Grain boundary, crystalline defects (including dislocation) provide the source and sink for vacancies.

See the additional reading for more about these basic concepts and application in real-world materials science and engineering.

#### 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 usually the result of uneven growth when the solid is crystallising. Grain sizes vary from 1  $\mu$ m to 1 mm.



45.98° tilt grain boundary in SiC. A projection along the <110> direction is shown



#### **Grain Boundary HRTEM**



Using high-resolution transmission electron microscopy (HRTEM), researchers obtained structure images of strontium titanate (SrTiO<sub>3</sub>) with a clearly resolved oxygen sublattice along different crystallographic directions in the bulk lattice and for a  $\Sigma$ 3 tilt grain boundary (GB). In this HRTEM image of a  $\Sigma$ 3(111)[1-10] GB of SrTiO<sub>3</sub> along the [1-10] direction the strontium, titanium, and oxygen are atomically resolved in both the bulk and the GB.

**Crystalline Defects** The ideal crystal has an infinite 3D repetition of identical units, which may be atoms or molecules.

Real crystals are limited in size, and they have some disorder in stacking which are called *defects*.

## **Point Defects**

A Point Defect involves a single atom change to the normal crystal array.

There are three major types of point defect: Vacancies, Interstitials and Impurities.

They may be built-in with the original crystal growth, or activated by heat.

They may be the result of radiation, or electric current etc, etc.



An empty lattice site is a vacancy

#### Vacancies

A Vacancy is the absence of an atom from a site normally occupied in the lattice.



An interstitial is an off-lattice atom which may be a foreign atom or a regular atom



An interstitial may form by an atom moving to an off-lattice site and create a vacancy at the same time

**Interstitials** An Interstitial is an atom on a non-lattice site.

There needs to be enough room for it, so this type of defect occurs in open covalent structures, or metallic structures with large atoms.

### Line Defects: Dislocation

A Dislocation is a line discontinuity in the regular crystal structure. There are two basic types: Edge dislocations, and Screw dislocations. An Edge dislocation in a Metal may be regarded as the insertion (or removal) of an extra half plane of atoms in the crystal structure.



In Ionic and Covalent solids edge dislocations involve extra half planes of *unit cells*.



The regions surrounding the dislocation line are made of essentially perfect crystal.

The only severe disruption to the crystal structure occurs along the dislocation line (perpendicular to the page).

Note that perpendicular to the page, the line may step up or down. These steps are known as *jogs*.

# **Dislocation Intersections:** when dislocations intersect, jogs and kinks are formed.

Kink : a step in the dislocation line in the slip plane Jog : a step in the dislocation line on another slip plane



# Movement and Generation of Dislocations: Kinks and Jogs

https://www.tf.uni-kiel.de/matwis/amat/def\_en/kap\_5/backbone/r5\_3\_1.html



Fig. 2. Distinctive difference in the growth rates of trunk and branch nanowires and the proposed dislocation-driven nanowire growth in the trunk of tree structures



M. J. Bierman et al., Science 320, 1060 -1063 (2008)





#### Fig. 1. SEM micrographs of PbS pine tree nanowires

M. J. Bierman et al., Science 320, 1060 -1063 (2008)



