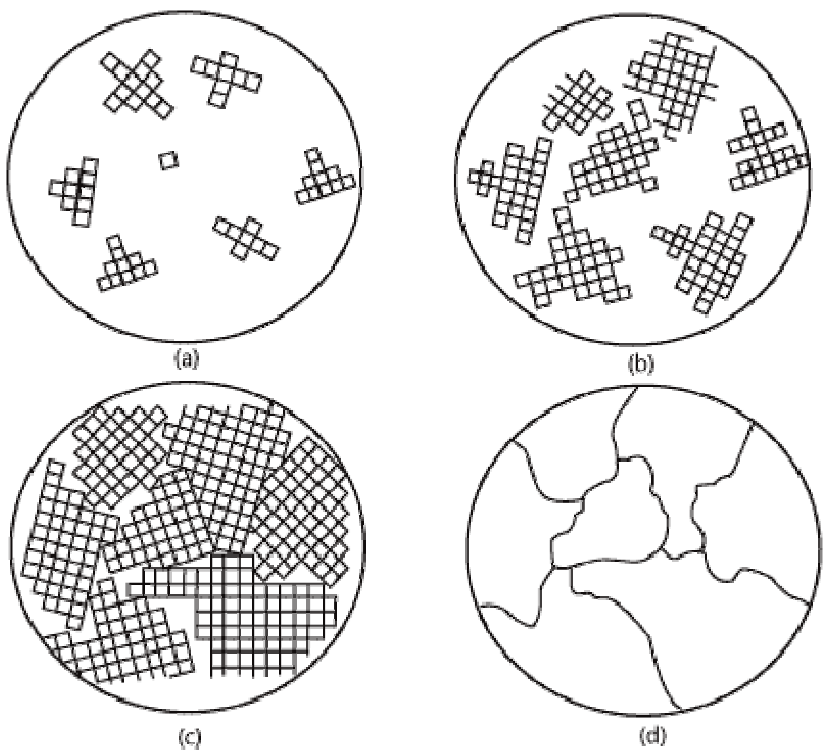
MATERIALS SCIENCE
CHAPTER 4: DEFECTS IN SOLIDS

Solids come with imperfections in their crystalline structures and these imperfections affect and contribute to the properties of materials. The imperfection is not always unfavourable. Under controlled conditions imperfections can be induced, to produce desired properties.

SOLIDIFICATION OF METALS

The solidification of metal takes place in the following steps:

1. the formation of stable nuclei in the melt (nucleation)
2. the growth of nuclei into crystals and the formation of a grain structure



The solidification of metal starts forms the point of nucleation. This is the moment when minute crystals are formed at the solidification temperature. As the temperature drops, atoms of the metal begin to bond together at the nucleation points and crystallization propagates. The crystals grow until they start to impinge upon adjacent growing crystals. The final size of the crystals depends on the number of nucleation points. More nucleation points mean smaller crystal and vice versa. The crystals are referred to as grains and the location where grains meet is called the grain boundary.

Crystal grains can be classified as **equiaxed grains** or **columnar grains**. Equiaxed grains grow equally in all direction but columnar grains are long, this, coarse grains.

METALLIC SOLID SOLUTION
A solid solution is a solid that consists of two or more elements atomically dispersed. They can be classified as substitutional solid solution or interstitial solid solution.

Substitution solid solution is where the solvent and solute atoms are located randomly at atom sites i.e. the solute replaces the solvent atoms. The solvent and solute have comparable atomic size.

Interstitial solid solution is where solute atoms have very small atomic size compared to the solvent atoms. Hence the solute atoms locate at interstitial sites between the solvent atoms.

Defects can be classified as **point defects linear defects, interfacial defects (or boundary).**

POINT DEFECTS
Point defects can be classified as self-interstitial or vacancy.

Vacancy

Vacancy is the absenteeism of an atom at an atoms site. All solids contain vacancies, it is impossible to create solid materials without.

Self-interstitial

We have self-interstitial when an atom in crowded into interstitial sites or small voids that is not normally occupied. This kind of defect produces distortions in the lattice. Their occurrence is much lower than vacancy defect.

