Chapter Four :
Semiconductor
Second stage: General Scienc
Types of defects in solid state 2024

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Crystalline solids are those where atoms or molecules or ions are arranged in a regular pattern (known as crystal lattice) that extends in all directions. A perfect crystal is one in which the arrangement of the atoms within the crystal lattice is periodic, i.e. each atom occupies its designated lattice site and there are no missing atoms . So crystal lattice is a highly ordered three-dimensional structure of atoms or molecules or ions base shown in figure (1).

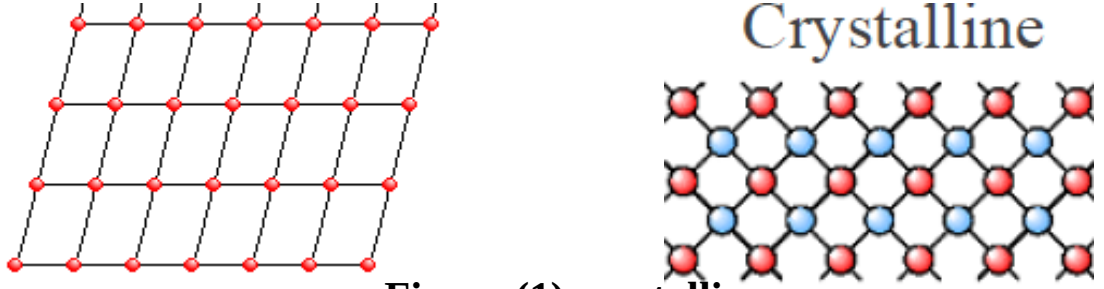


Figure (1) crystalline

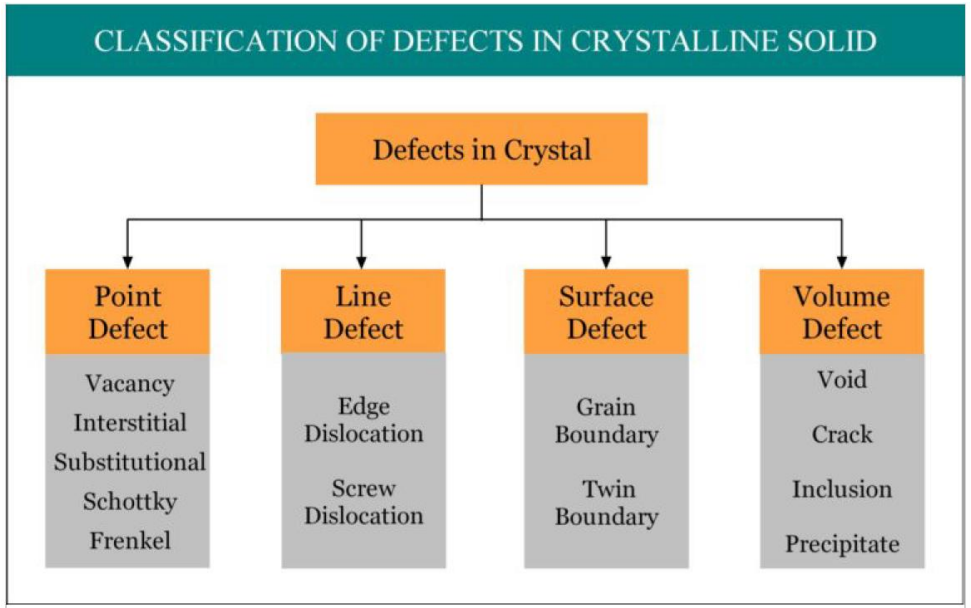
Imperfections in crystal structures

Crystal defect, **imperfection** in the regular geometrical arrangement of the atoms in a crystalline solid. ... These **imperfections** result from deformation of the solid, rapid cooling from high temperature, or high-energy radiation (X-rays or neutrons) striking the solid or thermal vibration or lattice vibration(phonon).

