# VI   IMPERFECTIONS: Point, Line, Surface and Volume

6.1 CRYSTAL DEFECTS

A perfect crystal is an idealization; there is no such thing in nature. It is useful to classify crystal lattice defects by their dimension.

- The 0-dimensional defects affect isolated sites in the crystal structure, and are hence called **point defects.** An example is a solute or impurity atom, which alters the crystal pattern at a single point.
- The 1-dimensional defects are called **dislocations**. They are lines along which the crystal pattern is broken.
- The 2-dimensional defects are surfaces, such as the external surface and the grain boundaries along which distinct crystallites are joined together.
- The 3-dimensional defects change the crystal pattern over a finite volume. They include precipitates, which are small volumes of different crystal structure, and also include large voids or inclusions of second-phase particles.
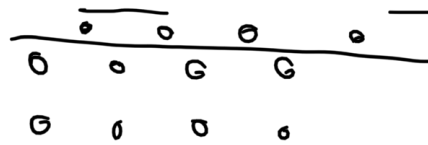
6.1.1 Point Defects:

A point defect disturbs the crystal pattern at an isolated site. It is useful to distinguish intrinsic defects, which can appear in a pure material, from extrinsic defects, which are caused by solute or impurity atoms.

Intrinsic defects
An intrinsic defect is formed when an atom is missing from a position that ought to be filled in the crystal, creating a vacancy,
or when an atom occupies an interstitial site where no atom would ordinarily appear, causing an interstitialcy.
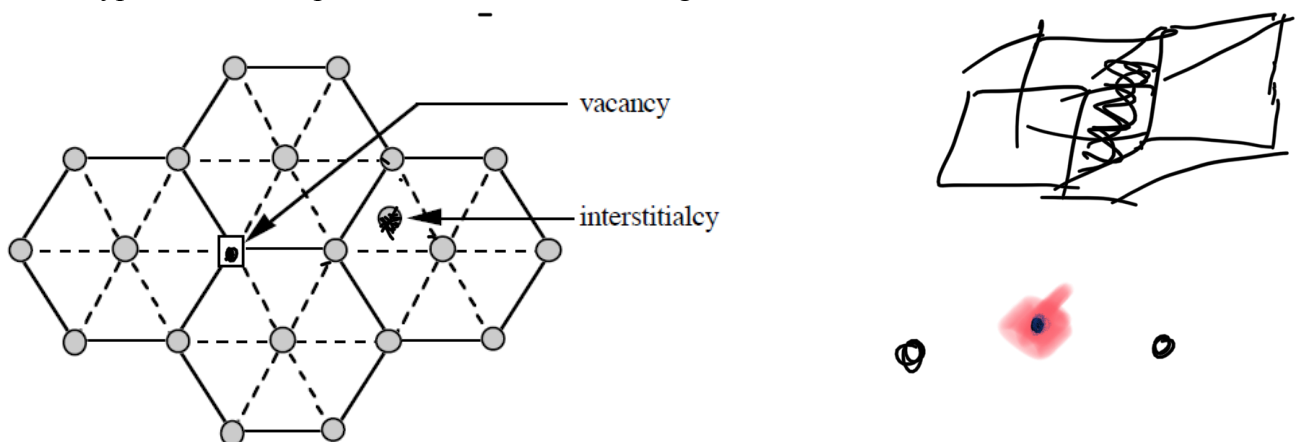The two types of intrinsic point defects are shown in fig. 35.

Figure 35: Illustration of a vacancy and interstitial in a hexagonal lattice.

Because the interstitial sites in most crystalline solids are small (or have an unfavorable bonding configuration, as, for example, in the diamond lattice) interstitialcies are high-energy defects that are relatively uncommon.

Vacancies, on the other hand, are present in a significant concentration in all crystalline materials. Their most pronounced effect is to govern the migration of atoms on the crystal lattice (solid state diffusion). In order for an atom to move easily from one crystal lattice site to another the target site must be vacant.

Ordered compounds can have more complex intrinsic defects. In most compounds the different species are charged to at least some degree.

An intrinsic defect destroys the local charge balance, which must be restored in some way. The compound defects that preserve charge are easiest to visualize in binary ionic solids like NaCl. An isolated vacancy in an ionic solid creates an excess charge. The excess charge can be compensated by a paired vacancy on the sublattice of the other specie; for example, the excess charge associated with a Na vacancy is balanced if there is a Cl vacancy nearby.

A neutral defect that involves paired vacancies on the cation and anion sublattices is called a **Schottky defect**. The concentration of Schottky defects decreases the density of the crystal. Alternatively, the charge imbalance caused by the vacancy can be corrected by adding an interstitial of the same specie; a Na vacancy is compensated by a Na interstitial.

