THE UNIVERSITY OF ZAMBIA
SCHOOL OF ENGINEERING
DEPARTMENT OF MECHANICAL ENGINEERING

MEC 2309 – PROPERTIES OF ENGINEERING MATERIALS I

GMM/FKC 2022

LECTURE 5

CRYSTAL DEFECTS IN MATERIALS

G. M. MUNAKAAMPE / F. K. CHITALU (2022)

INTRODUCTION

- The properties of many materials are influenced by the presence of imperfections. It is therefore important to have a knowledge about the types of imperfections that exist and the roles they play in affecting the behavior of materials.

INTRODUCTION

- In this lecture we will discuss different types of imperfections or defects in the ideal arrangement of atoms in a crystal.
- We will see that the presence of a relatively small number of defects have a profound impact on the macroscopic properties of materials, and the control (and intentional introduction) of defects is important in many kinds of material processing.

CRYSTAL DEFECTS

- The crystal lattices we have described represent an idealized, simplified system that can be used to understand many of the important principles governing the behavior of solids.
- In contrast, real crystals contain large numbers of defects (typically more than 104 per milligram), ranging from variable amounts of impurities to missing or misplaced atoms or ions.

CRYSTAL DEFECTS

Crystal defects occur for three main reasons:

- It is impossible to obtain any substance in 100% pure form. Some impurities are always present.
- Even if a substance were 100% pure, forming a perfect crystal would require cooling the liquid phase infinitely slowly to allow all atoms, ions, or molecules to find their proper positions. Cooling at more realistic rates usually results in one or more components being trapped in the “wrong” place in a lattice or in areas where two lattices that grew separately intersect.
- Applying an external stress to a crystal, such as a hammer blow, can cause microscopic regions of the lattice to move with respect to the rest, thus resulting in imperfect alignment.

CRYSTAL DEFECTS

- Real crystals are never perfect, there are always defects., I.E. The atoms are not perfectly arranged according to their crystal structures.
- Defects affect the properties of materials.
- Crystalline defect refers to a lattice irregularity having one or more of its dimensions on the order of an atomic diameter. Classification of crystalline imperfections is frequently made according to geometry or dimensionality of the defect

CRYSTAL DEFECTS

Several different imperfections are will be discussed and can classified in the following categories: Crystal defects can be classified into the following categories:

- **Point defects** (vacancy, interstitial, etc.) - those associated with one or two atomic positions.
- **Line or linear defects** (dislocations) - one-dimensional defects
- **Surface defects** (grain boundaries) - interfacial defects, which are two-dimensional
- **Volume defects** (voids, impurity cluster, etc) which are three dimensional.

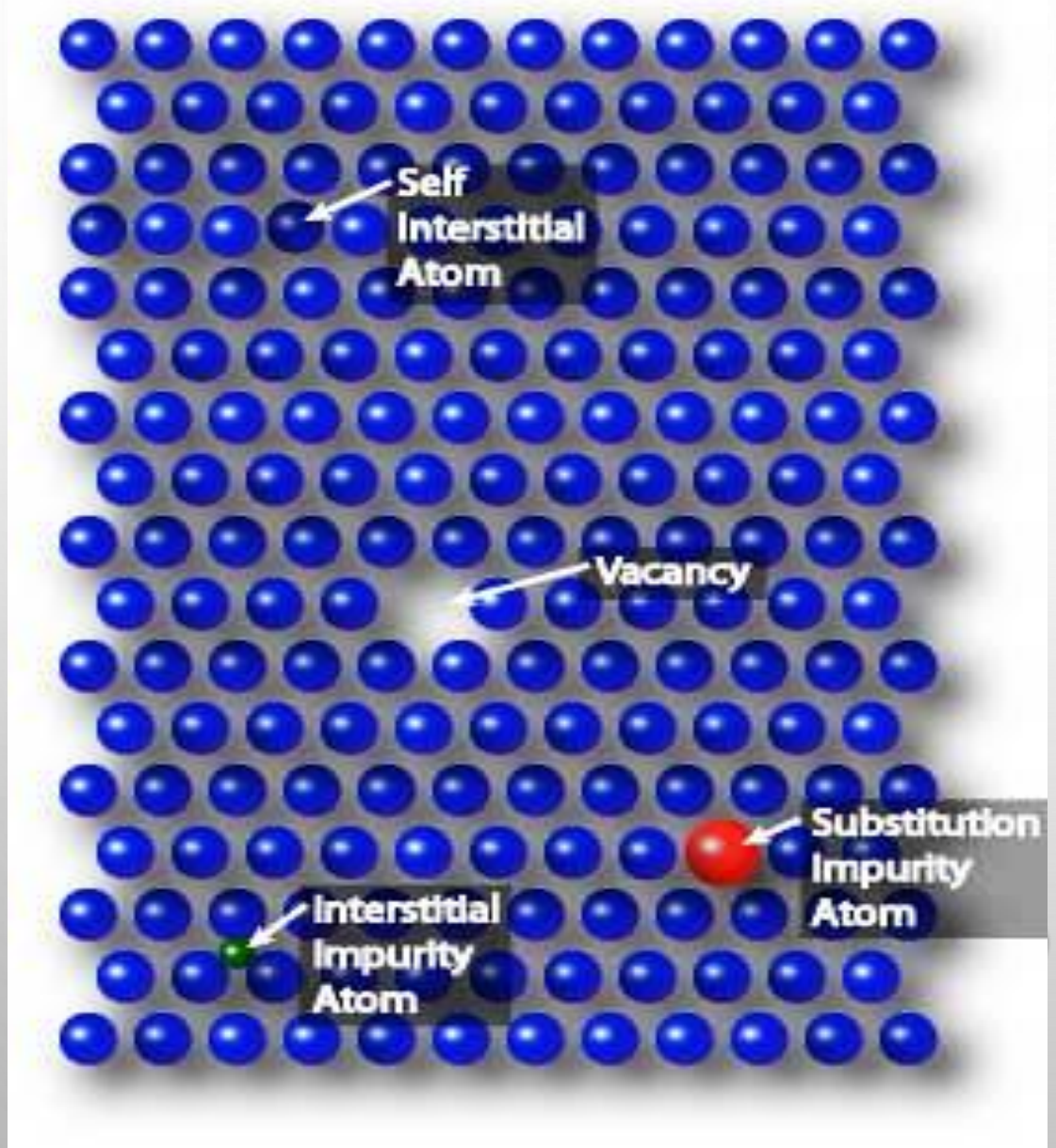
POINT DEFECTS

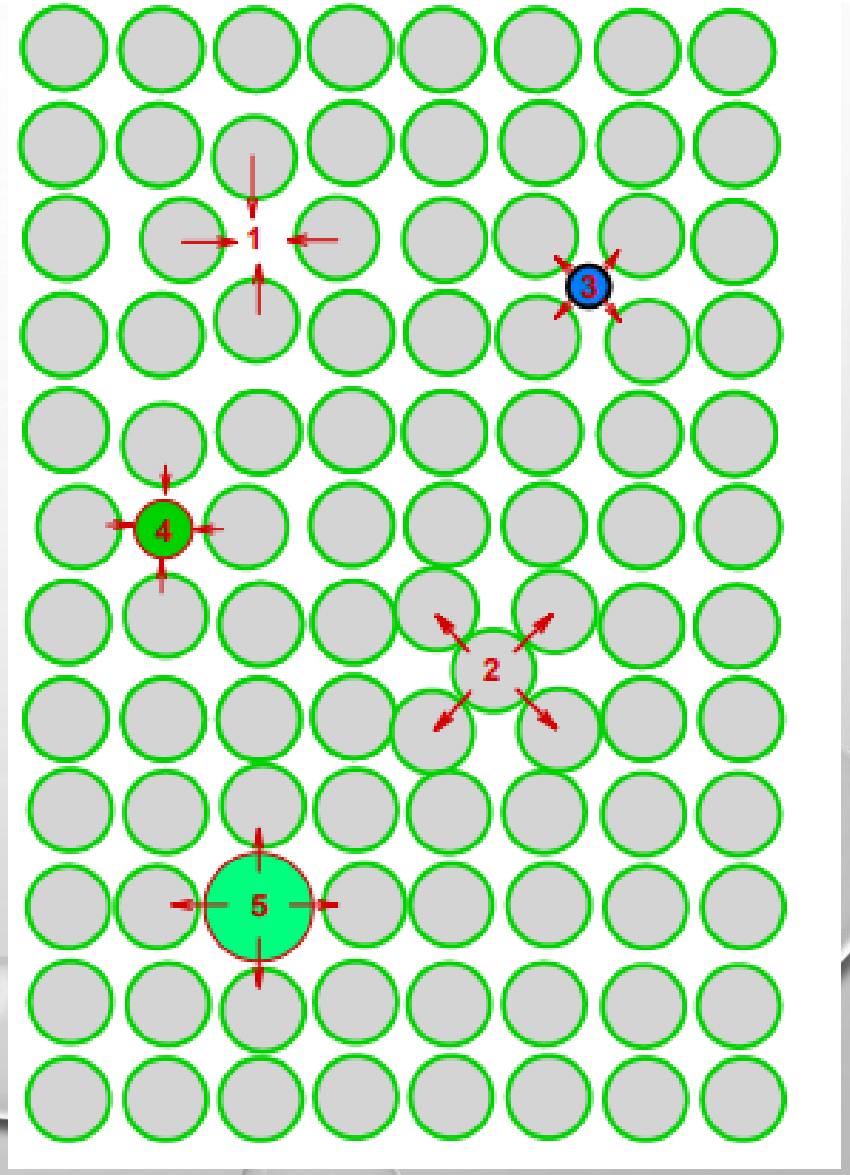
- Point defects are where an atom is **missing** or is in an **irregular place** in the lattice structure.
- Point defects include:
  - **Self-interstitial atoms** (an extra atom that has crowded its way into an interstitial void),
  - **Interstitial impurity atoms** (occur only in low concentrations in metals because they distort and highly stress the tightly packed lattice structure),.
  - Interstitial impurity atoms are much smaller than the atoms in the bulk matrix. Interstitial impurity atoms fit into the open space between the bulk atoms of the lattice structure.