The energies of thermal vibrations of a crystal have a quantum called phonons.

$$E_{ph} = \left(n + \frac{1}{2}\right)\hbar\omega$$

There are some types of crystal defect



Introduction

Defect classification

Structural **crystal defects are classified according to their dimensions.**

in thermo-dynamic equilibrium	
0-dimensional defects	**atomic size („point“) defects** **intrinsic** (vacancies, interstitials) **and extrinsic** (dopants) **defects**
in thermo-dynamic non-equilibrium	
1-dimensional defects	**dislocations** (edge, screw, 60° , 30° , mixed, mobile, sessile, bunched, ordered...)
2-dimensional defects	**stacking faults, twins grain and phase boundaries, facets ?** (expressing perfection !)
3-dimensional defects	**precipitates, inclusions, voids** (vacancy agglomerates), **bubbles, dislocation clusters**

The main kinds of static defects of crystal lattices

• **Point defects** - atoms missing or in irregular places in the lattice (lattice vacancies, substitutional and interstitial impurities, self interstitials

Linear defects - groups of atoms in irregular positions (e.g. screw and edge dislocations

• **Planar defects** – the interfaces between homogeneous regions of the material (grain boundaries, stacking faults, external surfaces}

Native point defects

Native defects are point defects due to atomic imperfections in the material. There are three types of native defects: vacancies, interstitials, and antisites. **Vacancies are atomic sites where a host atom in an ideal crystal structure is missing shown Figure (2)**

Interstitials are due to host atoms displaced from their regular crystal site Figures(2,3,4)

Antisite are atomic sites where the original atomic species has been replaced by another host atom in the crystal figure (2).

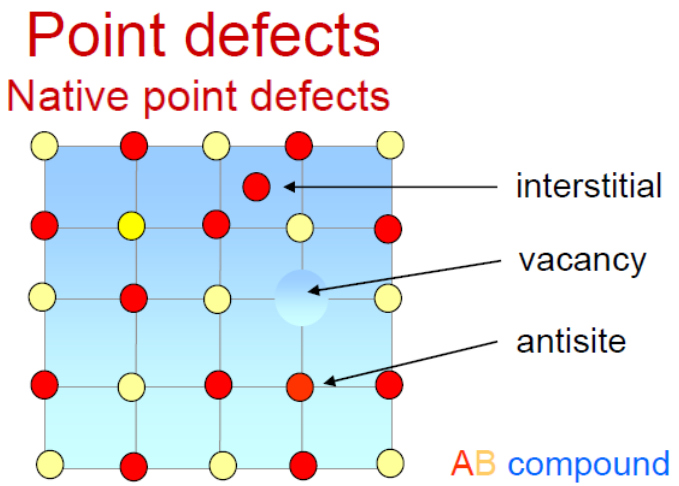


Figure (2): Native point defects

Native defects are thermodynamically equilibrium defects. They are always present in every material at any temperature above absolute zero with varying concentrations. In general, the native defect concentration increases with increase in growth temperature.

Point Defects

Naturally, point defects are the simplest kinds of defects that can exist within a crystal lattice example is a *vacancy* (also called a *Schottky defect*), a in which an atom is removed from a *lattice site* within the bulk of the crystal and transferred to the crystal surface.

Point Defects: Vacancies

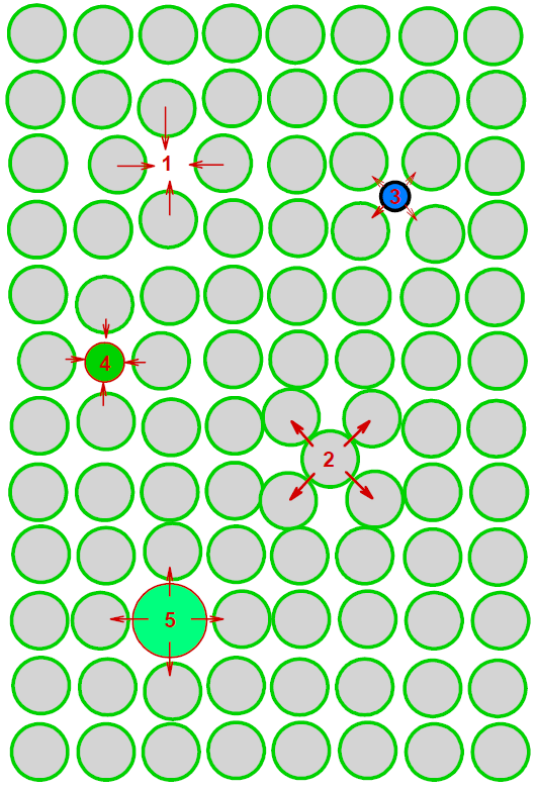
A perfect crystal with regular arrangement of atoms can not exist. There are always defects, and the most common defects are point defects.