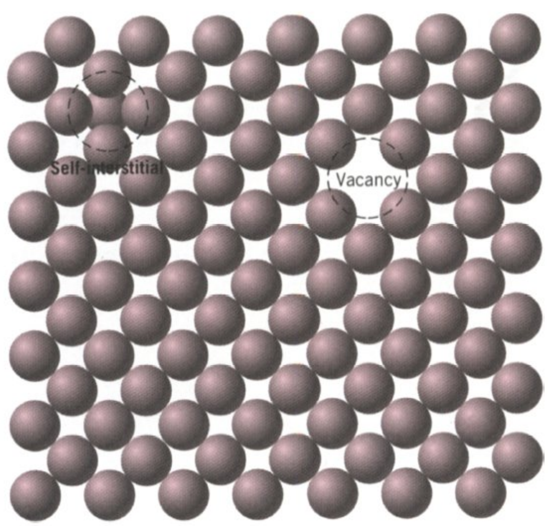
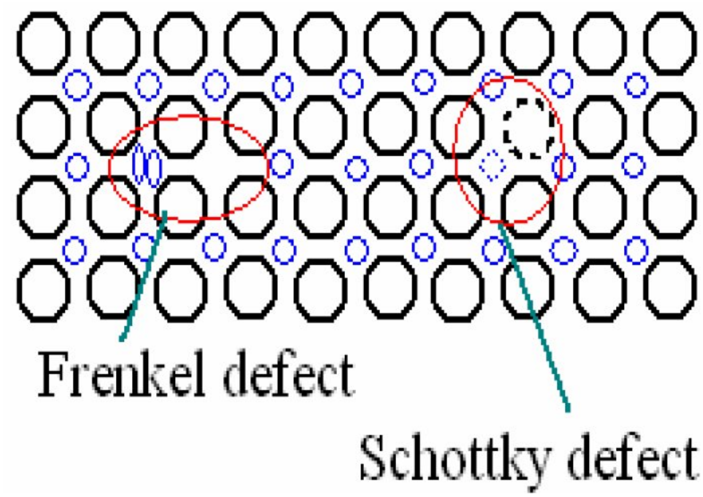


FIGURE 5.1 Two-dimensional representations of a vacancy and a self-interstitial. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 77. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

<u>There are two possibilities for point defects in ionic solids</u>

When an ion displaced from a regular position to an interstitial position creating a vacancy, the pair of vacancy-interstitial is called *Frenkel defect*. Cations are usually smaller and thus displace more easily than anions. Closed packed structures have fewer interstitials and displaced ions than vacancies because additional energy is required to force the atoms into the interstitial positions.

A pair of one cation and one anion can be missing from an ionic crystal, without violating the condition of charge neutrality. The pair of vacant sites, thus formed, is called *Schottky defect*.



DISLOCATIONS – LINEAR DEFECTS

Linear defects are one dimensional where some of the atoms are misaligned. There are two types of dislocations, edge and screw dislocation. Then there is a combination of the two. **Edge dislocation** is when an extra plane of atoms exist within the lattice but terminates within the crystal, it exist above the ⊥. The dislocation line is at the end of the extra half plane. The atoms above the dislocation line are squeezed together and those below are pulled apart. This type of defect is formed by tensional stress.