POINT DEFECTS

- An example of interstitial impurity atoms is the carbon atoms that are added to iron to make steel. Carbon atoms, with a radius of 0.071 nm, fit nicely in the open spaces between the larger (0.124 nm) iron atoms.
- **Substitutional impurity atoms** (atom of a different type than the bulk atoms, which has replaced one of the bulk atoms in the lattice).
- Usually close in size (within approximately 15%) to the bulk atom.
- An example of substitutional impurity atoms is the zinc atoms in **brass**. In brass, zinc atoms with a radius of 0.133 nm have replaced some of the copper atoms, which have a radius of 0.128 nm.
- **Vacancies or voids** (empty spaces where an atom should be but is missing). All crystalline solids contain vacancies and, in fact, it is not possible to create such a material that is free of these defects.

POINT DEFECTS





LINE OR LINEAR DEFECTS - DISLOCATIONS

- The smelting and forging of metals marks the beginning of civilization. Trial and error over this period of time lead to an astonishing degree of perfection, as can be seen all around us and in many museums.
- But why metals could be plastically deformed and why the plastic deformation properties could be changed to a very large degree by forging without changing the chemical composition, was a mystery for thousands of years.
- This became even bigger mystery when in the early 1900's scientists estimated that metals undergo plastic deformation at forces much smaller than the theoretical strength of the forces that are holding the metal atoms together.

LINE OR LINEAR DEFECTS - DISLOCATIONS

- A dislocation is a linear or one-dimensional defect around which some of the atoms are misaligned.
- The permanent deformation of most crystalline materials is by the motion of dislocations.
- Virtually all crystalline materials contain some dislocations that were introduced during solidification, during plastic deformation, and as a consequence of thermal stresses that result from rapid cooling. Dislocations are involved in the plas tic deformation of crystalline materials, both metals and ceramic

LINE OR LINEAR DEFECTS - DISLOCATIONS

- Dislocations are generated and move when a stress is applied.
- Dislocations are line-defects: the interatomic bonds are significantly distorted only in the immediate vicinity of the dislocation line.

LINE OR LINEAR DEFECTS - DISLOCATIONS

- Motion of dislocations allows slip – plastic deformation to occur. Properties of a metal could be greatly changed by solely by forming (without changing the chemical composition).
- strength and ductility of metals are controlled by dislocations.

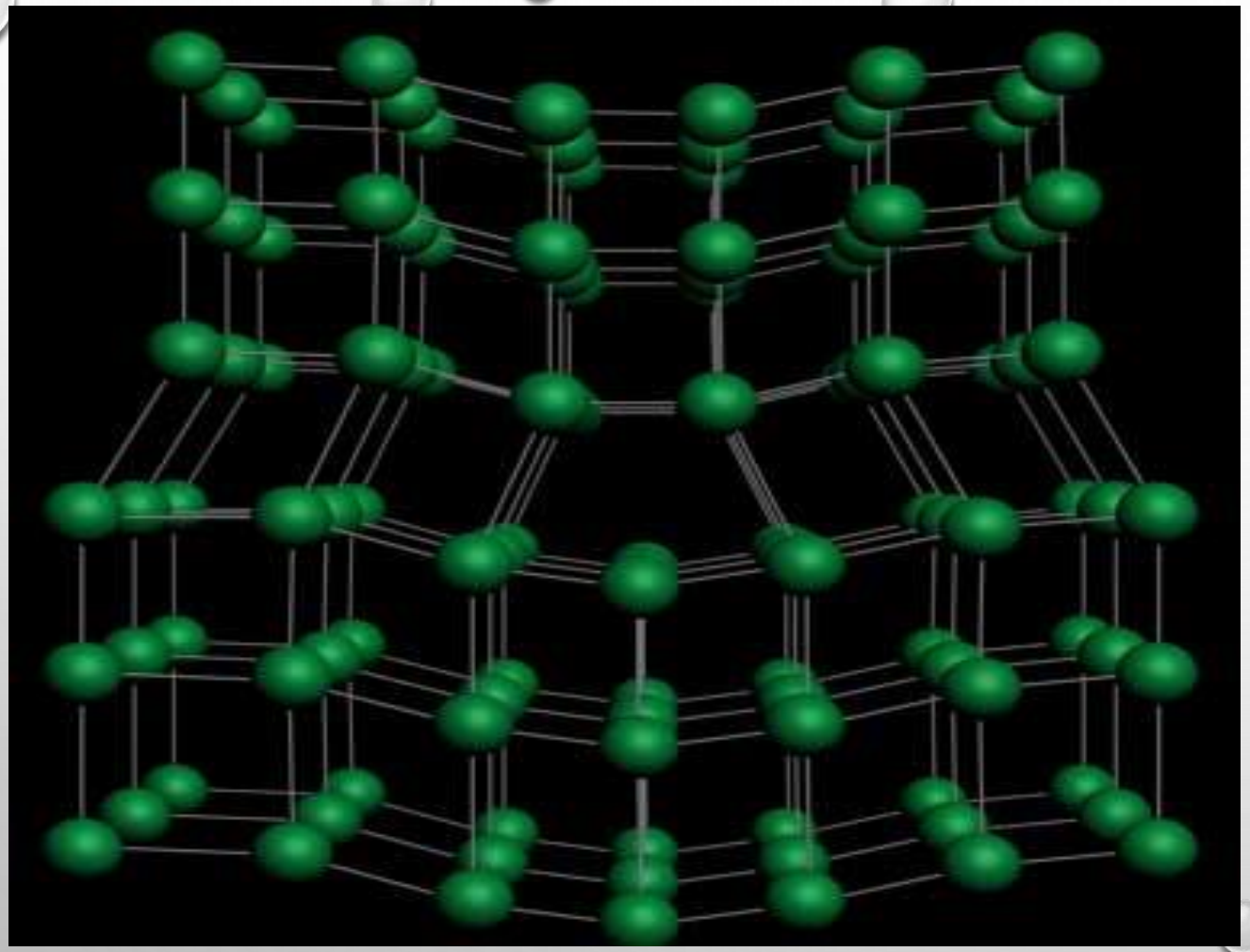
Two basic types of dislocations: **Edge dislocation** and **Screw dislocation**.

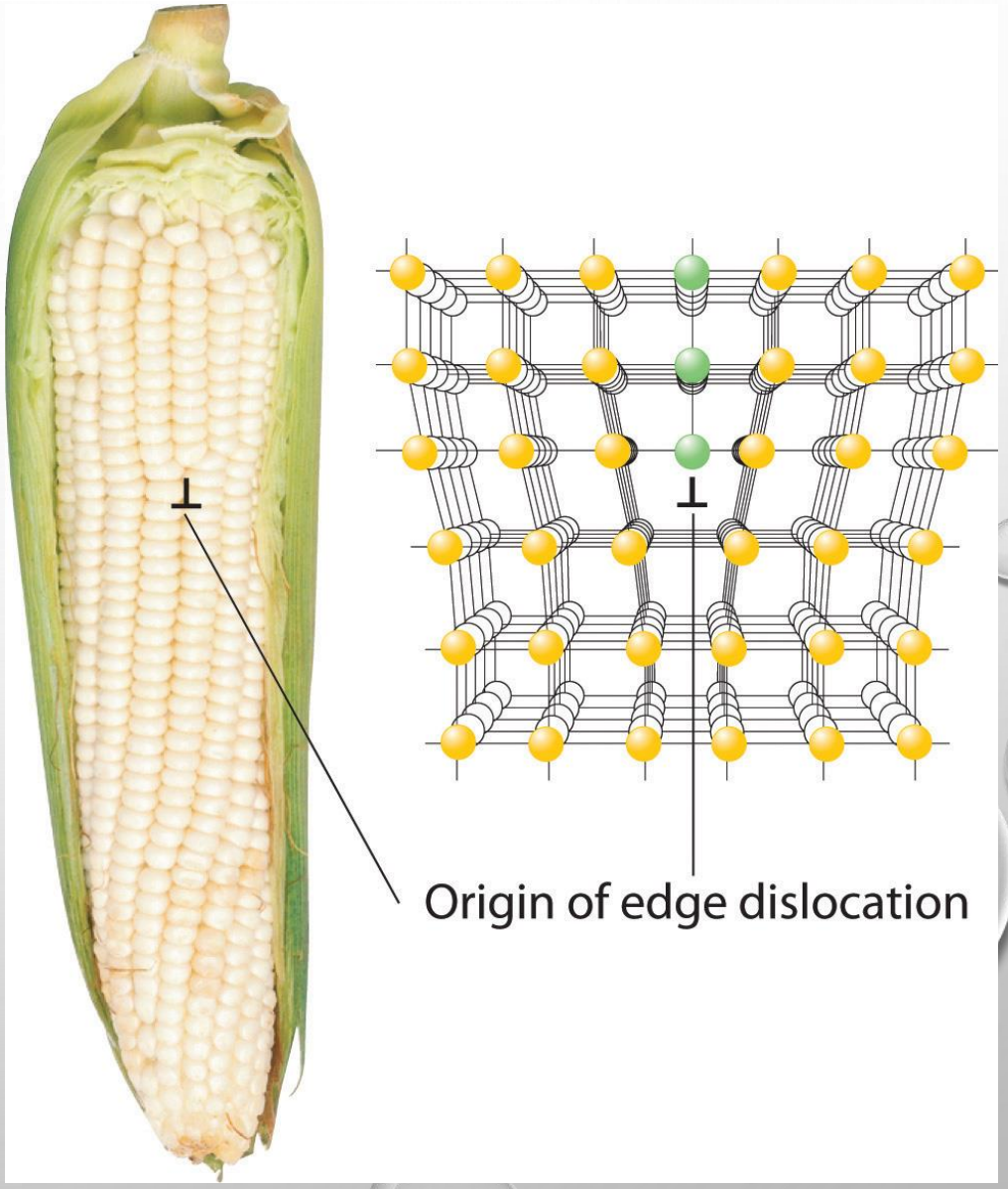
- Many dislocations are a hybrid of the edge and screw forms.