A neutral defect that is made up of a paired vacancy and interstitial is called **a Frenkel defect**. The concentration of Frenkel defects does not change the density of the crystal.

In compounds whose atoms are less strongly ionized it is energetically possible for species to exchange sites, so that an A-atom appears on the B sublattice or vice versa.

This type of point defect is called an **anti-site defect**, and is fairly common in semiconducting compounds such as GaAs.

Extrinsic defects

The extrinsic point defects are foreign atoms, which are called solutes if they are intentionally added to the material and are called impurities if they are not.

The foreign atom may occupy a lattice sites, in which case it is called a substitutional solute (or impurity) or it may fill an interstitial site, in which case it is called an interstitial solute. Since, the interstitial sites are relatively small, the type of the solute is largely determined by its size. Small atoms, such as hydrogen, carbon and nitrogen are often found in interstitial sites. Larger atoms are usually substitutional.

6.1.2 Line Defects - Dislocations

Dislocations are another type of defect in crystals. Dislocations are areas were the atoms are out of position in the crystal structure. Dislocations are generated and move when a stress is applied. It is responsible for the phenomenon of slip by which most metals deform plastically.

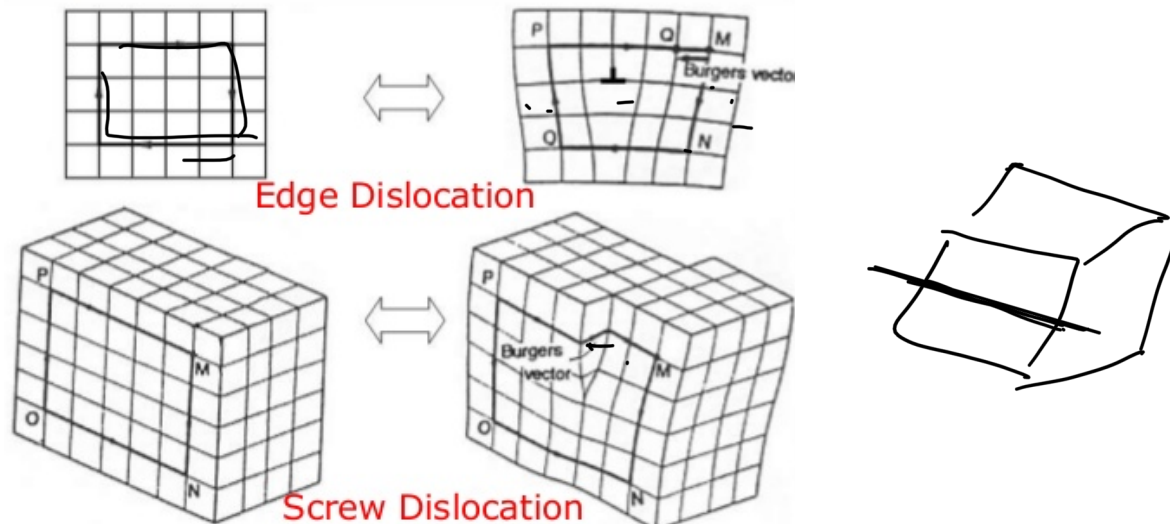There are two basic types of dislocations, the edge dislocation and the screw dislocation (fig. 36).
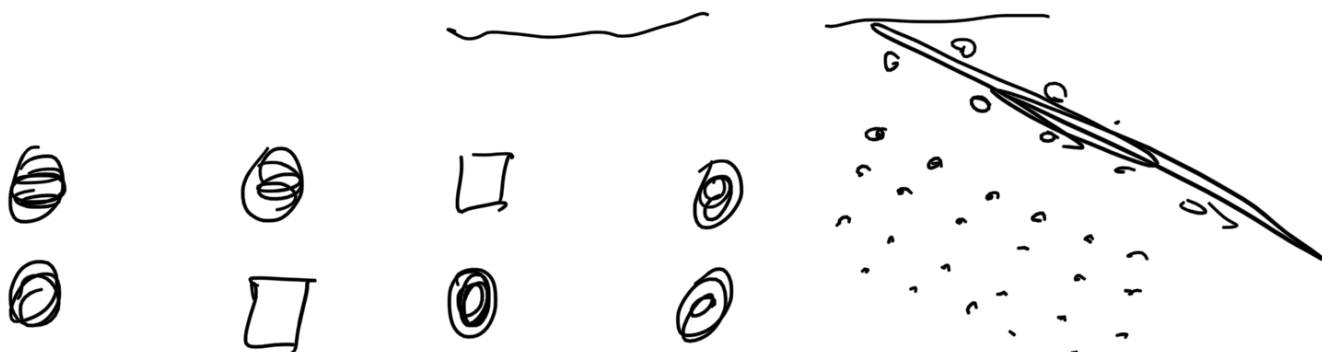
Figure 36: Illustration of an edge and screw dislocation.

