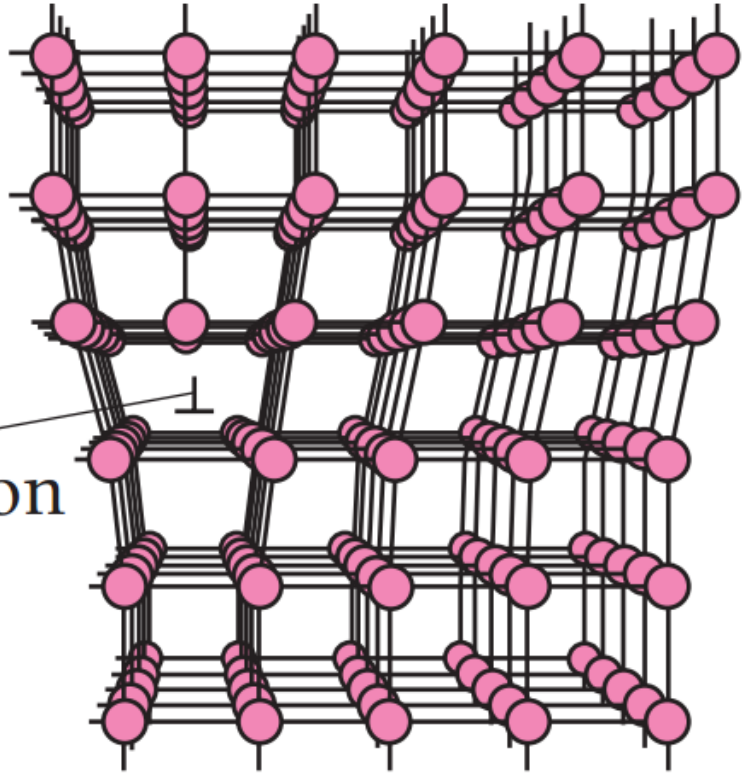
3.7 Color centers

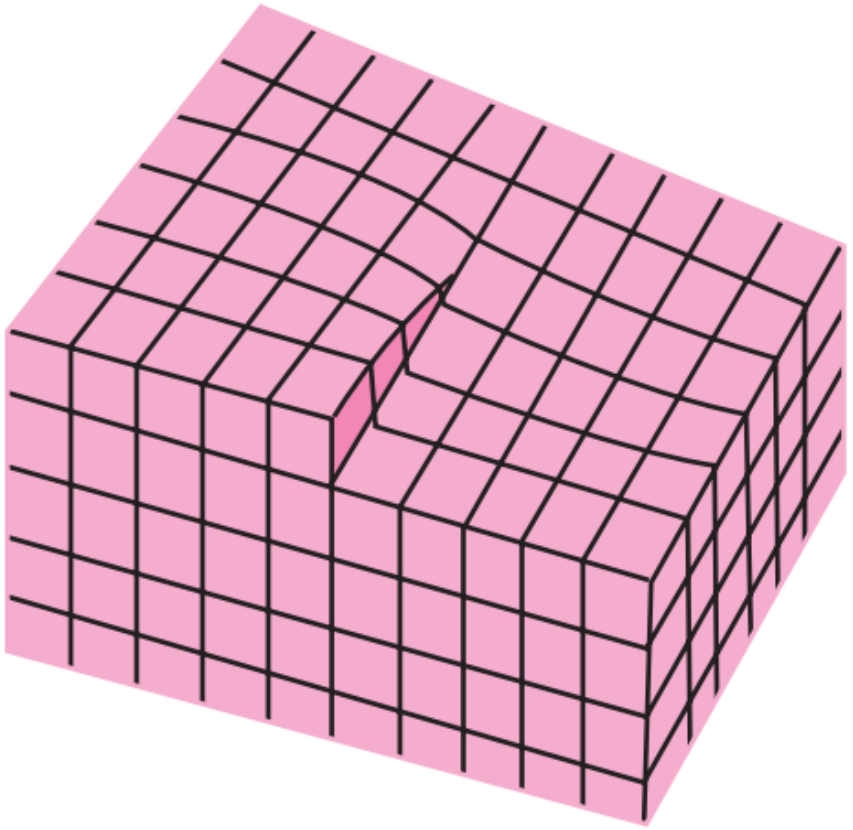
A color center is a defect-related electronic state that absorbs selected wavelengths of visible or other electromagnetic radiation.

F-center: In an alkali-halide crystal, an anion vacancy occupied by an electron is called an F-center. The trapped electron can undergo optical transitions, causing selective absorption and giving the crystal a characteristic color.

Color centers may form through irradiation, heating, or chemical treatments. They are particularly important in optical materials and defect spectroscopy.