If an atom is removed from its regular lattice site the empty lattice site is called a vacancy defect (V), and is shown in Fig. (3, 4 and 5) .

How many vacancies are there? The higher is the temperature, more often atoms are jumping from one equilibrium position to another and larger number of vacancies can be found in a crystal. Actually, the number of vacancies, Nv, increases exponentially with the absolute temperature, T, v:

$$N_V = N_S e^{\left(-\frac{N_V}{K_B T}\right)}$$

where N_S is the number of regular lattice sites, k is the Boltzmann constant, and N_V is the energy needed to form a vacant lattice site in a perfect crystal.



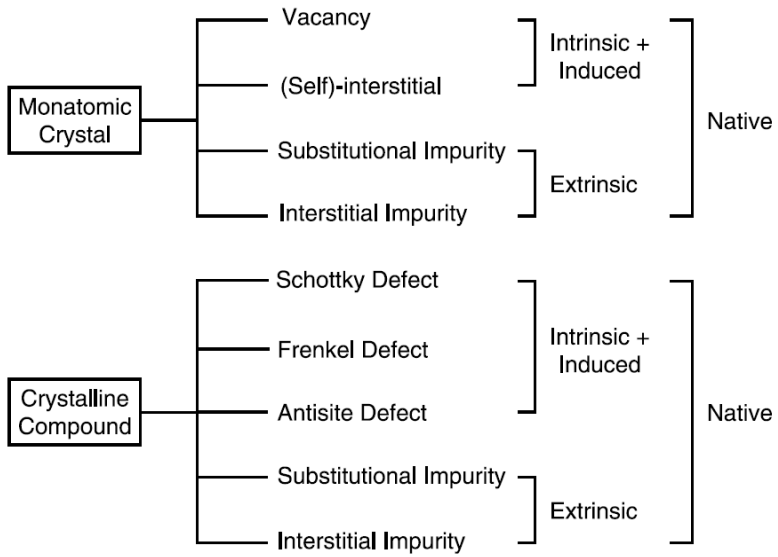
Schematic (3) representation of different point defects in a crystal. (1) vacancy; (2) self interstitial; (3) interstitial impurity; (4), (5) substitutional impurities. The arrows show the local stresses introduced by the point defects.