EDGE DISLOCATIONS

- Easily visualised as an extra half-plane of atoms in a lattice.
- Called a line defect because the locus of defective points produced in the lattice by the dislocation lie along a line.
- This line runs along the bottom of the extra half-plane.
- The inter-atomic bonds are significantly distorted only in the immediate vicinity of the dislocation line.

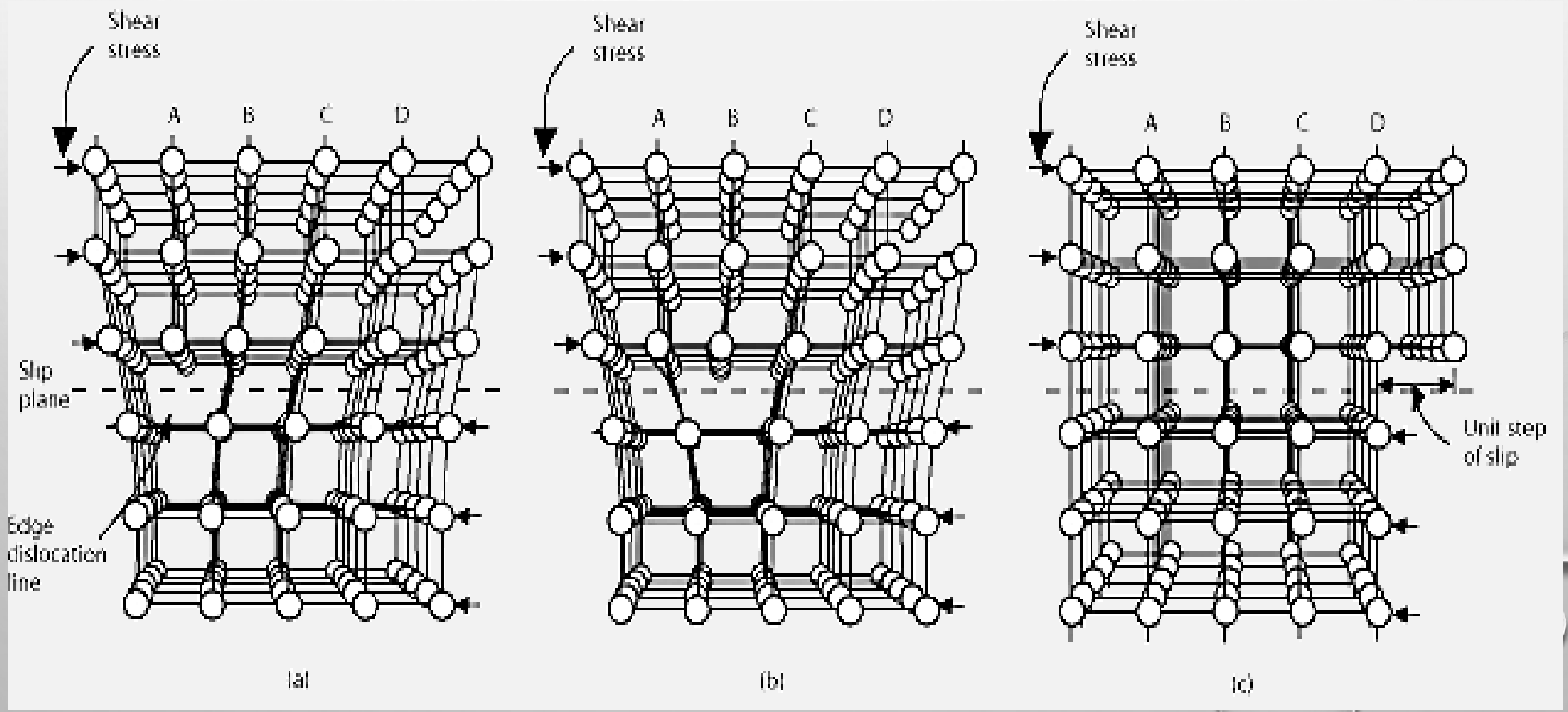
EDGE DISLOCATIONS





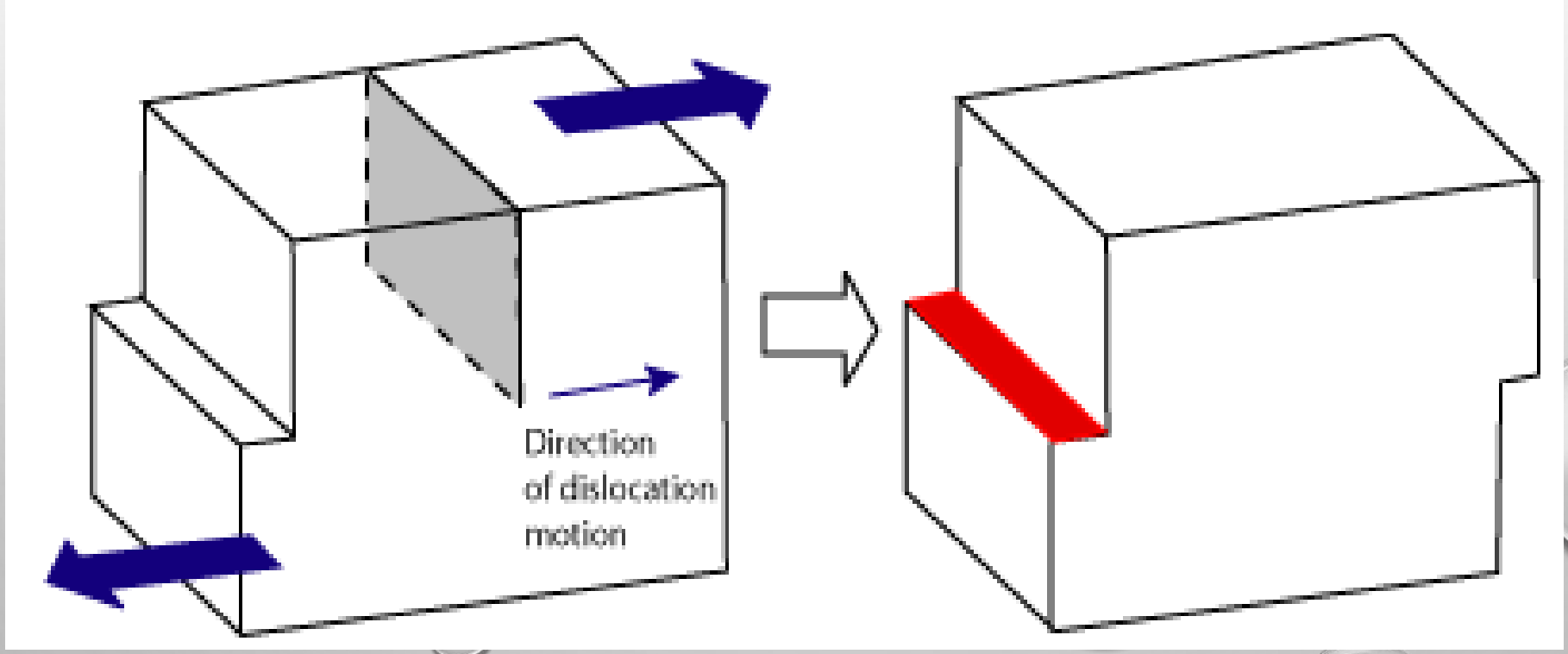
EDGE DISLOCATIONS

- The dislocation moves similarly moves a small amount at a time. The dislocation in the top half of the crystal is slipping one plane at a time as it moves to the right .
- In the process of slipping one plane at a time the dislocation propagates across the crystal. The movement of the dislocation across the plane eventually causes the top half of the crystal to move with respect to the bottom half.
- However, only a small fraction of the bonds are broken at any given time. Movement in this manner requires a much smaller force than breaking all the bonds across the middle plane simultaneously.