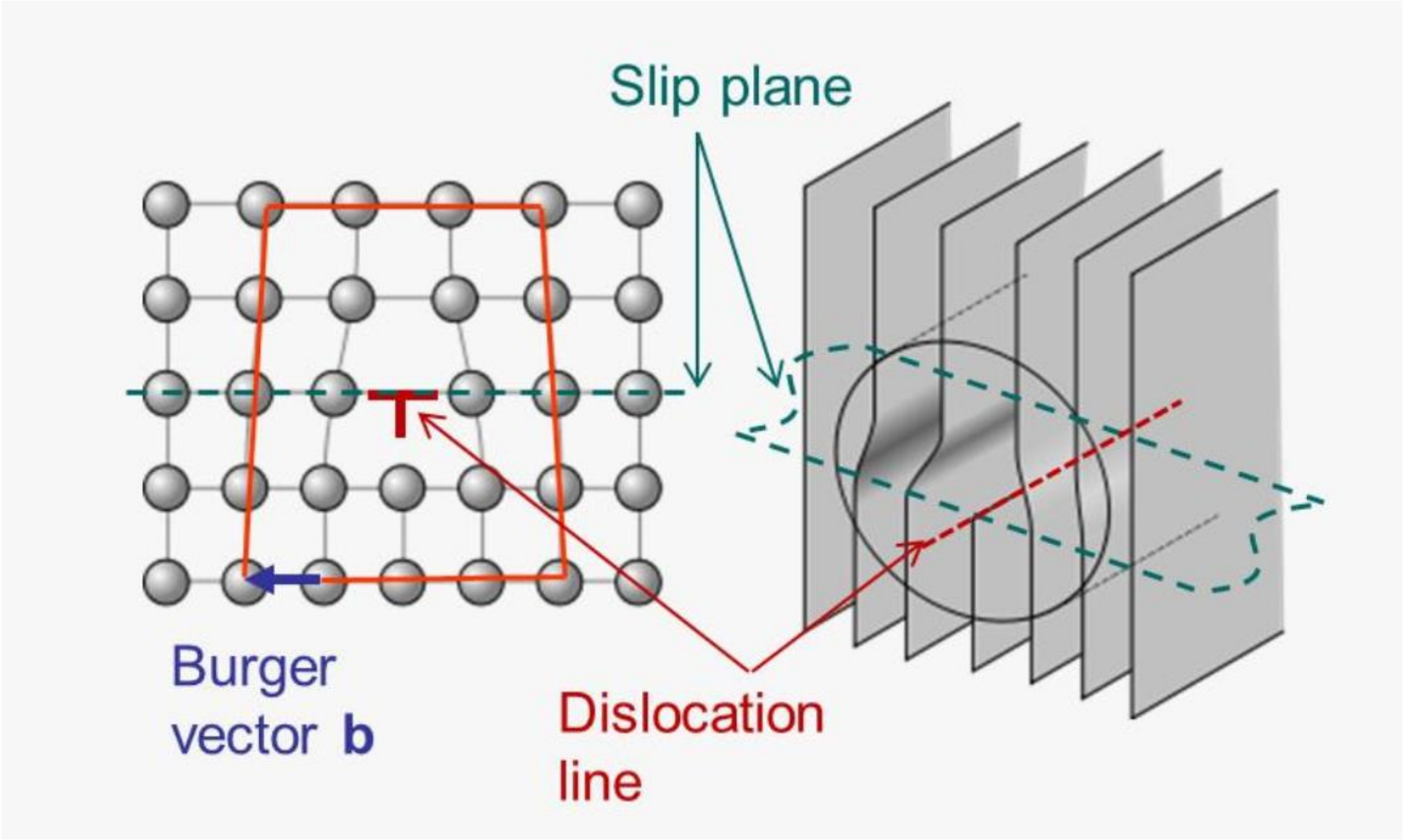
Crystal Defects





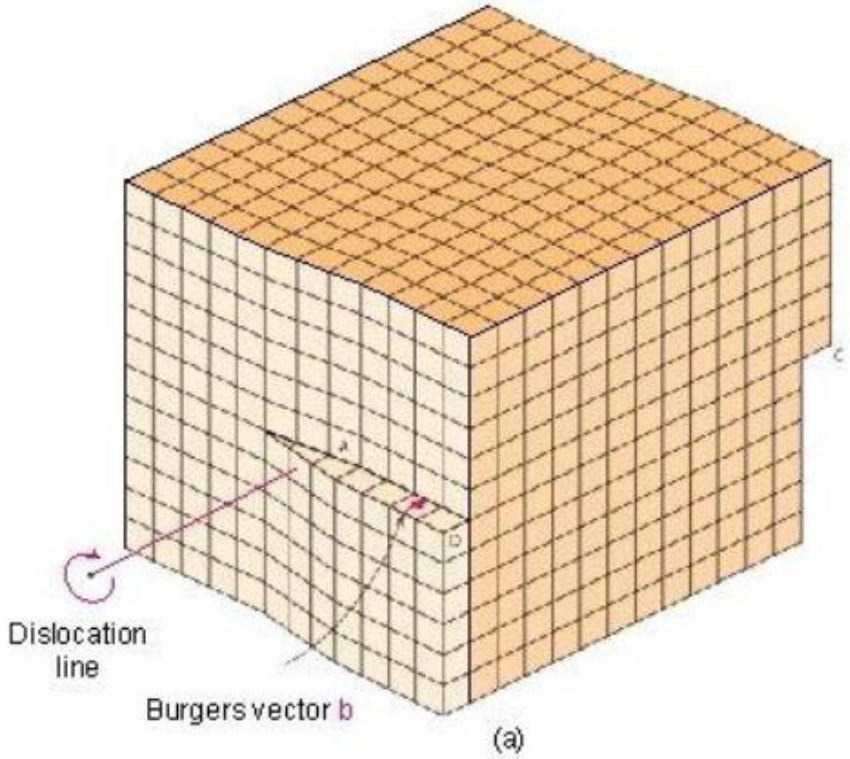
A screw dislocation.

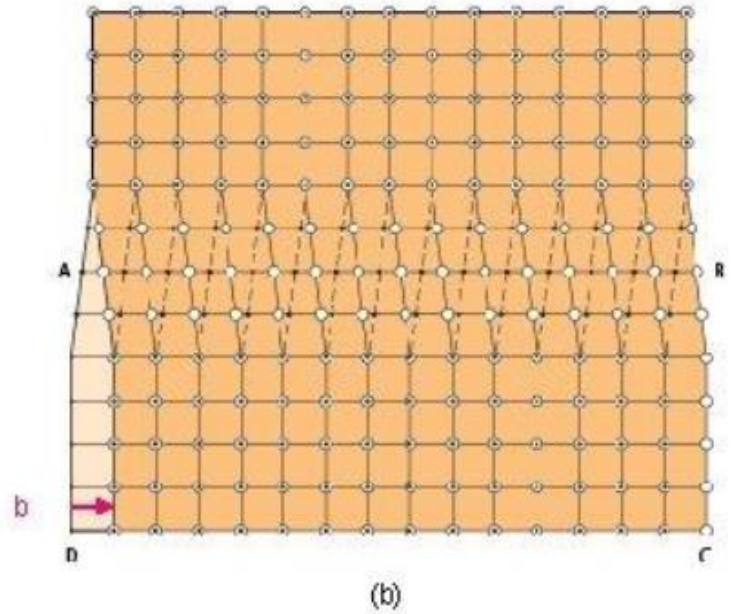
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Slip plane
T
Burger
vector b
Dislocation
line

Screw Dislocation

1. spiral planar ramp resulting from shear deformation.
2. **b** parallel (||) to dislocation line.