Edge Dislocation

In perfect crystal, atoms are arranged in both vertical and horizontal planes. If one of these vertical planes does not extend to full length, but ends in between within the crystal, then it is called edge dislocation.

Just above the edge of the complete plane the atoms are squeezed and are in a state of compression. Just below the edge of the incomplete plane, the atoms are pulled apart and are in the state of tension. The distorted configuration extends all along the edge into the crystal. The inter-atomic bonds are significantly distorted only in the immediate vicinity of the dislocation line. Edge dislocation are represented by T or ⊥ depending on whether the incomplete plane starts from top or from the bottom of the crystal, called as positive or negative edge dislocation. The magnitude and the direction of the displacement are defined by a vector called Burgers vector. The Burgers vector is perpendicular to the edge dislocation line.

Burgers vector

To describe the size and the direction of the main lattice distortion caused by a dislocation a so-called Burgers vector *b* is introduced. To find the Burgers vector, a circuit from atom to atom counting the same number of atomic distances in all directions is made. If the circuit encloses a dislocation, it will not close. The vector that closes the loop is the Burgers vector (fig.37).
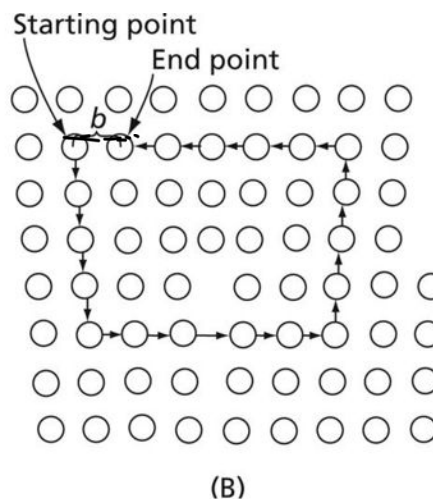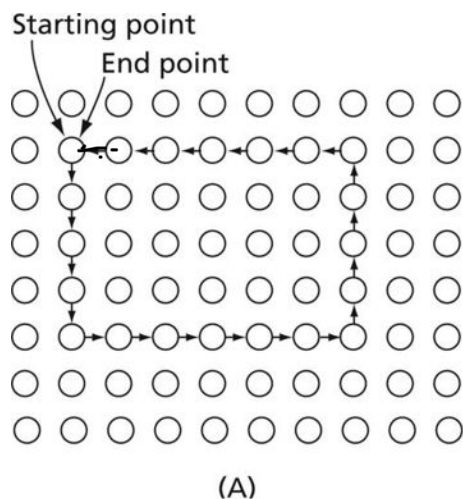
Figure 37: The Burgers circuit for an edge dislocation:

(A) Perfect crystal and

(B) crystal with distortion.

Screw Dislocations

There is a second basic type of dislocation, called screw dislocation. The motion of a screw dislocation is also a result of shear stress, but the defect line movement is perpendicular to direction of the stress and the atom displacement, rather than parallel. The Burgers vector is parallel to screw dislocation line. The speed of movement of a screw dislocation is lesser compared to edge dislocation

6.1.3 Planar Defects

A disruption of the long-range stacking sequence can produce two other common types of crystal defects: 1) **a stacking fault** and 2) a **twin boundary**.

Stacking fault: A change in the stacking sequence over a few atomic spacing produces a stacking fault whereas a change over many atomic spacing produces a twin region. So, if the hcp structure is going along as ABABAB and suddenly switches to ABABABCABAB, there is a stacking fault present.

Twin boundary: Twin boundaries occur when two crystals of the same type intergrow, so that only a slight misorientation exists between them. It is a highly symmetrical interface, often with one crystal the mirror image of the other; also, atoms are shared by the two crystals at regular intervals. This is also a much lower-energy interface than the grain boundaries that form when crystals of arbitrary orientation grow together.
Twin boundaries occurs in pairs, such that the orientation change introduced by one boundary is restored by other. The region between the pair of boundaries is called twin region.

Another type of planer defect is the **grain boundary**.

Grains can range in size from nanometers to millimeters across and their orientations are usually rotated with respect to neighboring grains. Where one grain stops and another begins is known as

a grain boundary. Grain boundaries limit the lengths and motions of dislocations. Therefore, having smaller grains (more grain boundary surface area) strengthens a material. The size of the grains can be controlled by the cooling rate when the material cast or heat treated. Generally, rapid cooling produces smaller grains whereas slow cooling result in larger grains.

6.1.4 *Volume Defects*

Volume defects occur on a much bigger scale than the rest of the crystal defects. Voids are regions where there are a large number of atoms missing from the lattice.

Another type of bulk defect occurs when impurity atoms cluster together to form small regions of a different phase. Other examples of bulk defects are pores, cracks and foreign particles.