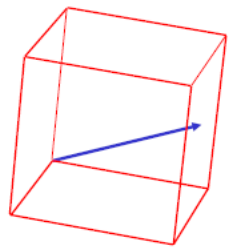
Lec.4 Crystallographic Directions, and Planes

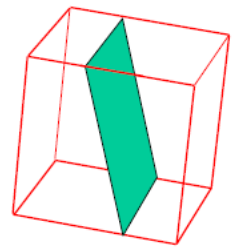
Dr.AMIR NAJAH SAUD AL-HUMAIRI
AL-MUSTAQBAL UNIVERSITY/ DEPARTMENT OF BIOMEDICAL ENGINEERING
Class: second
subject : Biomaterials science
Email: amir_najah@mustaqbal-college.edu.iq

Crystallographic Directions, and Planes

we need a way to identify directions and planes of atoms. Why?

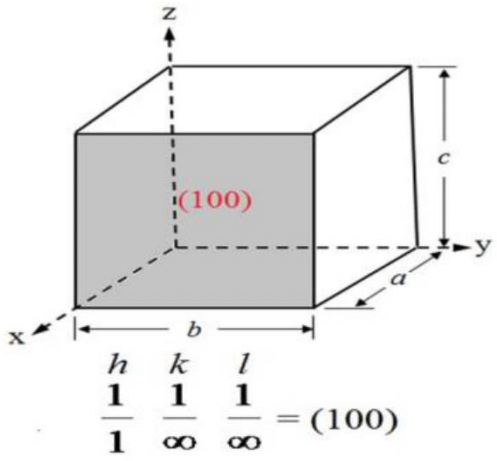
- Deformation under loading (*slip*) occurs on certain crystalline planes and in certain crystallographic directions.
- Before we can predict how materials fail, we need to know what modes of failure are more likely to occur.
- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.
- Directions and planes are described using three integers -**Miller Indices**

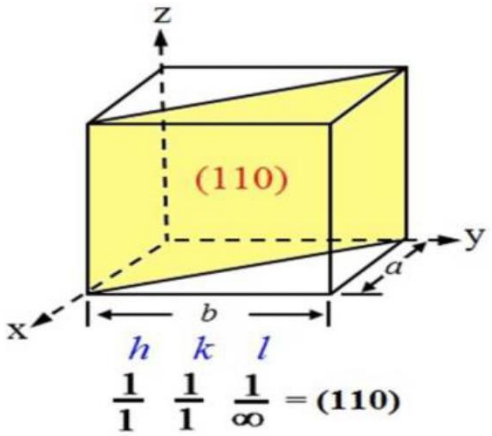

direction

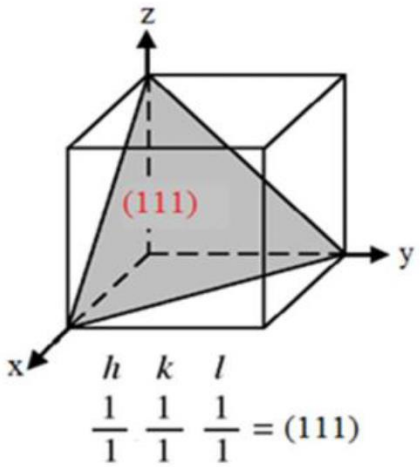

plane

Crystal Planes

- **Miller Indices**
- Planes in a crystal are described by notations called Miller indices
- Miller indices of a plane, indicated by h k l, are given by the reciprocal of the intercepts of the plane on the three axes.
- Miller indices of some other planes in the cubic system are shown in the figures