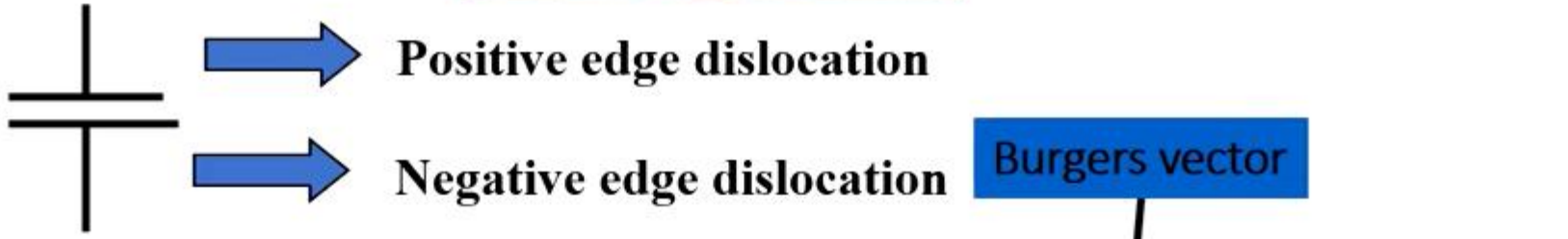
The screw dislocation in (a) as viewed from above. The dislocation line extends along line AB. Atom positions above the slip plane are open circles and those Below are solid circles.

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Crystalline Imperfections –
2. Line Defects (Dislocations)

Edge Dislocations

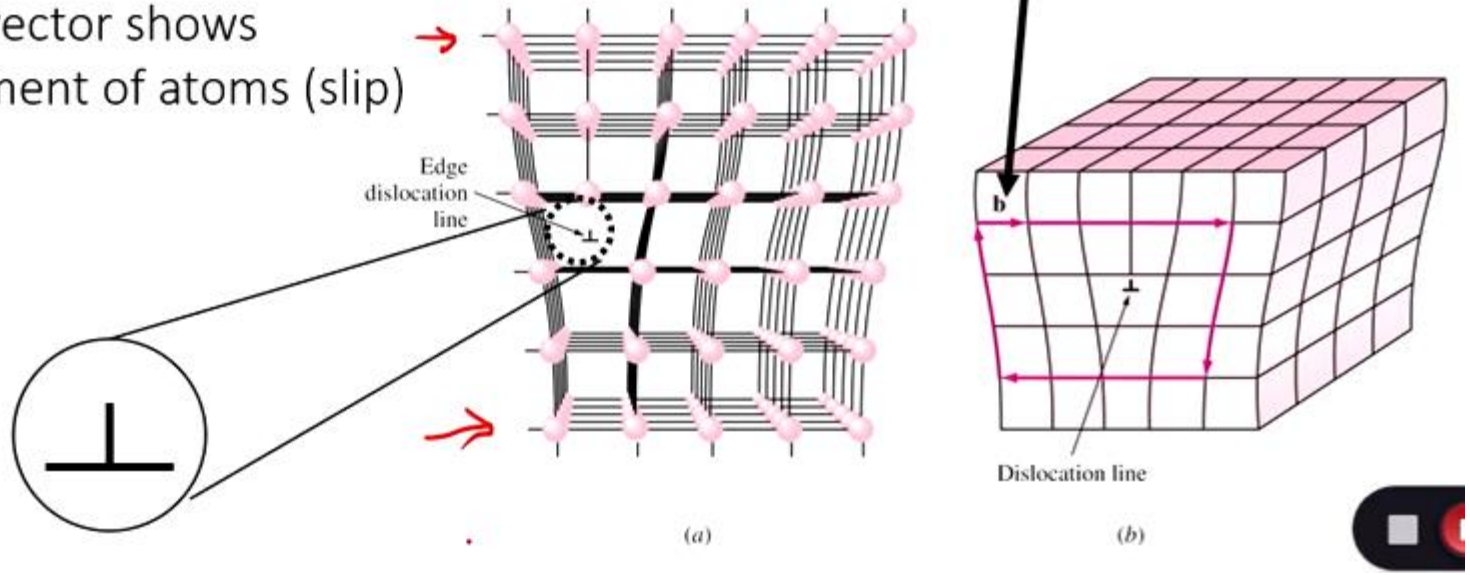
- Created by insertion of extra half planes of atoms



Positive edge dislocation

Negative edge dislocation

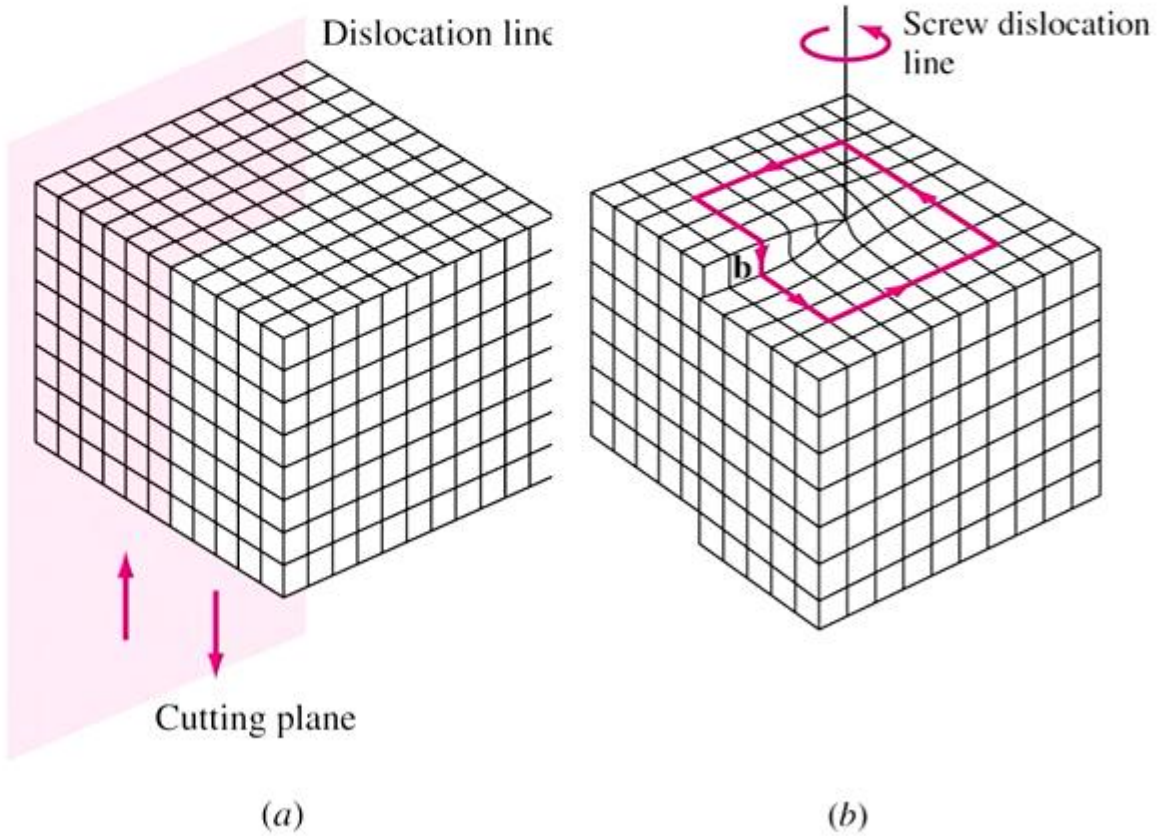
- Burgers vector shows displacement of atoms (slip)