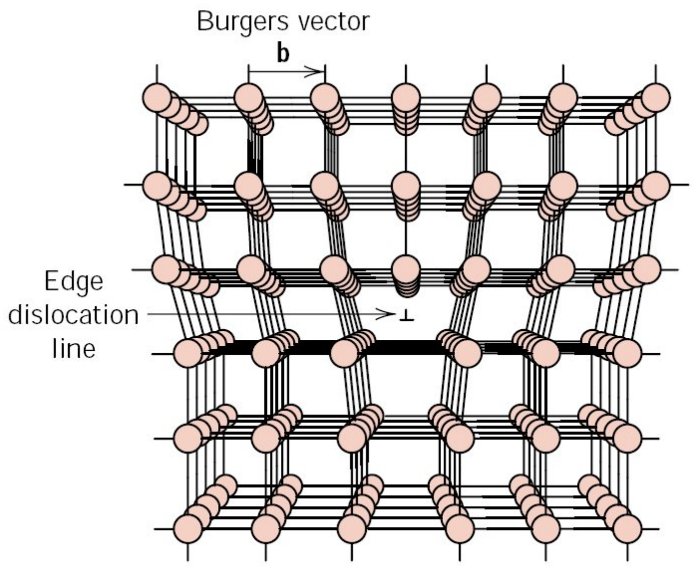
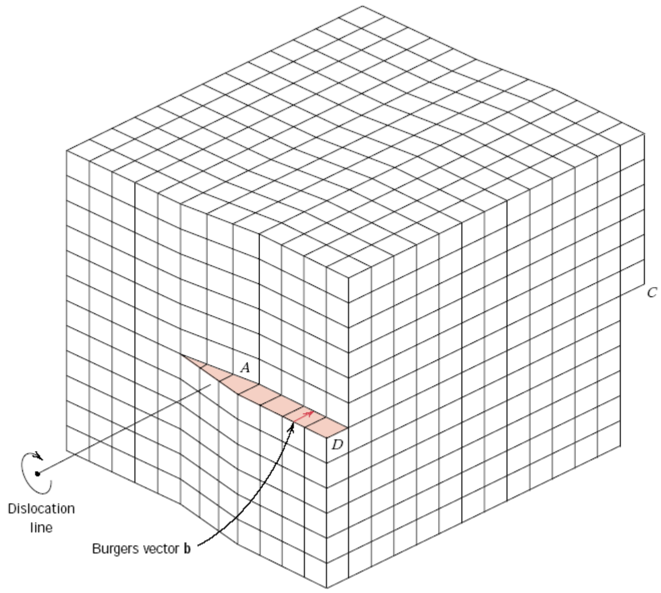


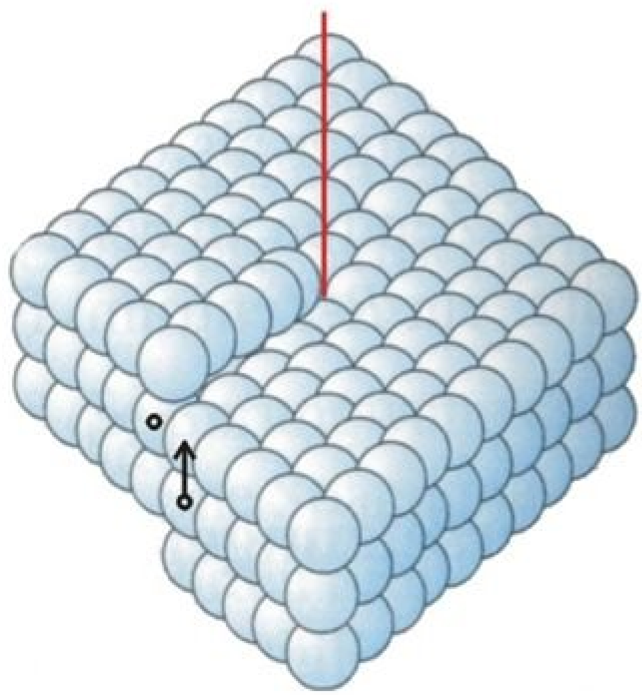
FIGURE 5.7 The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective. (Adapted from A. G. Guy, *Essentials of Materials Science,* McGraw-Hill Book Company, New York, 1976, p. 153.)