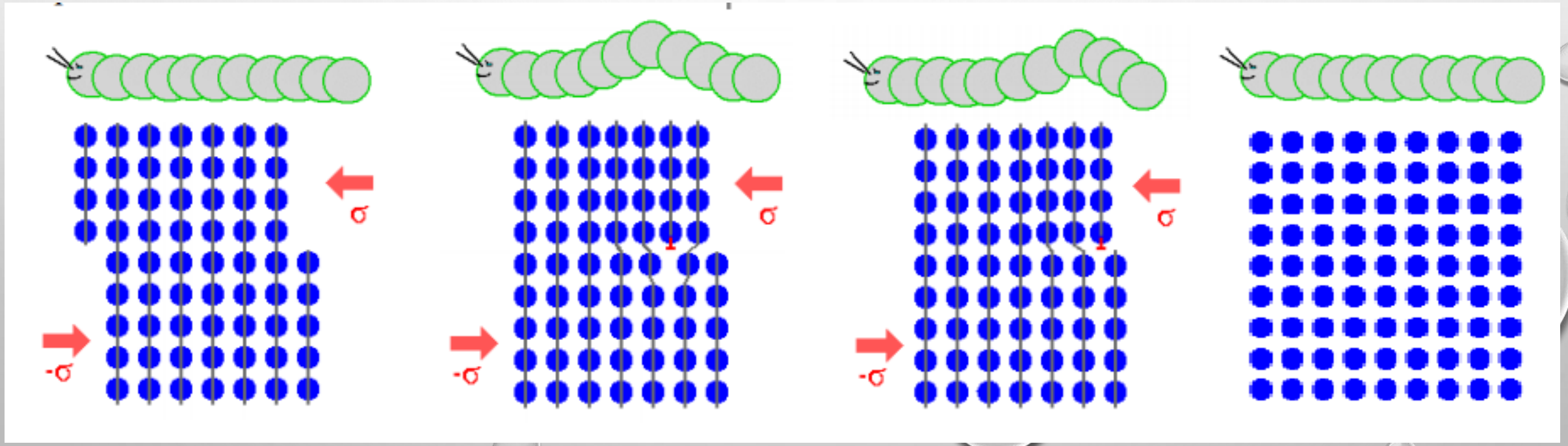
EDGE DISLOCATIONS

- Understanding the movement of a dislocation is key to understanding why dislocations allow deformation to occur at much lower stress than in a perfect crystal



EDGE DISLOCATIONS

- Dislocation motion is analogous to movement of a caterpillar. The caterpillar would have to exert a large force to move its entire body at once. Instead it moves the rear portion of its body forward a small amount and creates a hump. The hump then moves forward and eventual moves all of the body forward by a small amount.

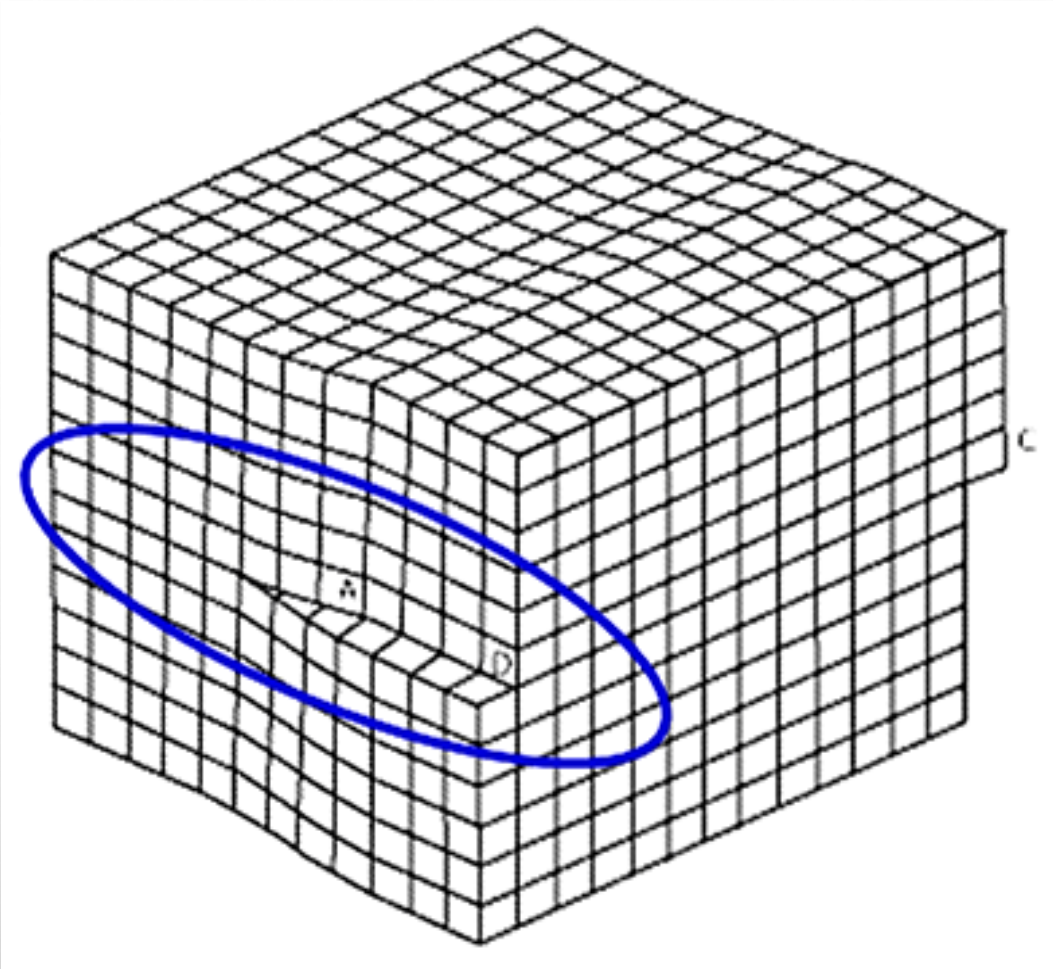


SCREW DISLOCATIONS

- Slightly more difficult to visualize.
- 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.
- Recall that the edge dislocation moves parallel to the direction of stress. As shown in the image below, the net plastic deformation of both edge and screw dislocations is the same, however.

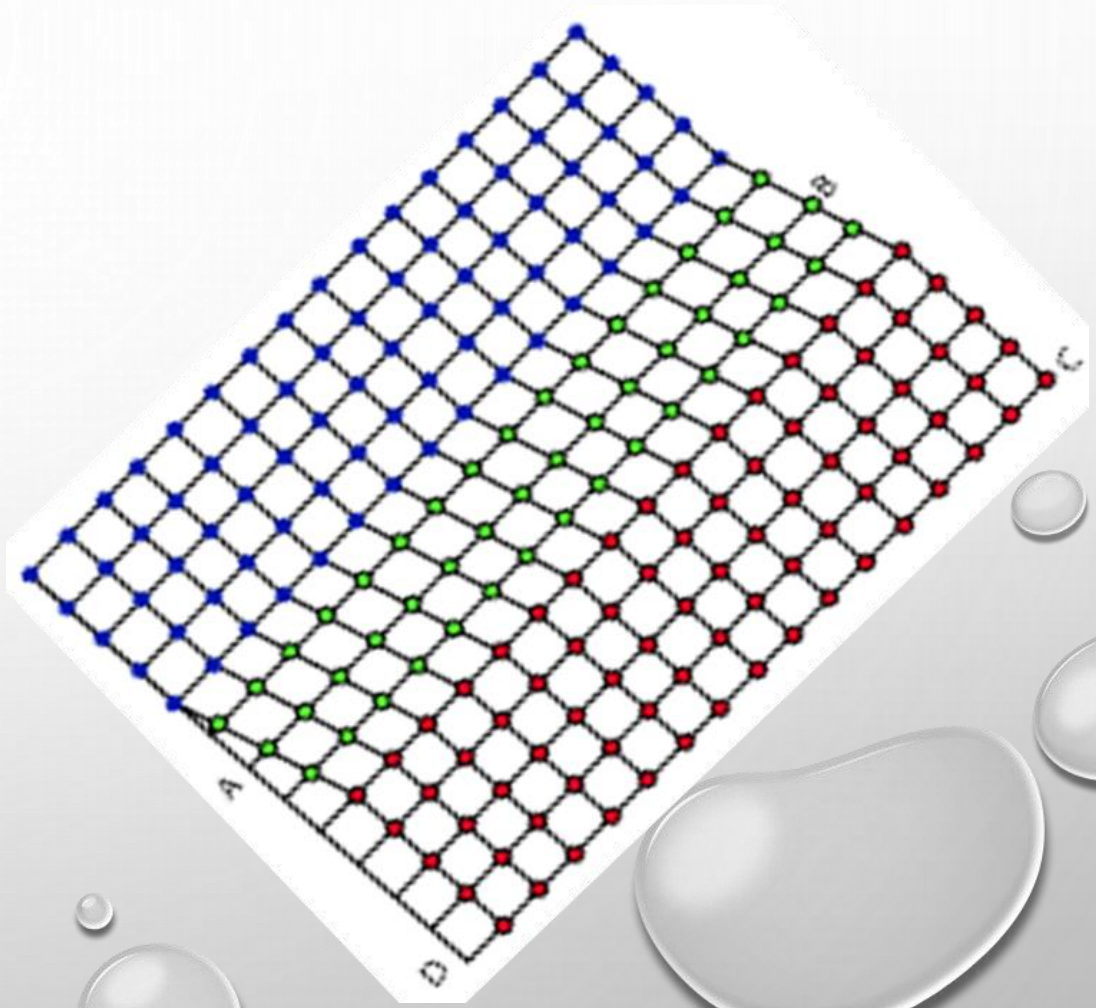
SCREW DISLOCATIONS

- To visualize a screw dislocation, imagine a block of metal with a shear stress applied across one end so that the metal begins to rip, shown in the upper image.