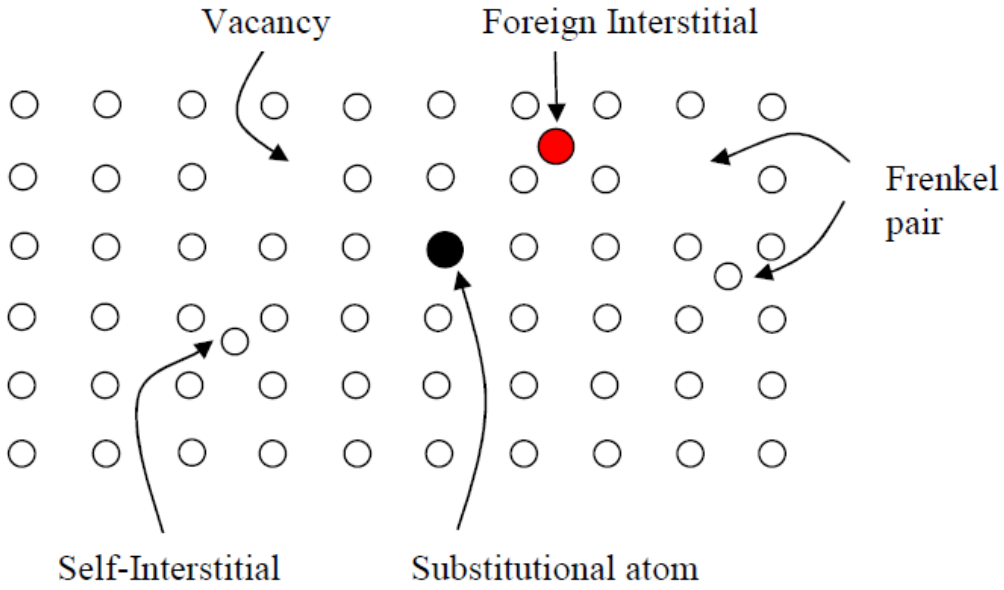
Primary Defects

Defects in semiconductors can be divided into two main categories; point defects and extended defects. Point defects are not extended in space in any dimension and this implies that the perturbation of the lattice is localized about a lattice site and involves only a few nearest neighbours

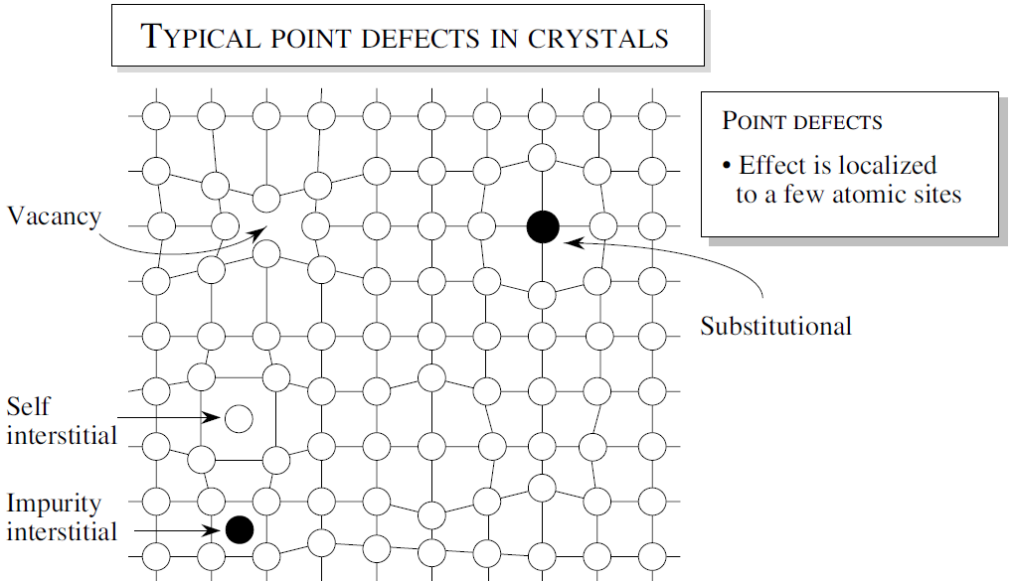
There are two kinds of point defects of great interest in semiconductor crystals, intrinsic (e.g. vacancies or self-interstitial) and extrinsic point defects (e.g. impurity atoms occupying substitutional or interstitial lattice sites.

Extended defects are extended in nature (such as, grain boundaries, dislocations).