Screw dislocation

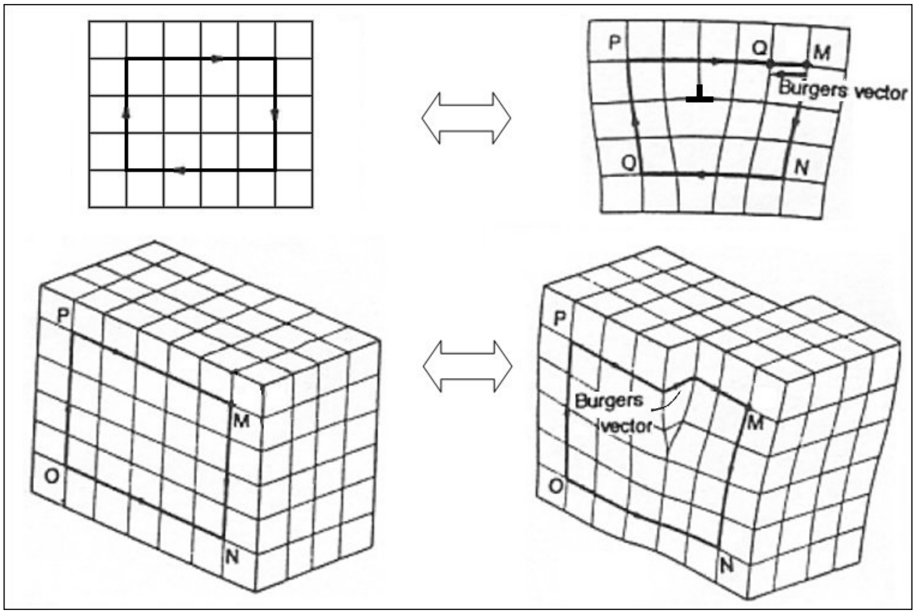
Screw dislocation can be formed in a perfect crystal by applying shear stress. The upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion forming a spiral ramp of atoms.



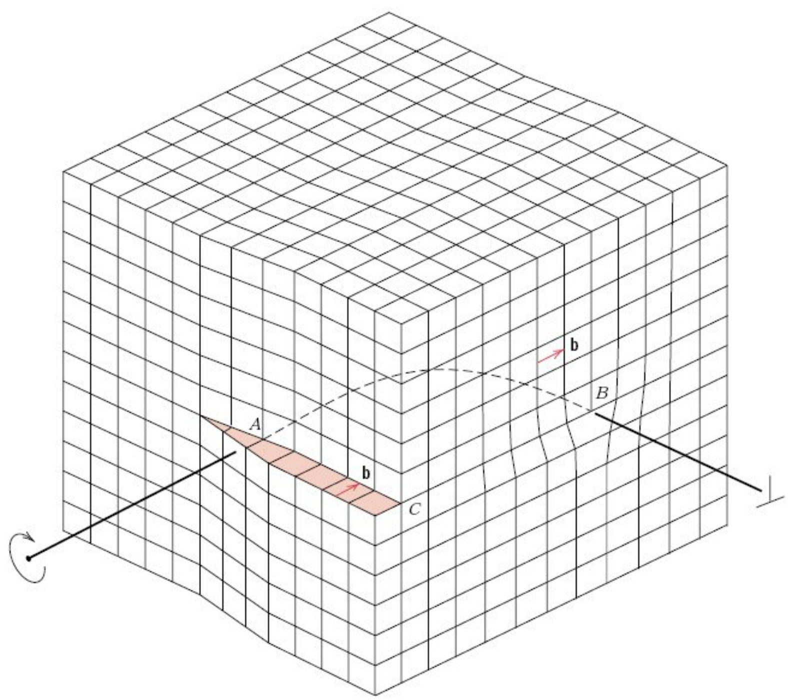
(a)



The **Burgers vector**, often denoted by **b**, is a vector that represents the magnitude and direction of the lattice distortion of dislocation in a crystal lattice.



A combination of the two gives mixed dislocations, which have edge and screw components.