Crystalline Imperfections –
2. Line Defects (Dislocations)

Screw Dislocations

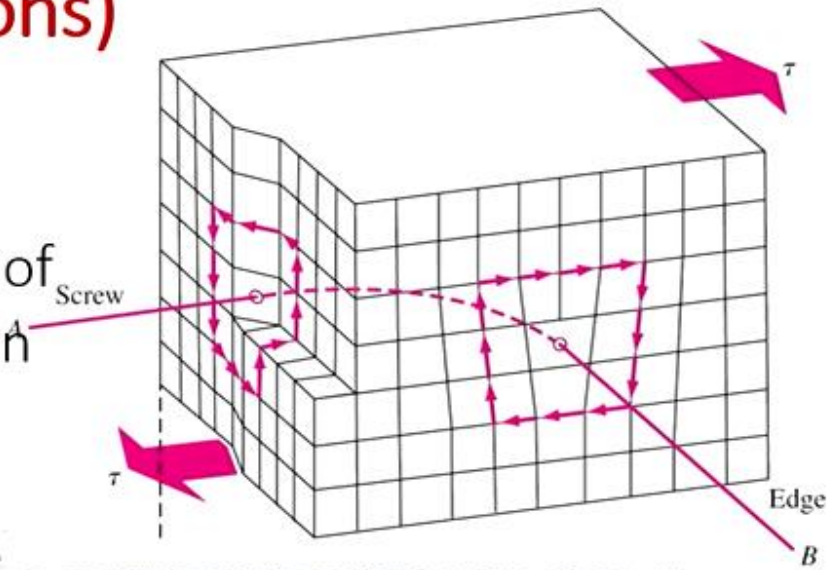
- Created due to upward and downward *shear stresses* applied to regions of a perfect crystal separated by cutting plane
- Distortion of lattice in form of a spiral ramp
- Slip vector is parallel to dislocation line



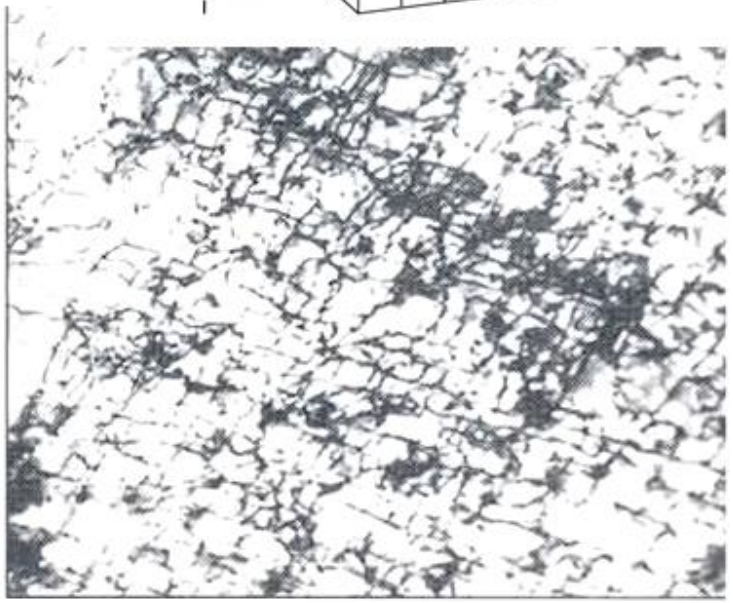
Crystalline Imperfections –
2. Line Defects (Dislocations)

Mixed Dislocations

- Most crystal have components of both edge and screw dislocation

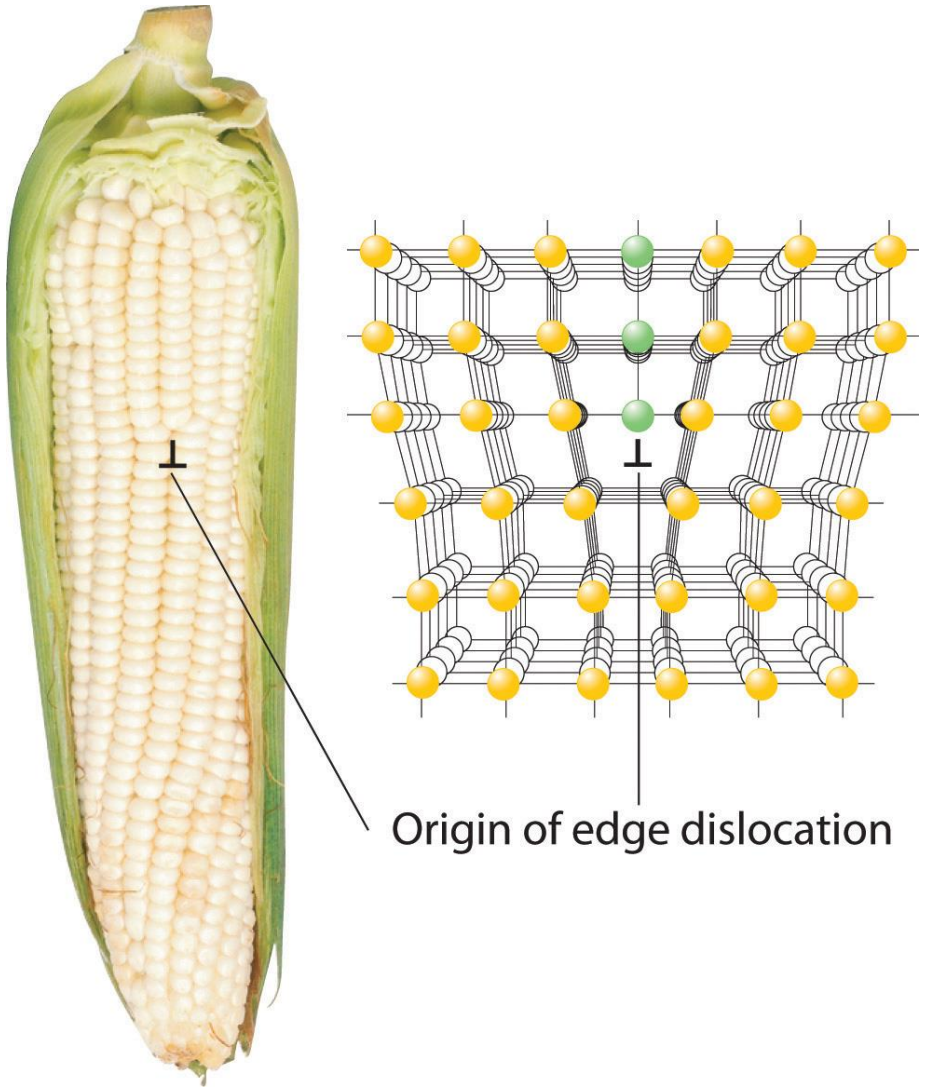


- Dislocation appear as dark lines when observed in electron microscope (due to irregular atomic arrangement)