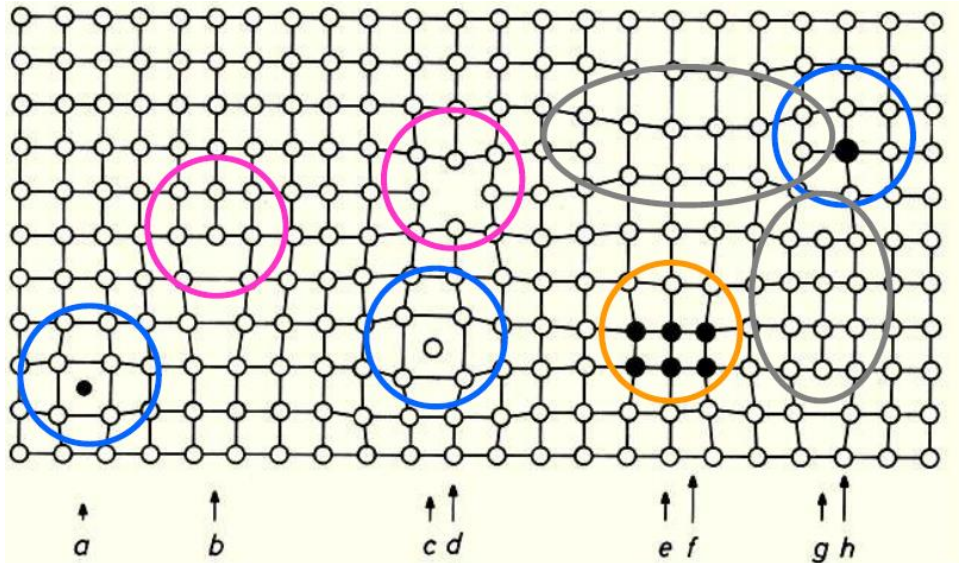




Figure(5a) A diagram of typical point defects in crystal



A schematic showing some important point defects in a crystal.



a – interstitial impurity atom
b – edge dislocation
c – self interstitial atom
d – vacancy
e – precipitate of impurity atoms
f – vacancy type dislocation loop
g – interstitial type dislocation loop
h – substitutional impurity atom

Figure (5) :Defect types

Interstitial Defect

Interstitials are atoms, which occupy a site in the crystal structure, which is not a regular lattice site as shown in Fig. (5 and 6). An interstitial defect can be of the same species as the atoms of the lattice (self-interstitial) or of a different nature (an interstitial impurity).

Foreign, usually smaller atoms (carbon, nitrogen, hydrogen, oxygen) are called **interstitial impurities.** They introduce less distortion to the lattice and are more common in real materials and more mobile. If the foreign atom atom replaces or substitutes for a matrix atom, it is called a **substitutional impurity**

More on Point Defects (A **Frenkel defect and Schottky defect)**

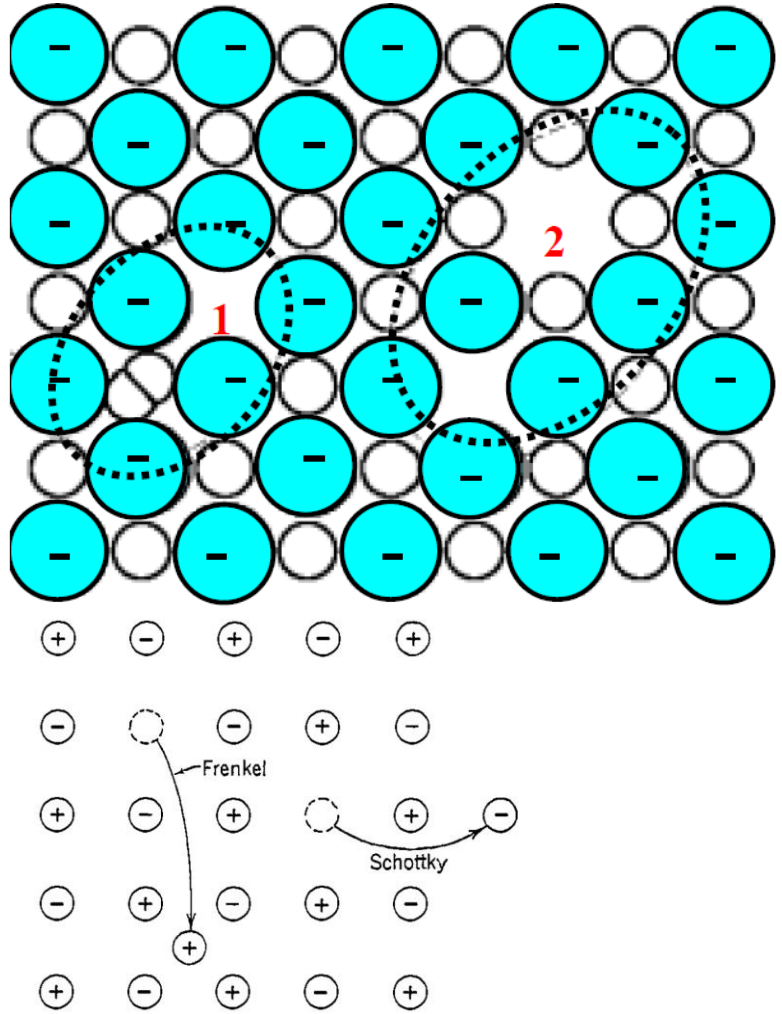
In ionic crystals (e.g. table salt Na^+, Cl^- the bonding is provided by columbic forces between positively and negatively charged ions. Point defects in ionic crystals are charged as well. The Columbic forces are very large and any charge imbalance has a very strong tendency to balance itself. To maintain charge neutrality several point defects can be created. A **Frenkel defect is a pair of cation (positive ion) vacancy and a cation interstitial. Or it may also be an anion (negative ion) vacancy and anion interstitial. Frenkel defect consists of one interstitial ion plus one vacant site in the sub lattice where that ion would normally be found**.