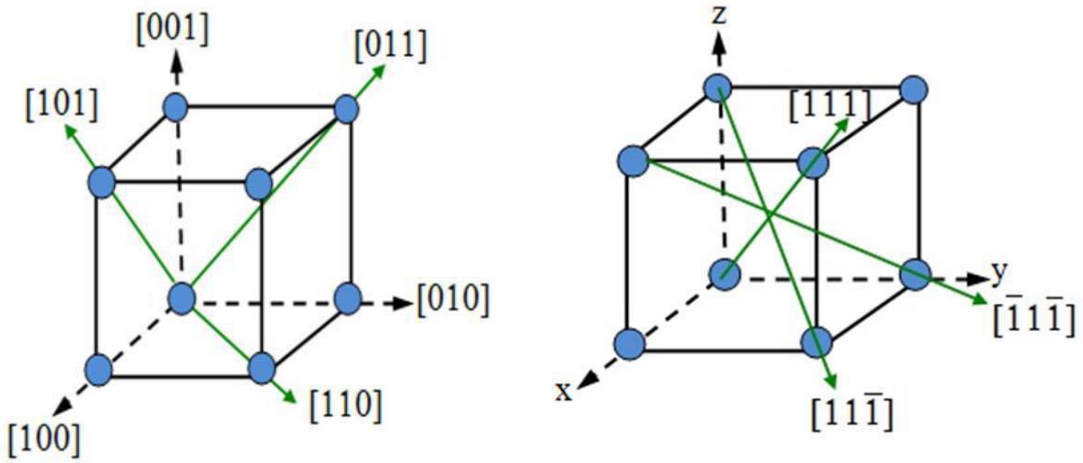






Crystal Planes

- **Crystal Directions**
- The directions in a crystal are given by specifying the coordinates (u, v, w) of a point on a vector (ruvw) passing through the origin. ruvw = ua + vb + wc. It is indicated as [uvw].
- For example, the direction [110] lies on a vector r110 whose projection lengths on x and y axes are one unit (in terms of unit vectors a and b).
- Directions of a form or family like [110], [101], [011] are written as <110> .



H.W// find the miller indices with direction for following

- 1-[101]
- 2-[002]
- 3-[301]
- 4-[011]
- 5-[222]
- 6-[210]

Linear and Planar density

- **Linear Density:**
- – Number of atoms per length whose centers lie on the direction vector for a specific crystallographic direction

$$LD = \frac{\#\text{ of atoms centered on a direction vector}}{\text{length of direction vector}}$$

ex. calculate linear atomic density ρ_l in [110] direction in Cu crystal lattice in atoms/mm. (Cu is FCC and lattice constant $a = 0.361$ nm)

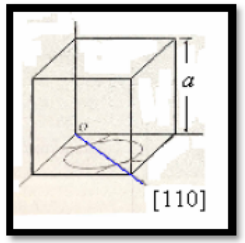
solution:

no. of atoms = ½ + 1 + ½ = 2 atoms

length = $\sqrt{2}\, a = \sqrt{2}\,(3.61 \times 10^{-7})$

$= 5.104 \times 10^{-7}$ mm

$$\rho_l = \frac{2 \text{ atoms}}{5.104 \times 10^{-7} \text{ mm}} = 3.92 \times 10^{6} \text{ atoms/mm}$$



Linear and Planar density

- **Planar Density**
- – Number of atoms per unit area that are centered on a particular crystallographic plane.

$$PD = \frac{\#\text{ of atoms centered on a plane}}{\text{area of plane}}$$

ex. calculate planar atomic density ρ_p on (110) plane of the α-Fe in BCC lattice in atoms/mm^2. (lattice constant a = 0.287 nm)

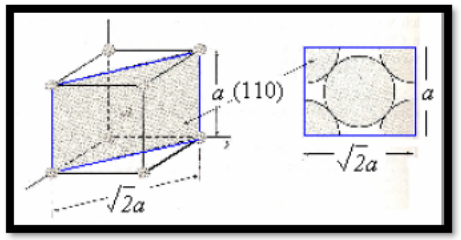
solution:

1 atom (center) + ¼ atom (corner) × 4 = 2 atoms

area = $a \times \sqrt{2}\, a = \sqrt{2}\, a^2 = \sqrt{2}\,(2.87 \times 10^{-7})^2$

$= 1.164 \times 10^{-13}$ mm^2

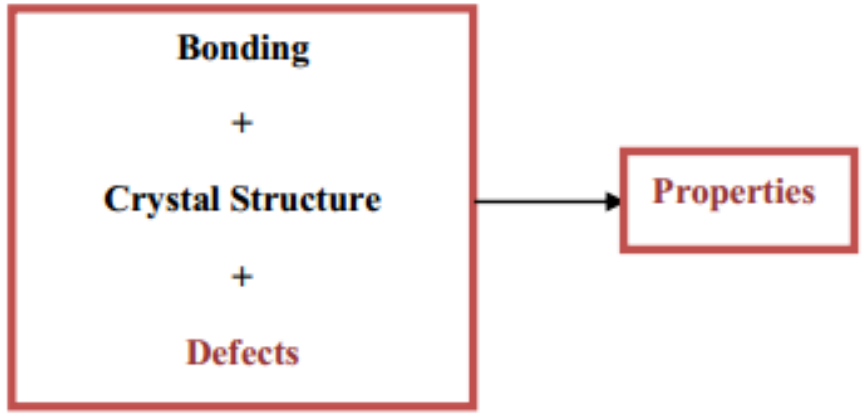
$$\rho p = \frac{2 \text{ atoms}}{1.164 \times 10^{-13} \text{ mm}^2} = 1.72 \times 10^{13} \text{ atoms/mm2}$$