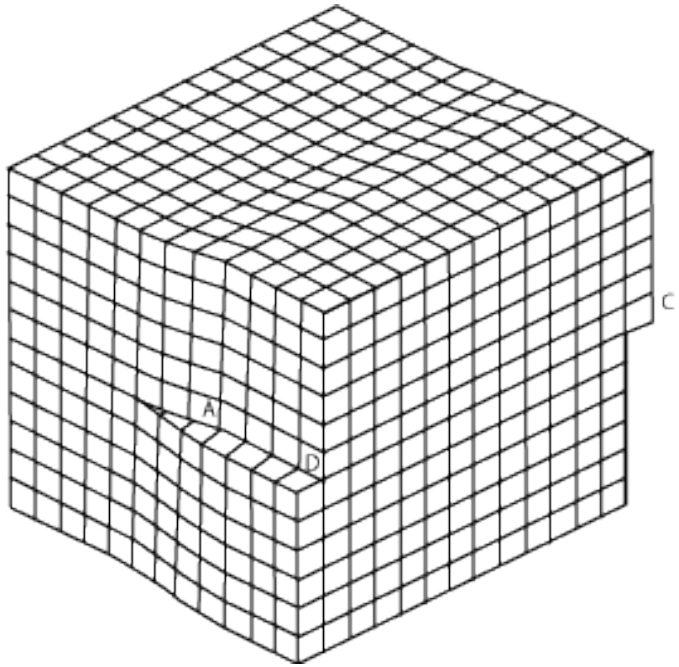


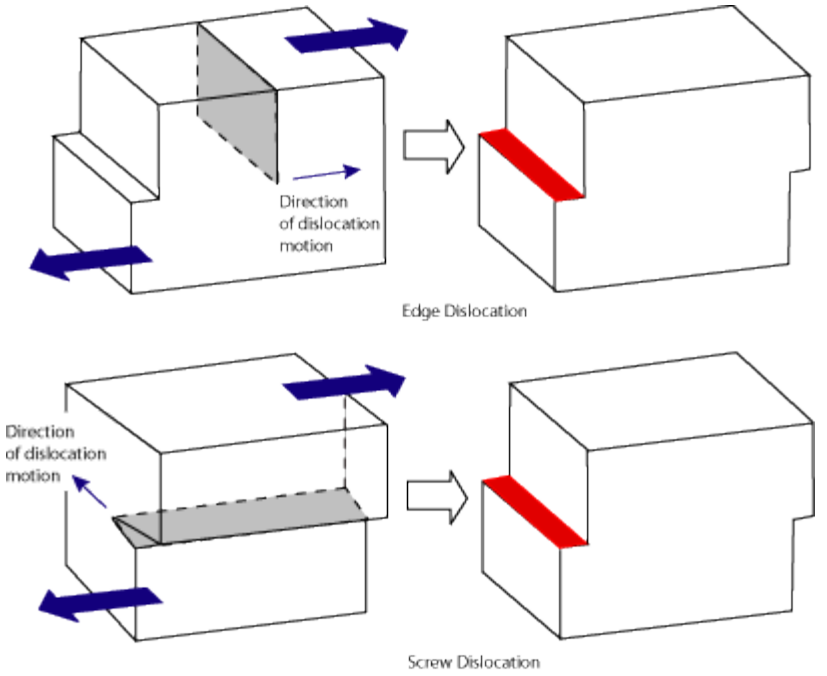
Dislocation structure of iron deformed 14% at -195^0C