SCREW DISLOCATIONS

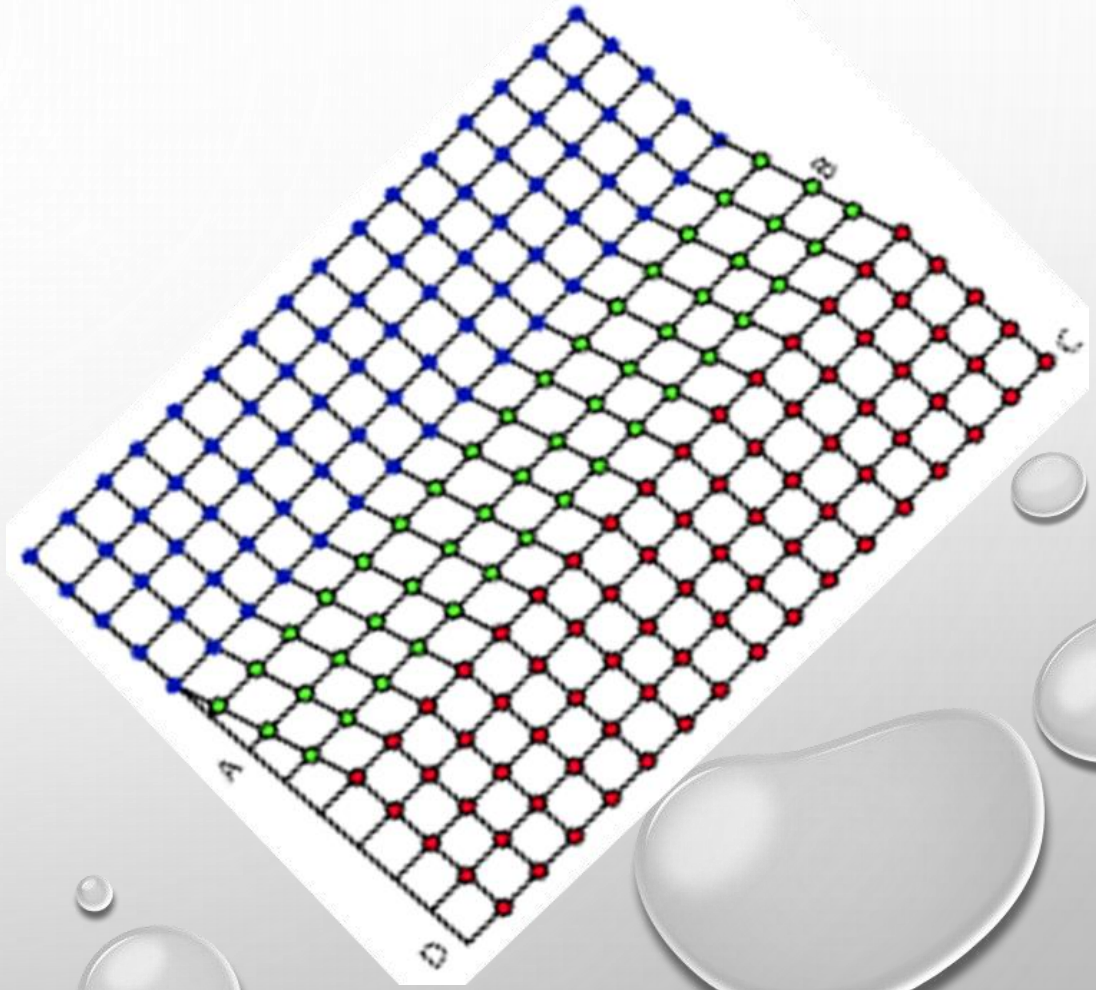
- This image shows the plane of atoms just above the rip.
- Blue atoms have not yet moved from original positions. Red atoms have moved to new positions and have re-established metallic bonds.
- Green atoms are in the process of moving.



SCREW DISLOCATIONS

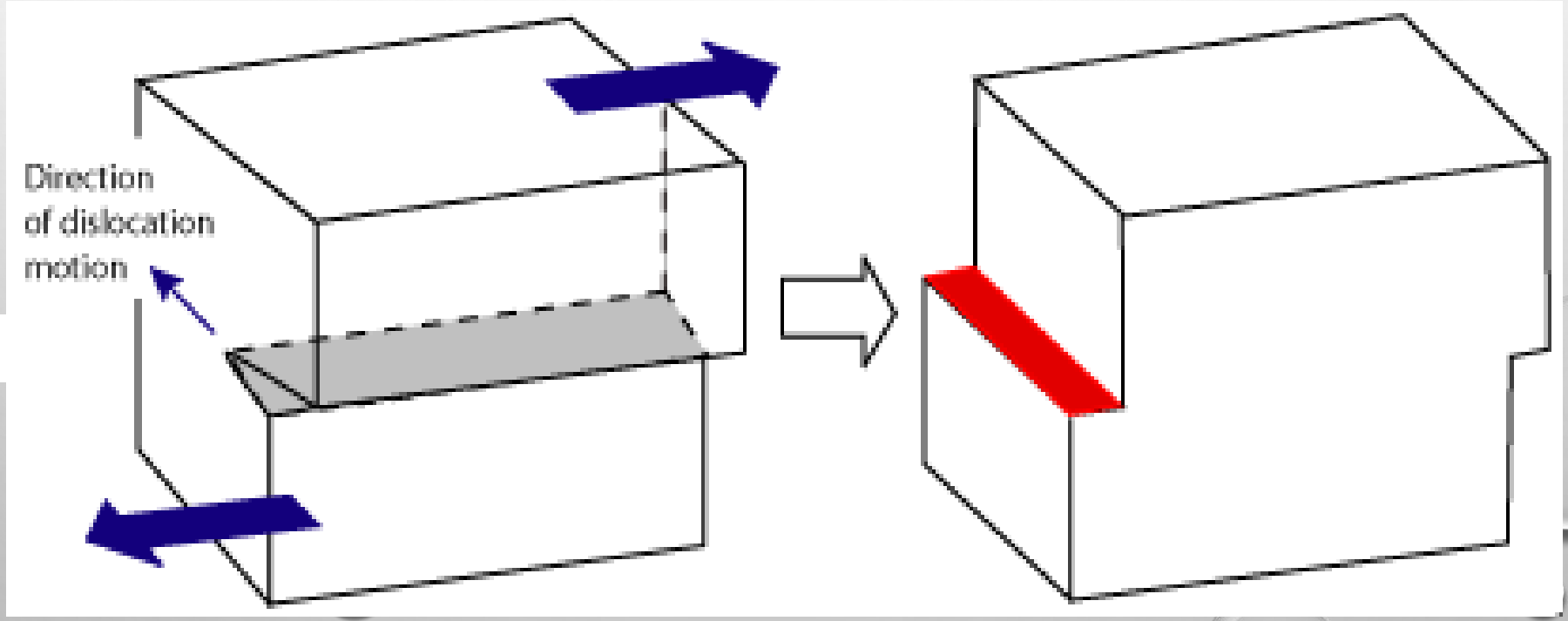
- If the shear force is increased, the atoms will continue to slip to the right. Into the red positions

- Only a portion of the bonds are broken at a time.



SCREW DISLOCATIONS

- Movement in this manner requires much smaller force than breaking all the bonds across the middle plane simultaneously.
- If the shear force is increased, the atoms will continue to slip to the right until the entire plane slips.



LINE AND LINEAR DISLOCATIONS

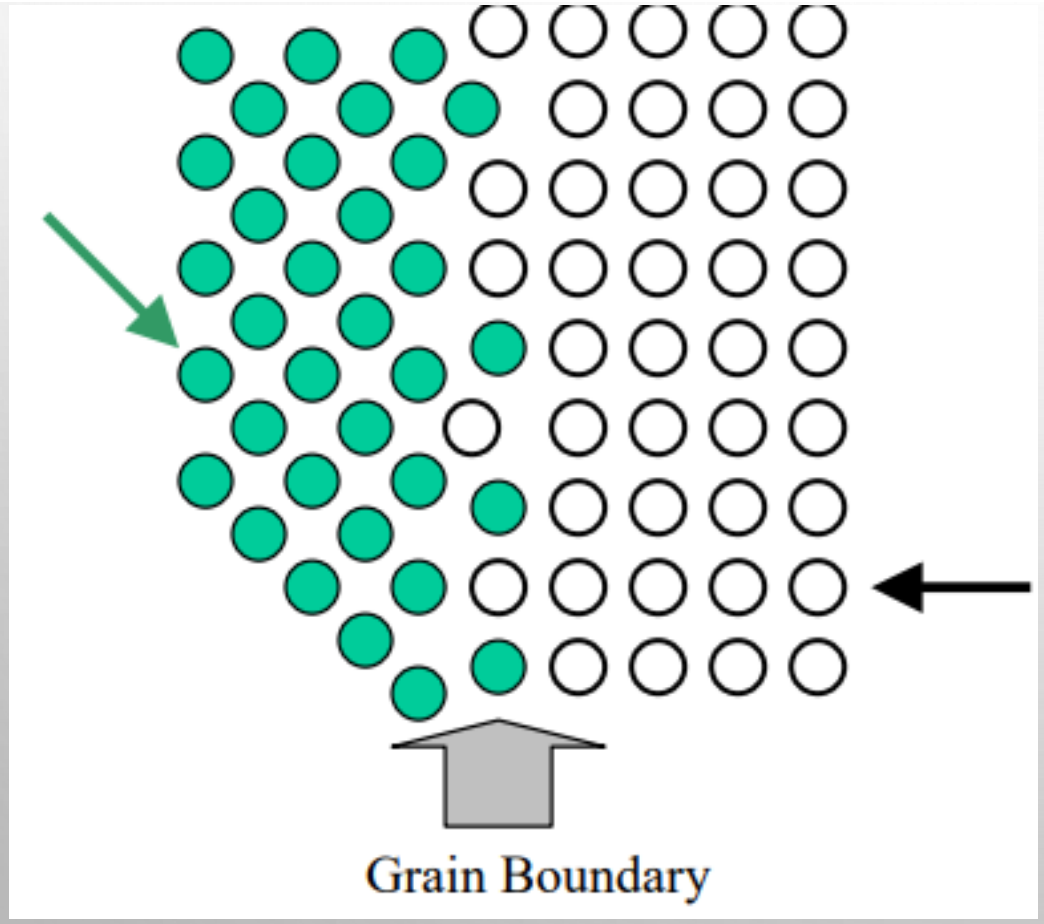
Transmission electron micrograph of a **titanium alloy** in which the dark lines are dislocations. 51,450 × (Courtesy of M. R. Plichta, Michigan Technological University.)