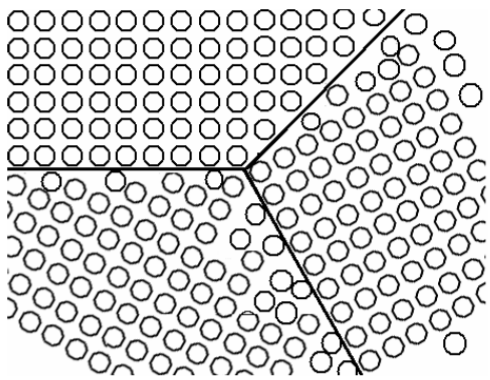


(a)

PLANAR DEFECTS

This defect includes external surfaces, grain boundaries, twins, low angles boundaries, high-angle boundaries, twists and stacking faults. The **external surface** of any material is most common type of planar defect. The atoms on the surface are bonded to other atoms only on one side. Therefore the surface atoms have lower number of neighbours hence they have higher energy level. This makes it susceptible to erosion and corrosion.

Grain boundaries are surface imperfections that separate grains of different orientations. The grain boundary itself is a narrow region between two grains of about two to five atomic diameters in width and is a region of lower atomic packing because of atomic mismatch. Some atoms may also be in strained positions that raise the energy level at the boundary. The higher energy level makes it susceptible to nucleation and growth of precipitates. The lower atomic packing of the grain boundaries allows for more rapid diffusion of atoms in the grain boundary region.



A **twin** is defined as a region in which a mirror image for the structure exists across a plane or a boundary. This occurs when permanent deformation has taken place or during recrystallization (repositioning). Twin boundaries tend to strengthen a material.

BULK OR VOLUME DEFECTS

Volume defects are three-dimensional in nature. These defects are introduced, usually, during processing and fabrication operations like casting, forming etc. E.g.: Pores, Cracks, Foreign particle. These defects act like stress raisers, thus affecting the mechanical properties of the parent solids. In some instances, foreign particles are added to strengthen the solid. Particles added act as hindrances to movement of dislocations thus increasing the strength.

EXPERIMENTAL TECHNIQUES FOR IDENTIFICATION OF MICROSTRUCTURE AND DEFECTS

Various instruments exist to study and understand the behaviour of materials based on their microstructure, existing defects, microconstituents and other features and characteristics.

<u>Optical Metallography</u>

Magnification level of up to 2000X.

Gives qualitative and quantitative information pertaining to grain size, grain boundary, existence of various phases and internal damage.

Metal preparation include:

Surface grinding stages that removes large scratches and thin plastically deformed layers.

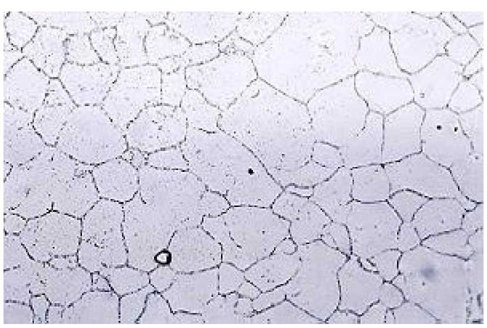
Polishing stage removes small scratches incurred during grinding to give smooth mirror like finish.

Chemical etching involves is where the atoms at the grain boundaries are attacked more rapidly than the rest of the material due lower atomic packing. Hence tiny groves are produced at the grain boundaries.

Under a metallurgical microscope where the sample is exposed to light, the groves do not reflect light as intensely as the remainder of the grain material. Therefore they appear as dark lines.

Impurities, other existing phases and internal defects can be detected this way too.

From this we can ascertain the grain size.



Scanning Electron Microscopy (SEM)