Crystal Defects

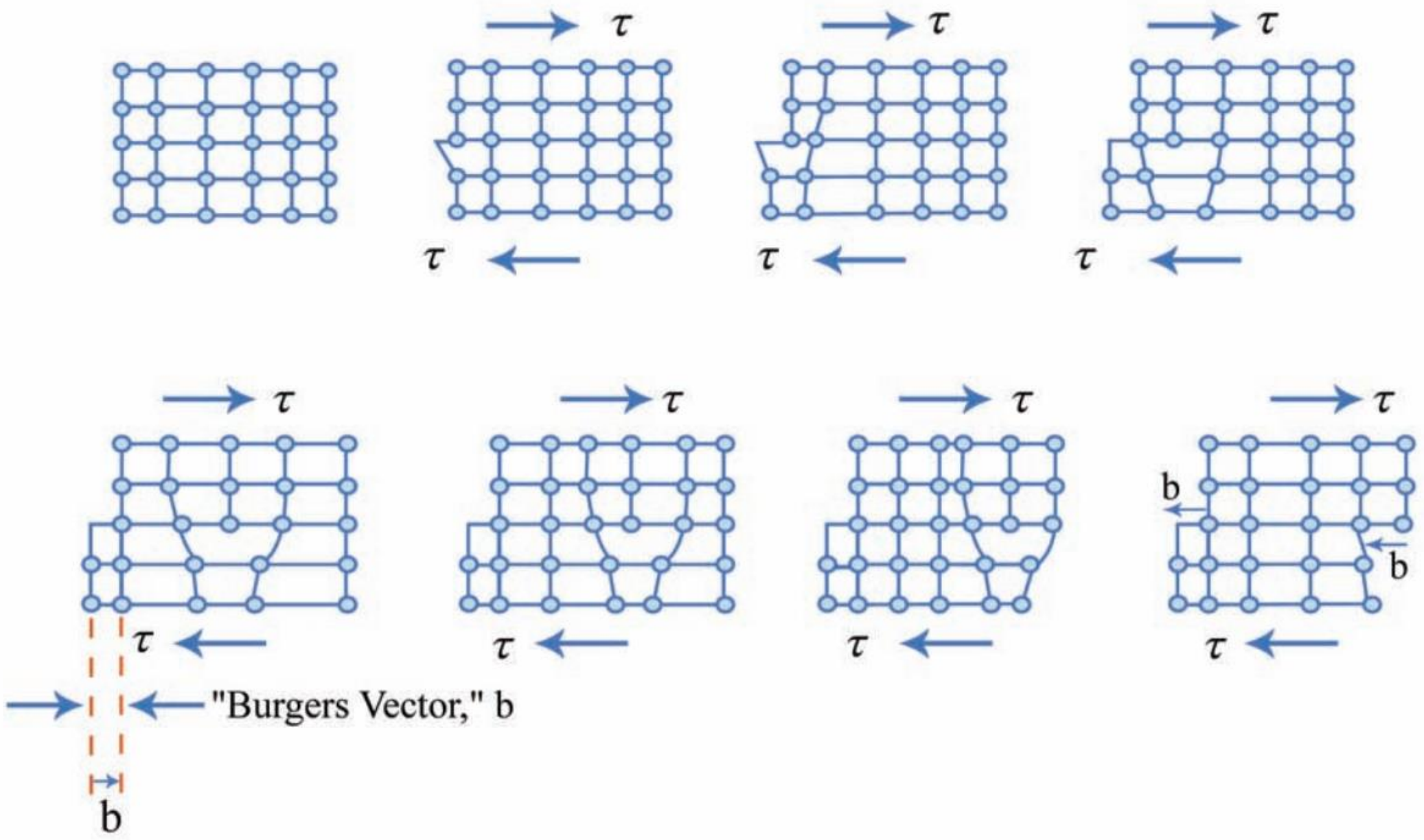


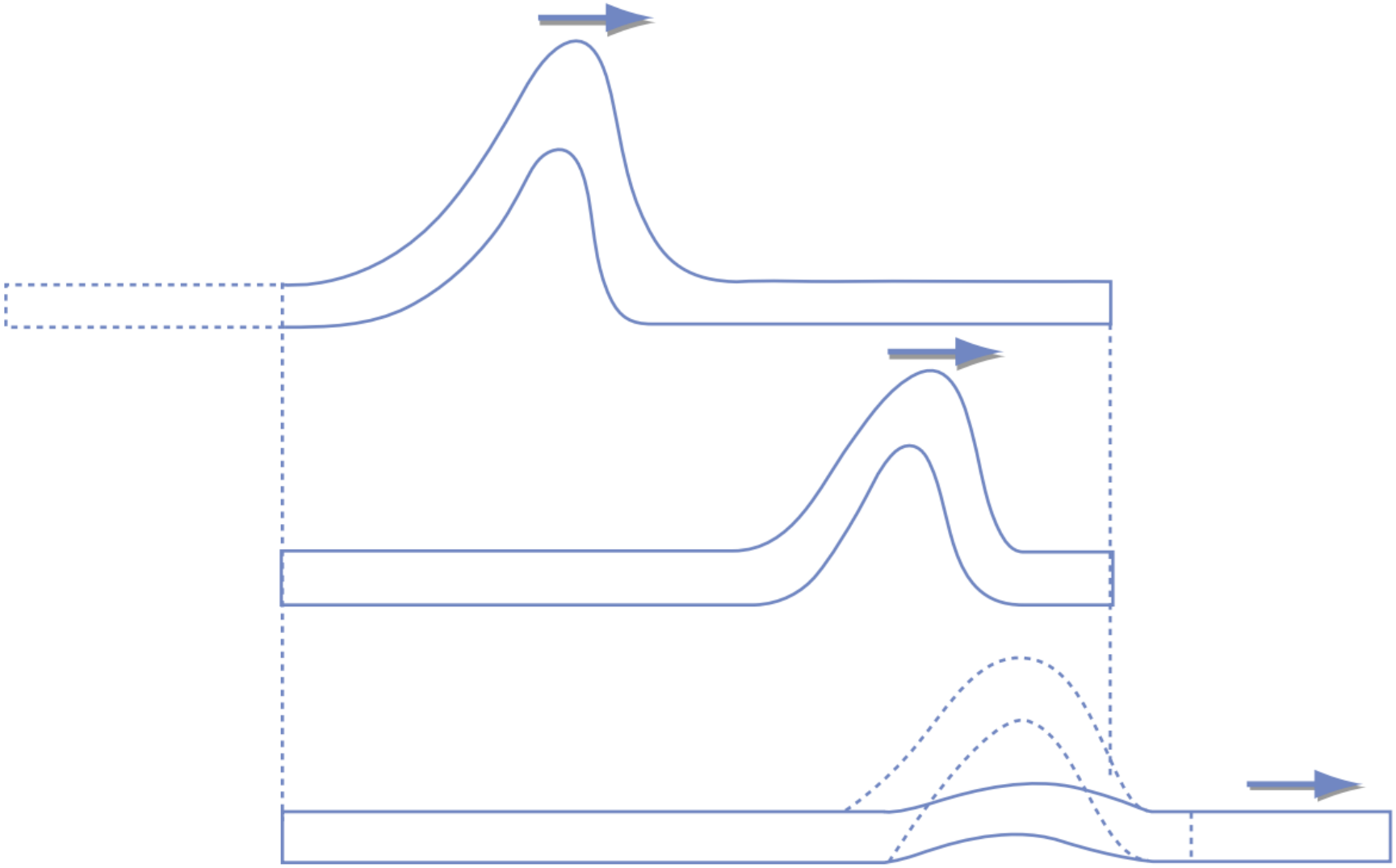
Crystal Defects



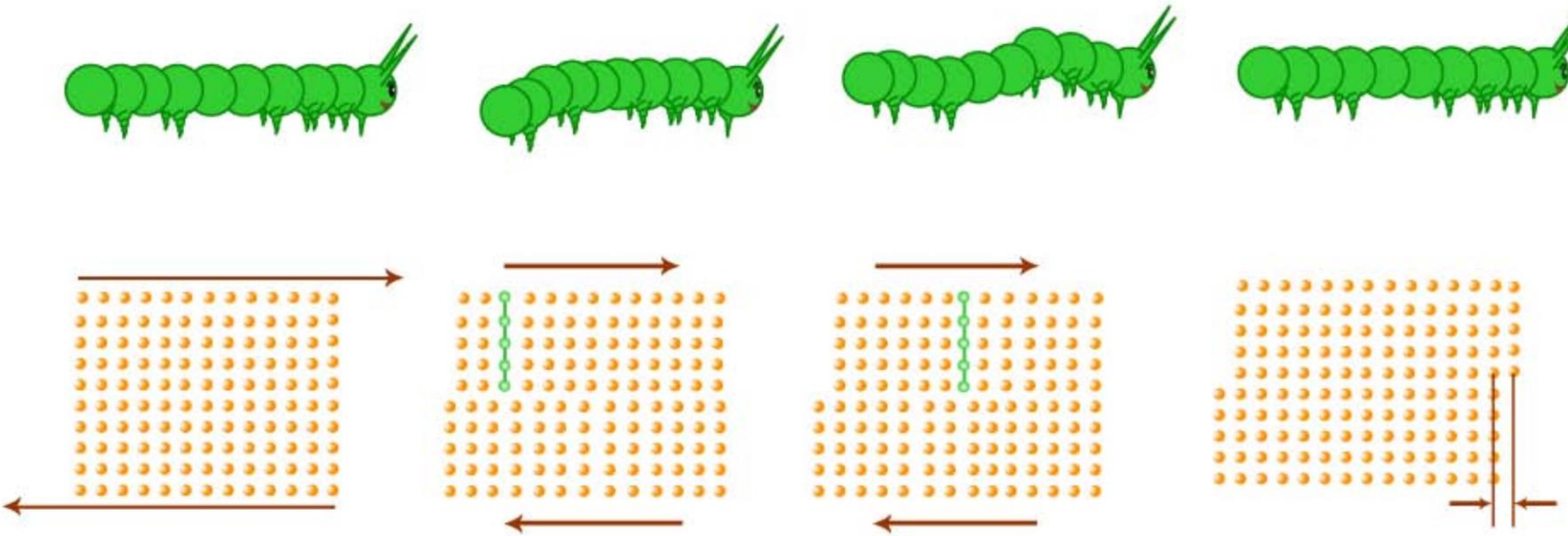