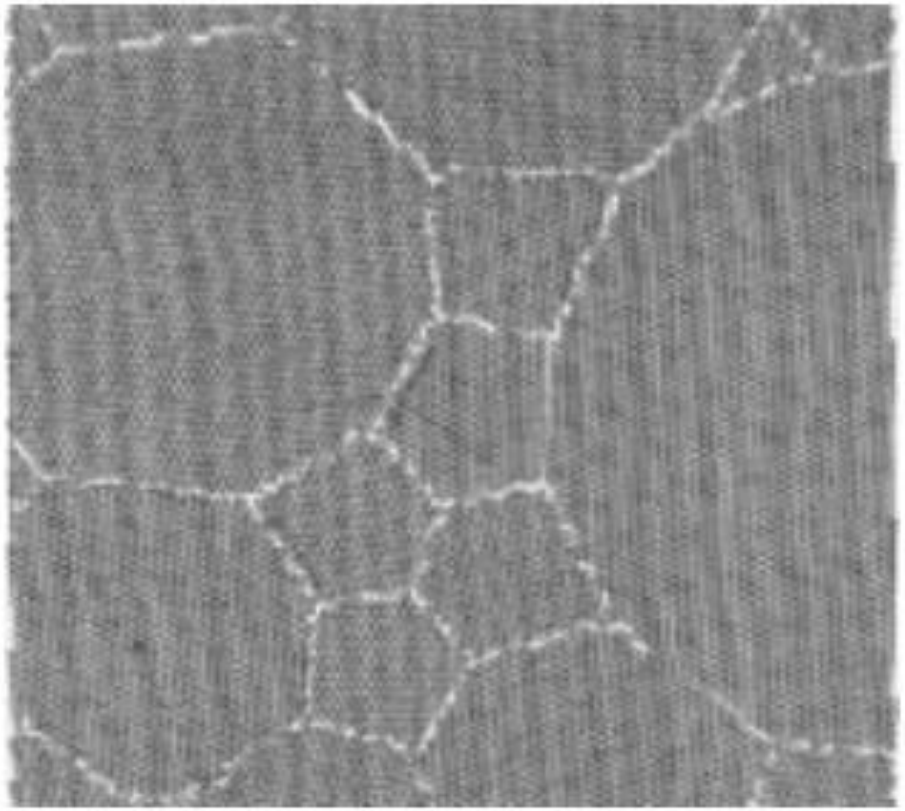
SURFACE, PLANE OR PLANAR DEFECTS

- Until now we considered structure and defects of single crystals that have periodic, regular atomic arrangement throughout the sample.
- Single crystals, however, can be rarely found in real materials unless the growth conditions are specially designed and controlled, as, for example, when producing silicon single crystals for microelectronic devices or blades for turbine engines made of superalloys.
- Instead, 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.

SURFACE, PLANE OR PLANAR DEFECTS

- The individual grains are separated by grain boundaries, regions of are less densely and regularly packed as compared to the bulk of the grains.





Atomistic model of a nanocrystalline solid
by Mo Li, JHU

SURFACE, PLANE OR PLANAR DEFECTS

Stacking Faults and Twin Boundaries

- 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 region.

- A change in the stacking sequence over a few atomic spacings produces a stacking fault whereas a change over many atomic spacings produces a twin region

SURFACE, PLANE OR PLANAR DEFECTS

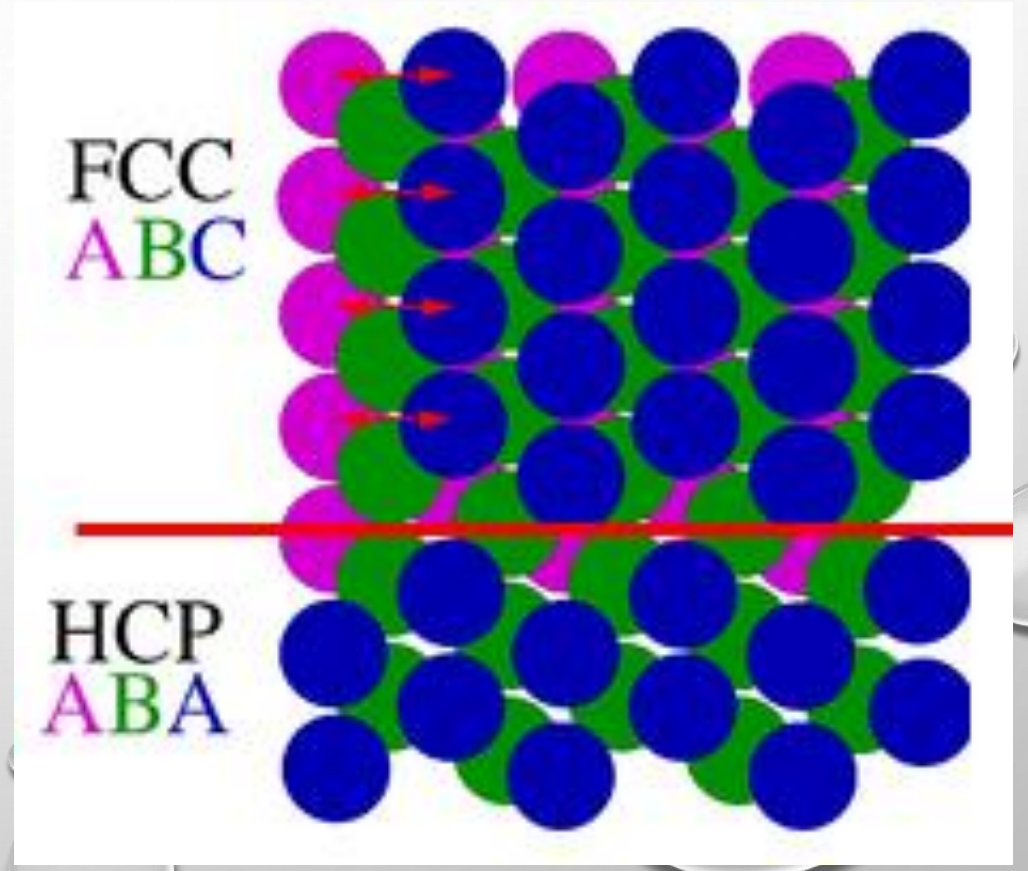
Stacking Fault

- is a one or two layer interruption in the stacking sequence of atom planes.
- occurs in a number of crystal structures, but is easiest to see how they occur in close packed structures.
- E.g.: face centred cubic (fcc) structures differ from hexagonal close packed (hcp) structures only in their stacking order.
- For hcp and fcc, the first two layers arrange themselves identically, and are said to have an AB arrangement

SURFACE, PLANE OR PLANAR DEFECTS

Stacking Fault

- If the third layer is placed so that its atoms are directly above those of the first (A) layer, the stacking will be ABA.
- This is the hcp structure, and it continues ABABABAB

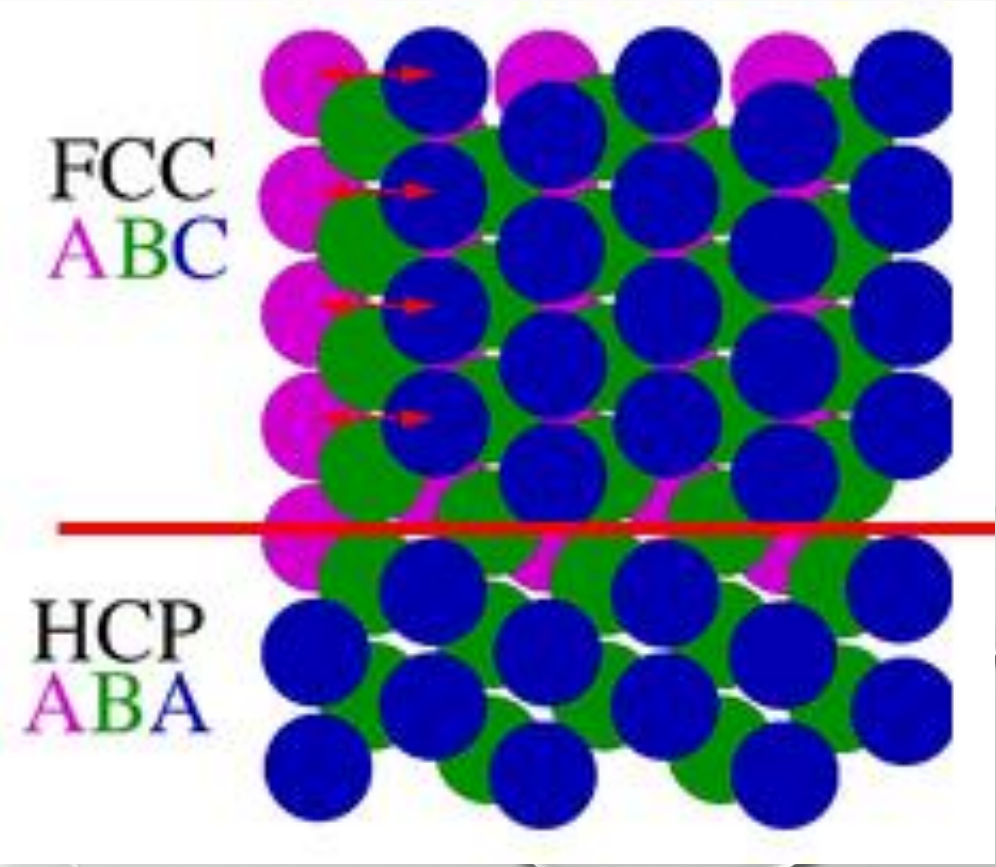


SURFACE, PLANE OR PLANAR DEFECTS

Stacking Fault

- But it is possible for the third layer atoms to arrange themselves so that they are in line with the first layer to produce an ABC arrangement which is that of the fcc structure.