However anions are much larger than cations and it is not easy for an anion interstitial to form.

A **Schottky defect** is a pair of anion and cation vacancies. Or (a in which an atom is removed from a *lattice site* within the bulk of the crystal and transferred to the crystal surface).

In both Frenkel and Schottky defects, the pair of point defects stay near each other because of strong columbic attraction of their opposite charges. As will be for conductors, insulators and semiconductors, some impurities in semiconductors can lead to transistor properties.

At all temperatures above 0K Schottky, Frenkel, and antisite point defects are present in thermodynamic equilibrium



Schematic representation of (1) Frenkel defect (vacancy-interstitial pair) and (2) Schottky defect (a pair of cation and anion vacancies) in an ionic crystal.

$N_v = N e^{-E_v/kT}$, the number of vacancies N_v

formation energy E_v of the vacancy.

where N is the total number of atoms in the crystal.

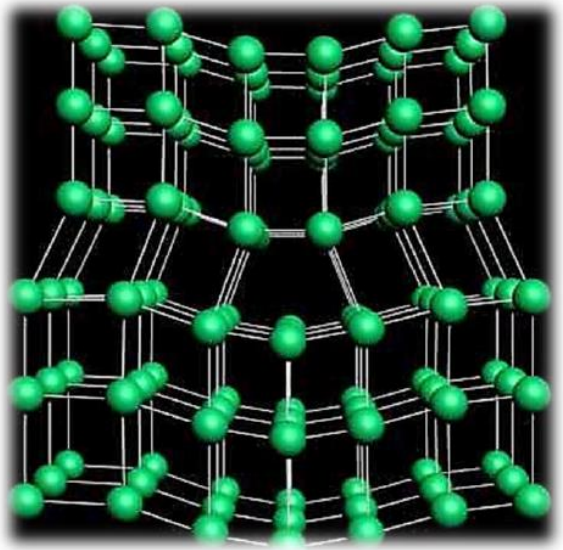
Dislocations defects

Dislocations can be explained as linear defects in which some of the atoms of the crystal lattice are misaligned .

The two basic types of dislocations are ***edge* dislocations and *screw* dislocations**.

If a plane of atoms in the middle of a crystal is terminated, edge dislocations are formed

Dislocations are line defects along which the crystal lattice is shifted by a certain amount.