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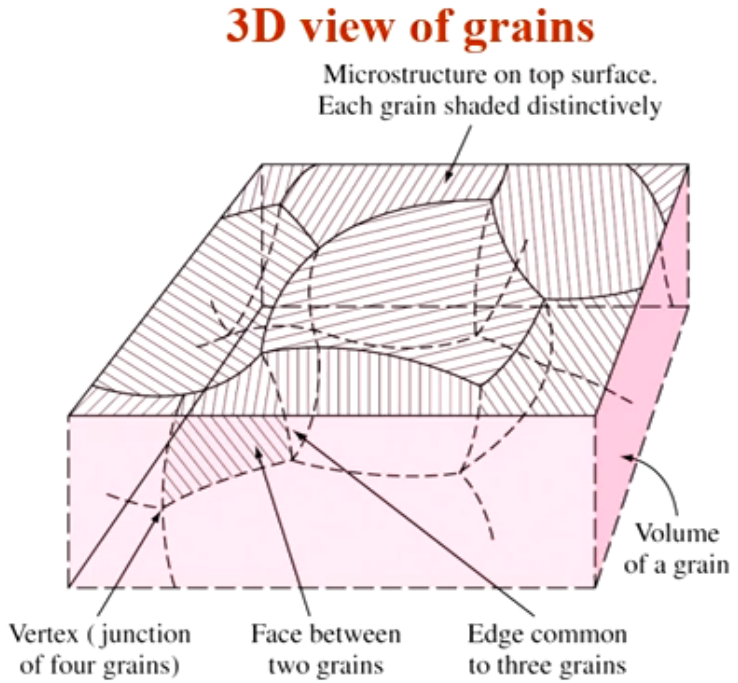
The 'carpet-ruck' analogy of an edge dislocation.