- So, if the hcp structure is going along as ABABAB and suddenly switches to ABABABCABAB, there is a **stacking fault** present, along the red line in the figure.



SURFACE, PLANE OR PLANAR DEFECTS

Stacking Fault

- Alternately, in the fcc arrangement the pattern is ABCABCABC.
- A stacking fault in an fcc structure would appear as one of the planes missing.
- In other words the pattern would become ABCABCAB_ABCABC.

SURFACE, PLANE OR PLANAR DEFECTS

Twin

- If a stacking fault does not correct itself immediately but continues over some number of atomic spacings, it will produce a second stacking fault that is the twin of the first one.
- E.g., if the stacking pattern is ABABABAB but switches to **ABCABCABC** for a period of time before switching back to ABABABAB, a pair of twin stacking faults, or simply a twin, is produced.

ABABABABABABCABCABCABCABCABCABABABABABABABA

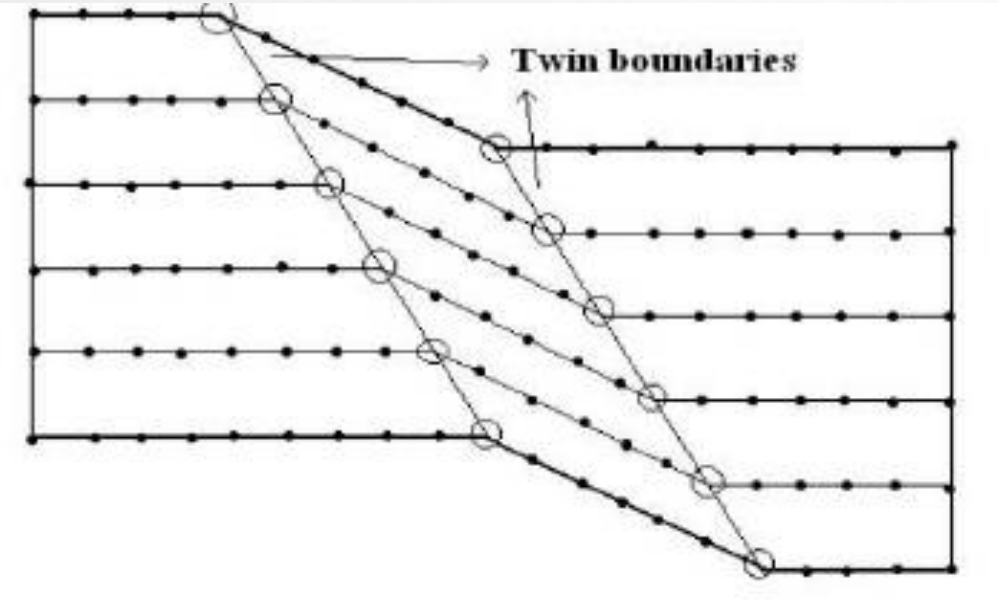
SURFACE, PLANE OR PLANAR DEFECTS

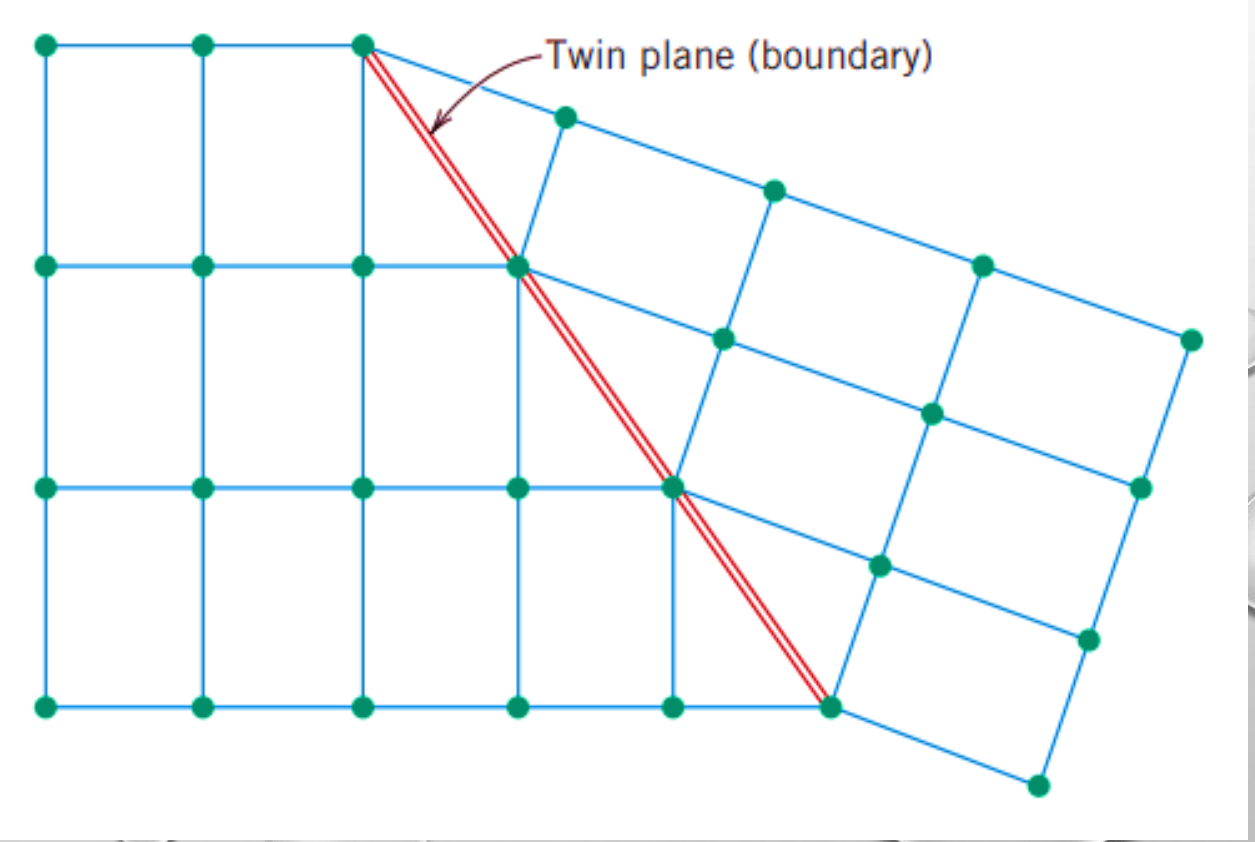
Twin

- The region in the stacking sequence that goes
- ABCABCACBACBABCABC is the twin plane and the twin boundaries are the A planes on each end of the highlighted region.
- Twin boundaries are the boundaries in the grains at which the atomic arrangement on one side of the boundary is the mirror image of the atoms on the other side
- They may be produced by shear deformation
- The region between the pair of boundaries is called the twinned region

SURFACE, PLANE OR PLANAR DEFECTS

Twin





SURFACE, PLANE OR PLANAR DEFECTS

Grain Boundaries in Polycrystals

- Solids generally consist of a number of crystallites or grains.
- Grains can range in size from nanometres to millimetres across
- Their orientations are usually rotated with respect to neighbouring grains.
- Where one grain stops and another begins is known as a grain boundary. Grain boundaries limit the lengths and motions of dislocations.

SURFACE, PLANE OR PLANAR DEFECTS

Grain Boundaries in Polycrystals

- Therefore, having smaller grains (more grain boundary surface area) strengthens a material.
- Grain size can be controlled by the cooling rate in heat treatment.
- Generally, rapid cooling produces smaller grains whereas slow cooling result in larger grains.

VOLUME OR BULK DEFECTS

These are defects occurring on a much bigger scale than the rest of the crystal defects. These include:

- **Voids**

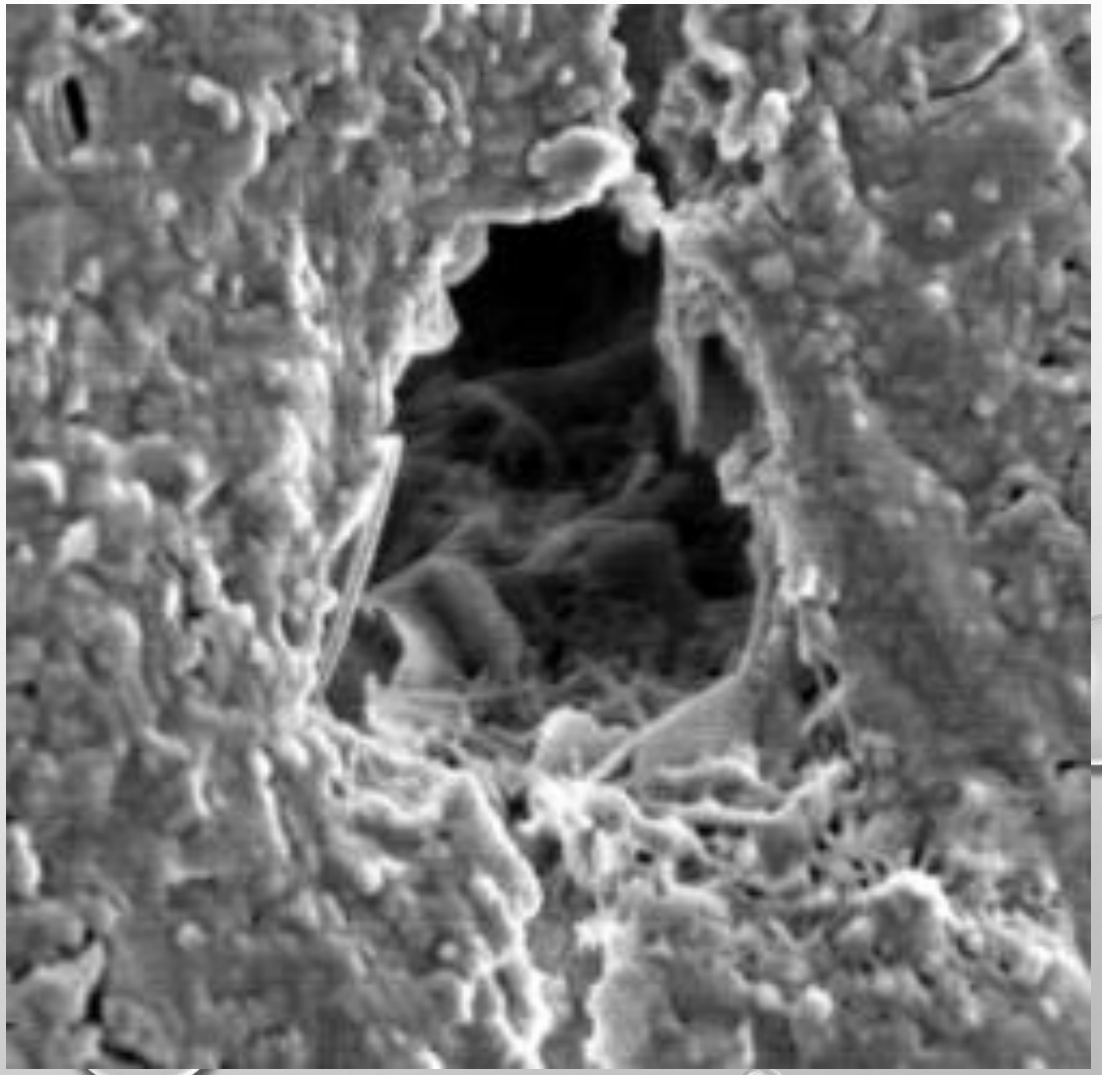
and

- **Impurity atoms cluster**

VOLUME OR BULK DEFECTS

Voids

- regions where there are one or a large number of atoms missing from the lattice. The image to the right is a void in a piece of metal (large number of atoms missing).

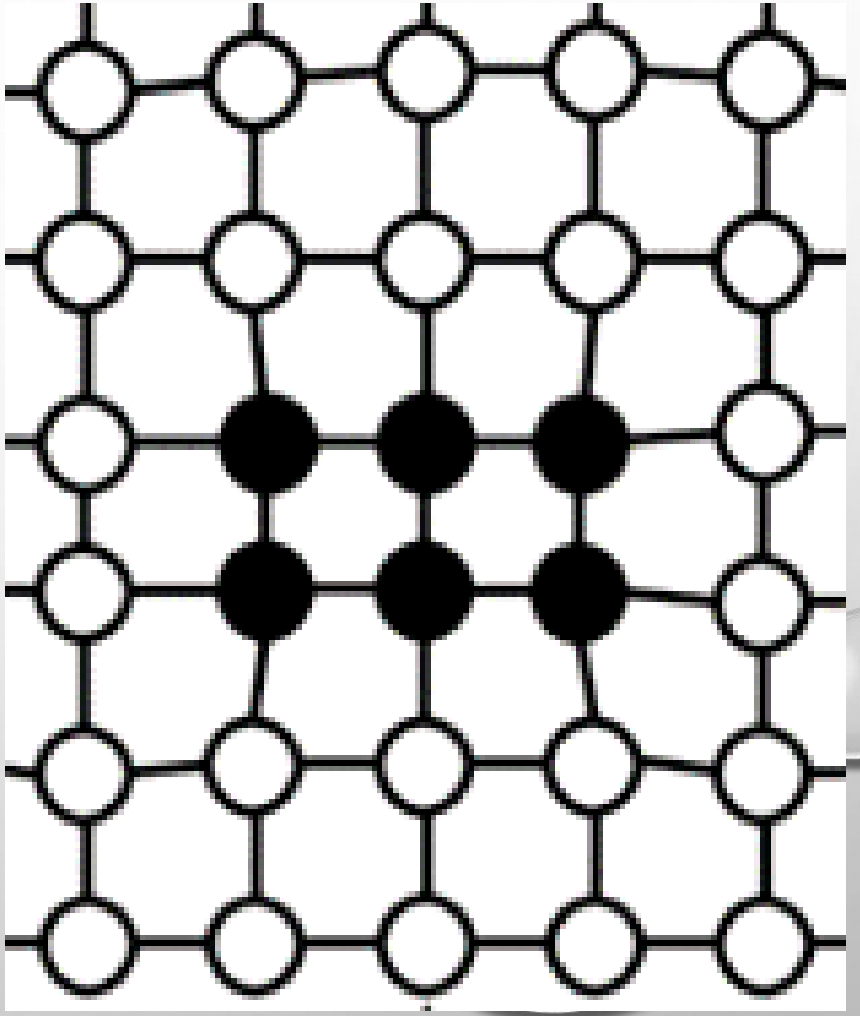


- Voids can occur for a number of reasons (due to entrapped air = **porosity**; due to shrinkage = **cavitation**).

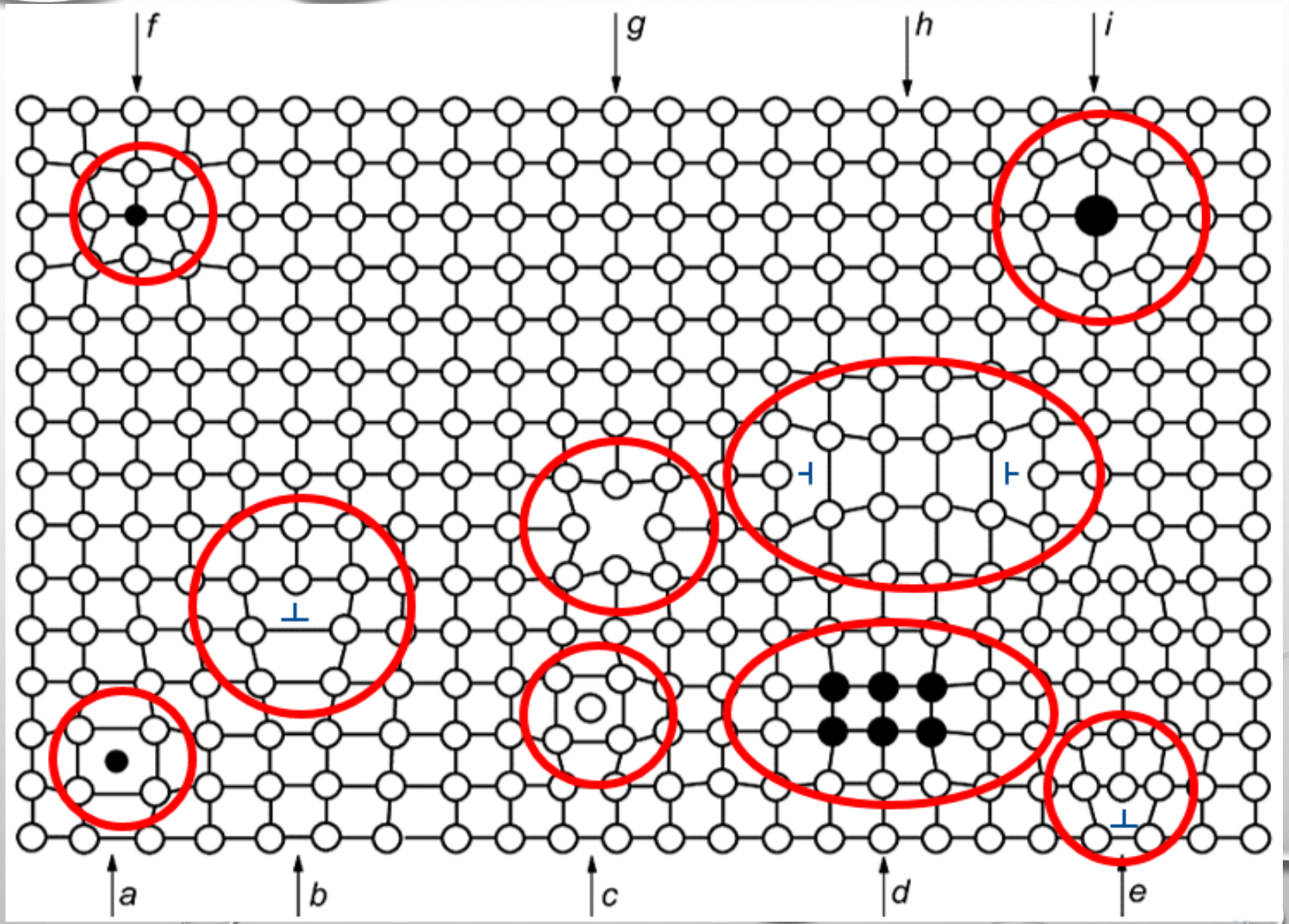
VOLUME OR BULK DEFECTS

Impurity atoms cluster

- When **impurity atoms cluster** together to form small regions of a different phase.
- The term ‘phase’ refers to that region of space occupied by a physically homogeneous material.
- These regions are often called precipitates.



SUMMARY OF CRYSTAL DEFECTS



SUMMARY OF CRYSTAL DEFECTS

From the figure, Crystal Defects can be summarized as follows:

a) Impurity interstitial
b) Dislocation
c) Self-interstitial
d) Cluster of impurity atoms
e) Extrinsic dislocation loop
f) Small substitutional impurity
g) Vacancy
h) Intrinsic dislocation loop
i) Large substitutional impurity

END OF LECTURE 5