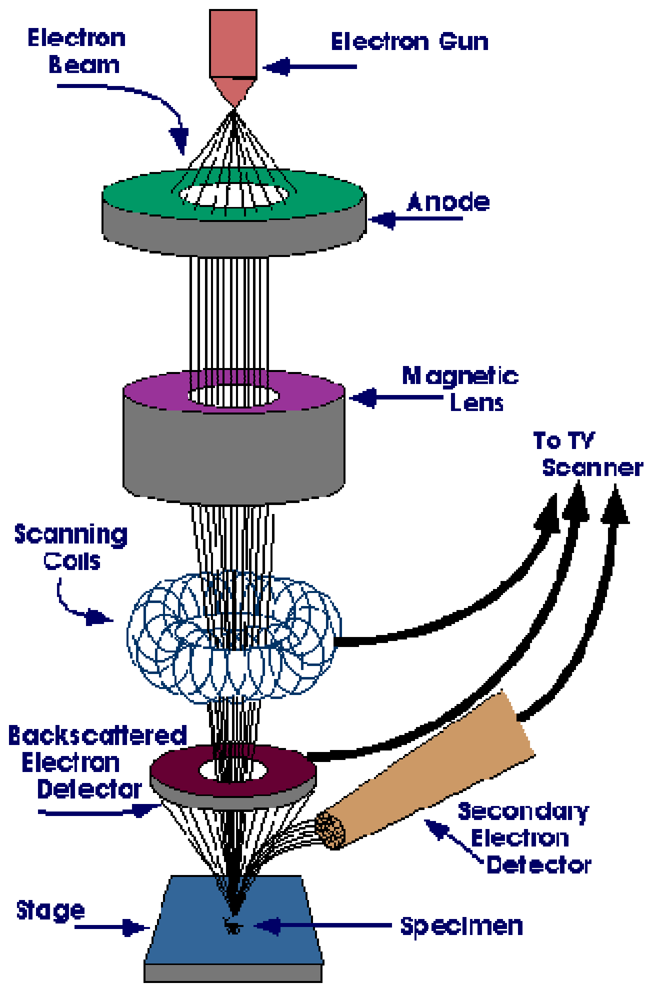
Used microscopic feature measurement, fracture characterization, microstructure studies, thin coating evaluations, surface contamination examination and most useful for failure analysis.

The SEM is a microscope that uses electrons rather than light to form an image.

A beam of electrons is produced at the top of the microscope by heating a metallic filament.

The electron beam follows a vertical path through the column of the microscope. It makes its way through electromagnetic lenses which focus and direct the beam down towards the sample.

The electrons from the sample and detectors collect the secondary or backscattered electrons, and convert them to a signal that is sent to a viewing screen that similar to the one in an ordinary television, producing an image.

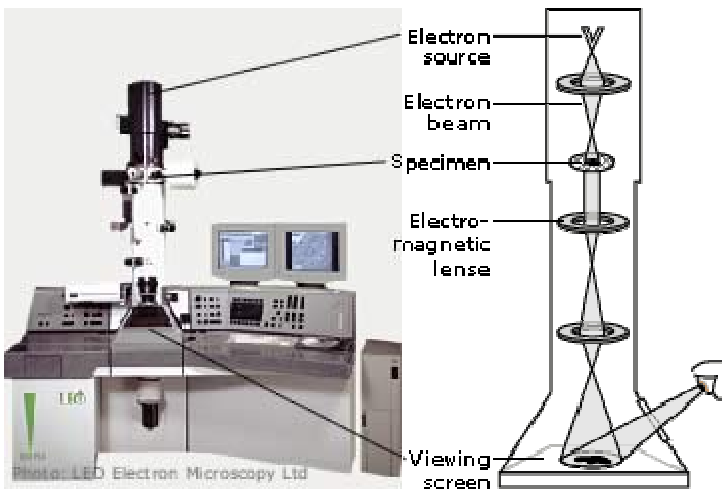


Transmission Electron Microscopy (TEM)

Used to study defects and precipitates in materials.

Sample preparation is very complex and requires specialized instruments. The sample is must be very thin only several hundred nanometres or less.

The concept is similar to the SEM but in this case the electron beam passes through the sample specimen. Depending on the density of the material present, some of the electrons are scattered and disappear from the beam. At the bottom of the microscope the unscattered electrons hit a fluorescent screen, which gives rise to a "shadow image" of the specimen with its different parts displayed in varied darkness according to their density. The image can be studied directly by the operator or photographed with a camera.



Scanning Probe Microscopes

This is a recently developed tool that allows the user to analyse materials at the atomic level.

Modern microscopes, such as the Scanning Tunnelling Microscope (STM), can image the surfaces of materials with unparalleled magnification. The magnification is so extreme, that individual atoms become visible. The STM consist of an extremely sharp tip (diameter in the range of a single atom) probes the surface of sample while scanning the surface.