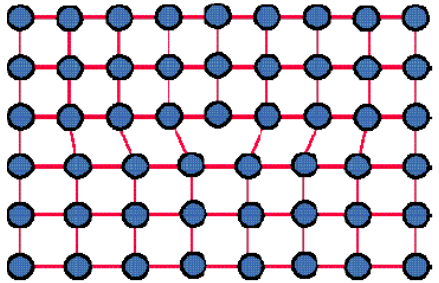


Lattice structure illustrating an edge dislocation within a semiconductor

Edge Dislocations

The simplest linear defect is a dislocation where there is a fault in the arrangement of atoms in a line through the crystal lattice.

Screw Dislocations

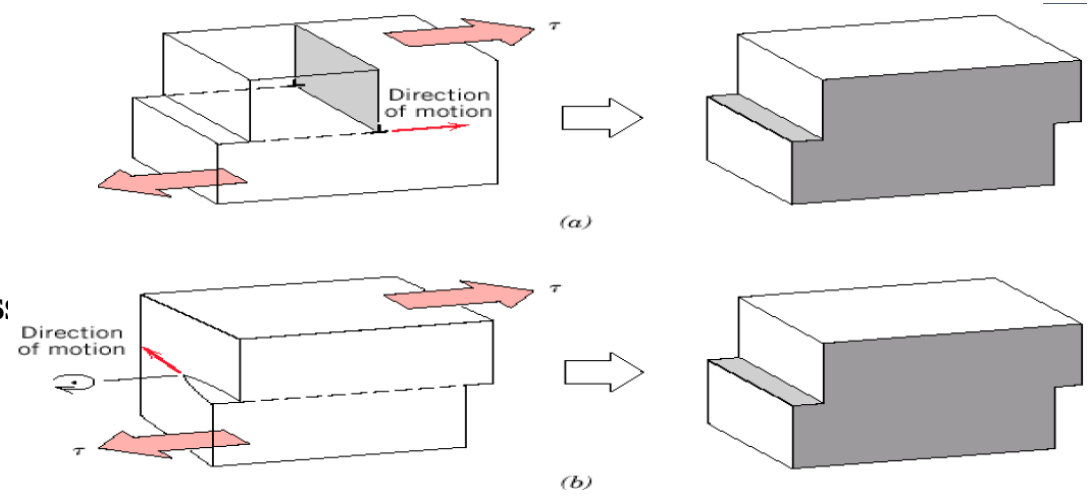


Another linear defect is a screw dislocation. This occurs when a stress is applied to the crystal and the dislocation of the line of atoms is perpendicular to the stress. A screw dislocation results from shear distortion. Many dislocations in crystalline materials have both edge and screws components; these are mixed dislocations

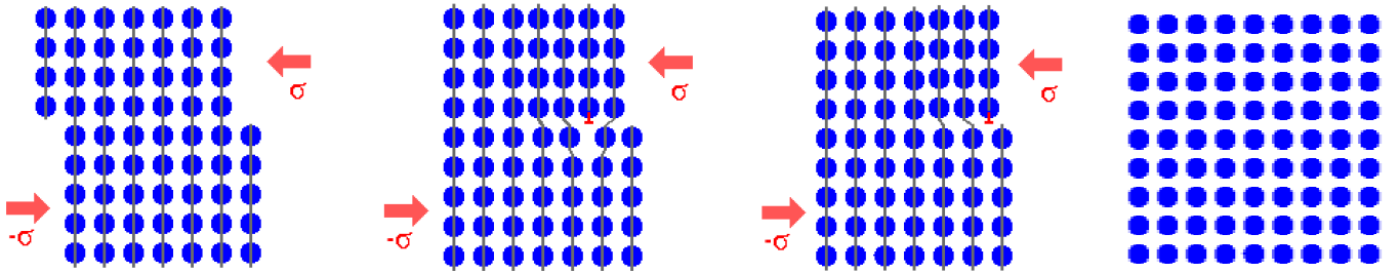
Direction of Dislocation Motion

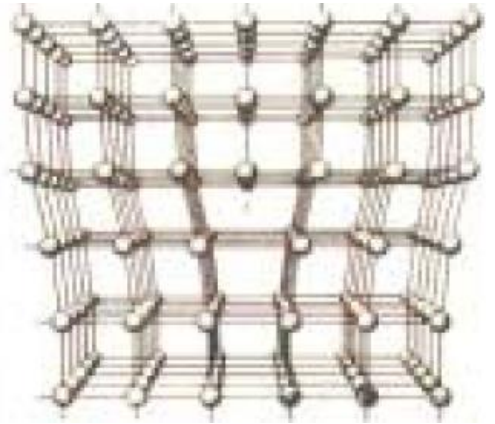
Edge dislocation line moves parallel to applied stress