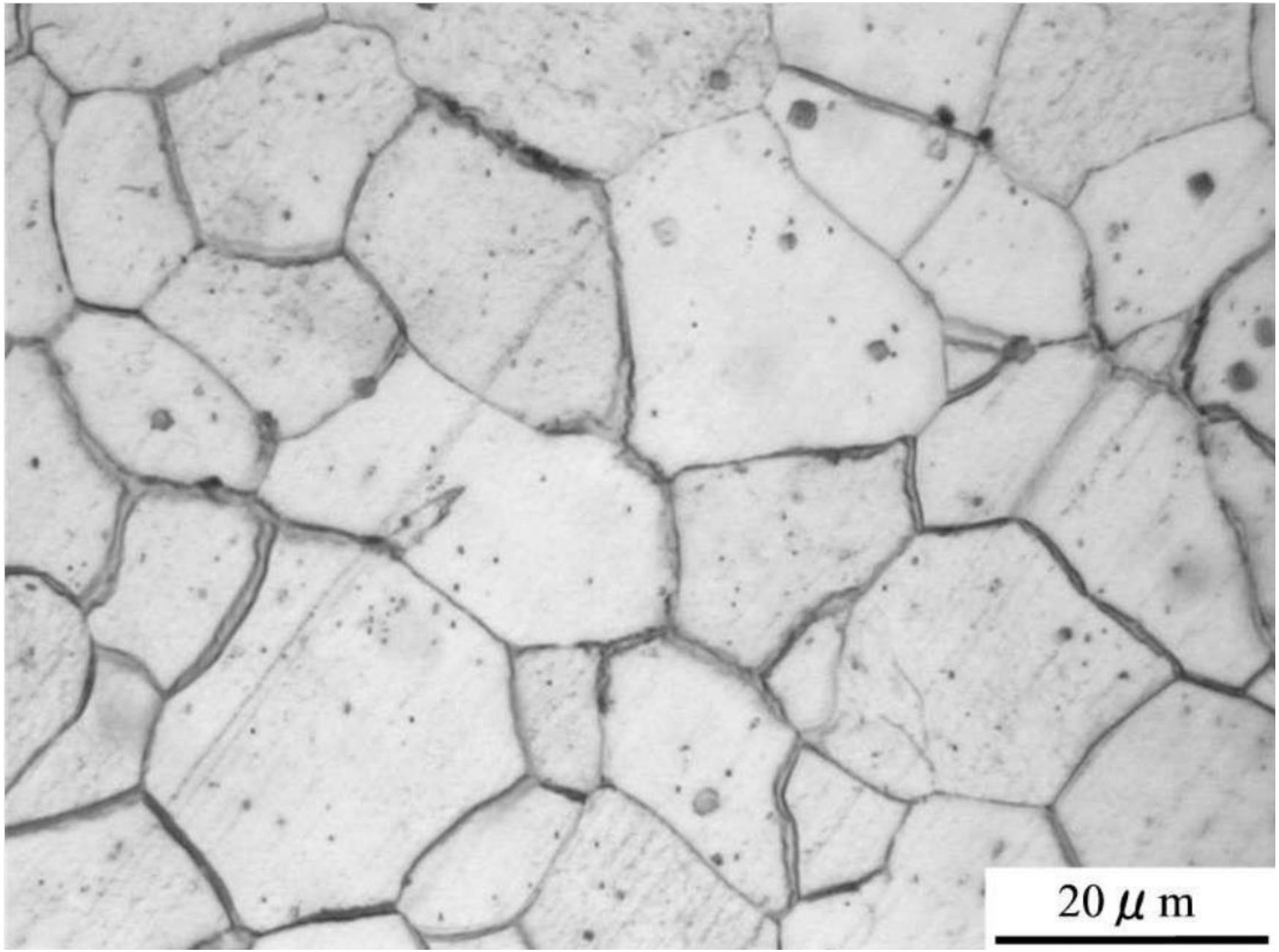


Crystalline Imperfections –
3. Planar Defects

Grain Boundaries

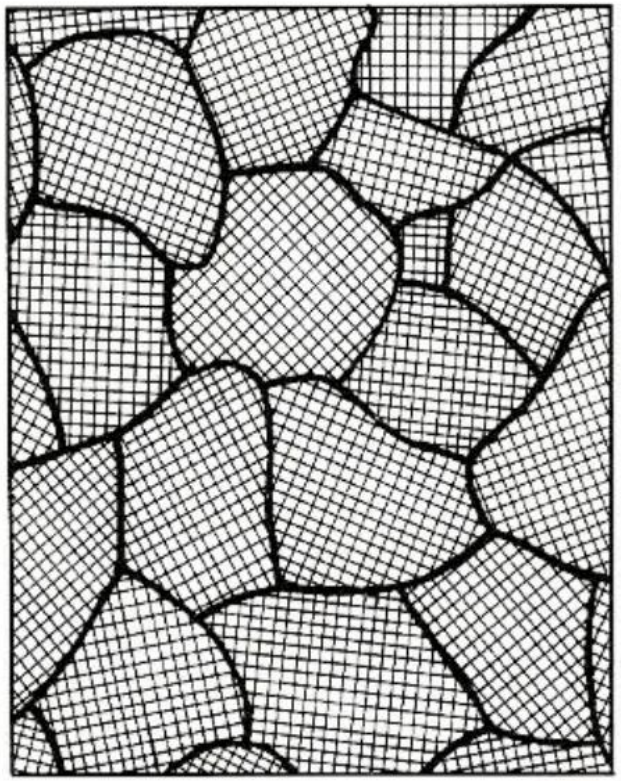
- Narrow region between two grains of about 2-5 atomic diameters in width, contains mismatched atoms from adjacent grains
- Separate grains of different orientations
- Formed due to simultaneously growing crystals meeting each other
- Favorable sites for nucleation and growth of precipitates
  - Irregular atom arrangement provides lower atomic packing and high energy
  - Atoms are thus able to diffuse more rapidly to form precipitates

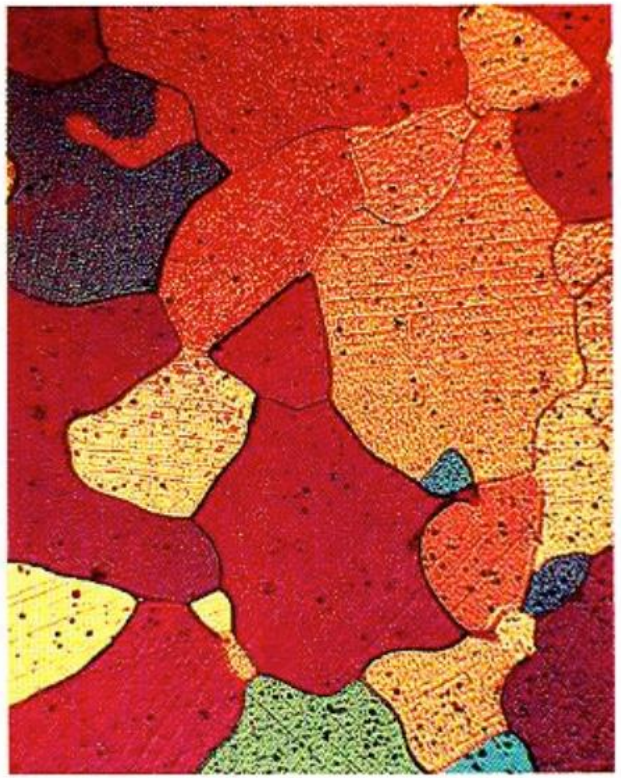


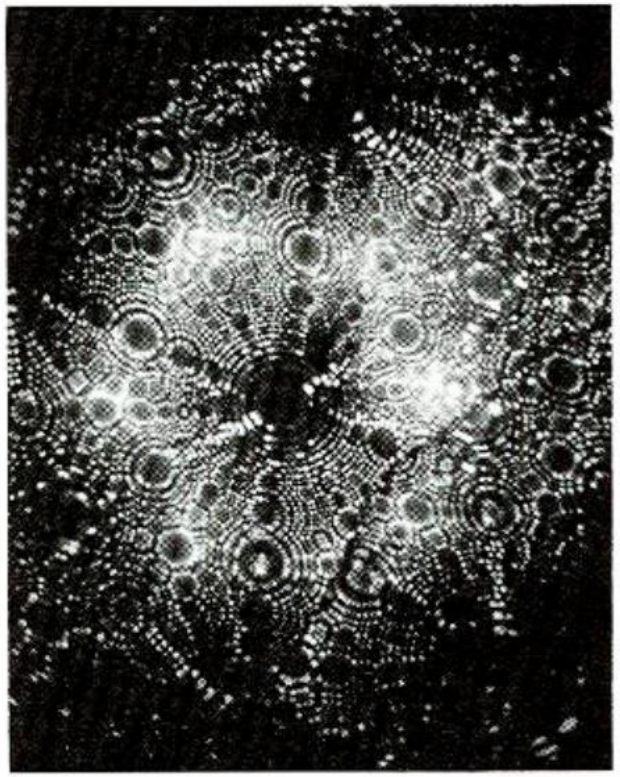

20 μ m

polycrystalline Cu

W bicrystal







optical microscope
polarized light

field ion
microscope