Screw dislocation line moves perpendicular to applied stress



Motion of dislocations allows slip – plastic deformation when interatomic bonds are fractured and reformed. Actually, slip always occurs through dislocations motion.



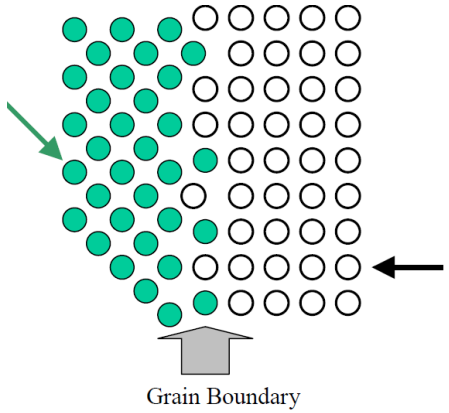


This 3D picture shows the inserted half-plane dislocation line goes through the center of the picture

The propagation of one dislocation across the plane causes the top half of the crystal to move with respect to the bottom half but we do not have to break all the bonds across the middle plane simultaneously (which would require a very large force).

Planar defects. Grain Boundaries. Polycrystals

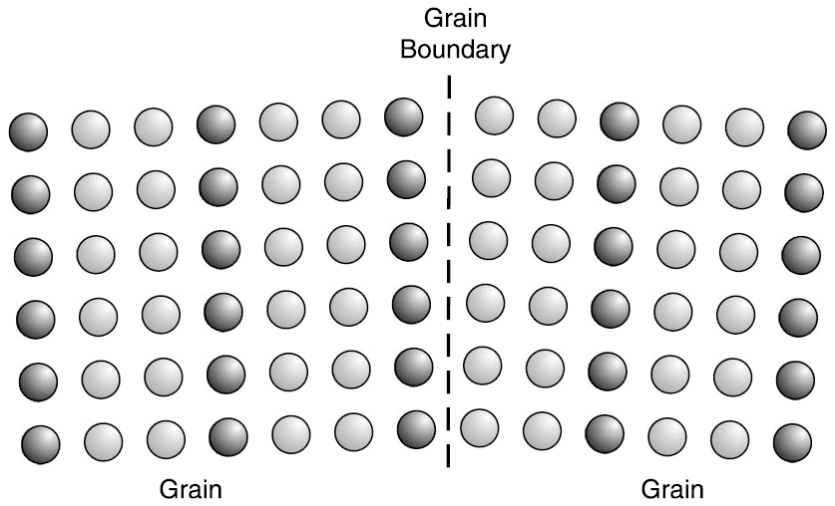
Solids generally consist of a number of small crystallites or *grains*. The grains can be from nanometers to millimeters in size and the orientations of atomic planes are rotated with respect to the neighboring grains. These materials are called **polycrystals.**



Grain Boundary

Figure :Planar defects in solids: (a) boundaries between slightly misaligned regions or domains

Planar Defects: Grain Boundaries



A Grain Boundary is a general planar defect that separates regions of different crystalline orientation (i.e. grains) within a polycrystalline solid.

The atoms in the grain boundary will not be in perfect crystalline arrangement.

Grain boundaries are important in several ways. They present paths for atoms to diffuse into the material and scatter light passing through transparent materials to make them opaque. They also affect mechanical properties. The boundaries limit the lengths and motions of dislocations that can move. This means that smaller grains (more grain boundary surface area) strengthens materials