Crystalline Defects

- The properties of some materials are profoundly influenced by the presence of defects.
- :For example
- The mechanical properties of pure metals experience significant alterations when alloyed. (i.e, when impurity atoms are added)- for example, brass (70% copper – 30% zinc) is much harder and stronger than pure copper.
- Crystals are like people, it is the defects in them which tend to make them Interesting "Colin Humphreys

Why are defects important?

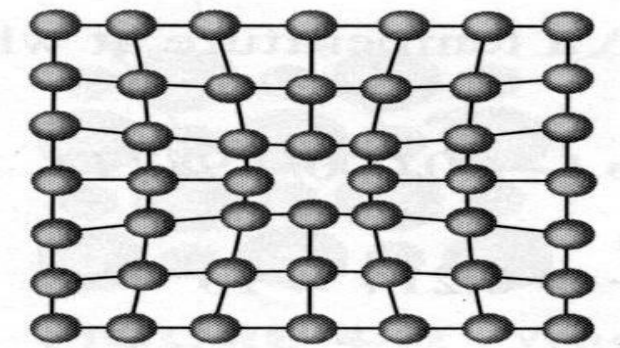


Types of Crystalline Defects

- Point Defects - Vacancies, Interstitial, and Substitutional

A. Vacancy Defects

- A vacancy defect is formed when an atom is missing from a normal atomic site in a crystalline structure.
- The number of vacancies present in a material increases exponentially as the temperature increases
- **How many vacancies are there?**
- Statistical thermodynamics predicts that the number of vacancies Nv, have very strong dependence on temperature, T, and can be estimated using the Boltzmann distribution**:**



$$Nv = N \exp\left(\frac{-Q_v}{K_B T}\right)$$

Where

N :- is the total number of regular lattice sites , (total number of atomic sites).

Q**V** :- is the energy required to form a vacant lattice site in a perfect crystal.

K**B** :- is the Boltzmann's constant , = 1.38 * 10^{-23} J/ atom .K

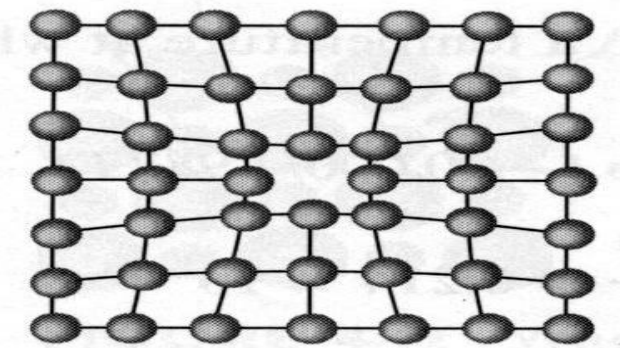
T :- is the temperature in Kelvin (K).

Types of Crystalline Defects

- Point Defects - Vacancies, Interstitial, and Substitutional

A. Vacancy Defects

- A vacancy defect is formed when an atom is missing from a normal atomic site in a crystalline structure.
- The number of vacancies present in a material increases exponentially as the temperature increases
- **How many vacancies are there?**
- Statistical thermodynamics predicts that the number of vacancies Nv, have very strong dependence on temperature, T, and can be estimated using the Boltzmann distribution**:**



$$Nv = N \exp\left(\frac{-Q_v}{K_B T}\right)$$

Where

N :- is the total number of regular lattice sites , (total number of atomic sites).

Q**V** :- is the energy required to form a vacant lattice site in a perfect crystal.

K**B** :- is the Boltzmann's constant , = 1.38 * 10^{-23} J/ atom .K

T :- is the temperature in Kelvin (K).

Vacancy Defects

Number of Vacancies Computation at a Specified Temperature

Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000°C) for copper are 63.5 g/mol and 8.4 g/cm^3, respectively.

Solution

$$N = \frac{N_A \rho}{A_{Cu}}$$

$$= \frac{(6.023 \times 10^{23}\ \text{atoms/mol})(8.4\ \text{g/cm}^3)(10^6\ \text{cm}^3/\text{m}^3)}{63.5\ \text{g/mol}}$$

$$= 8.0 \times 10^{28}\ \text{atoms/m}^3$$

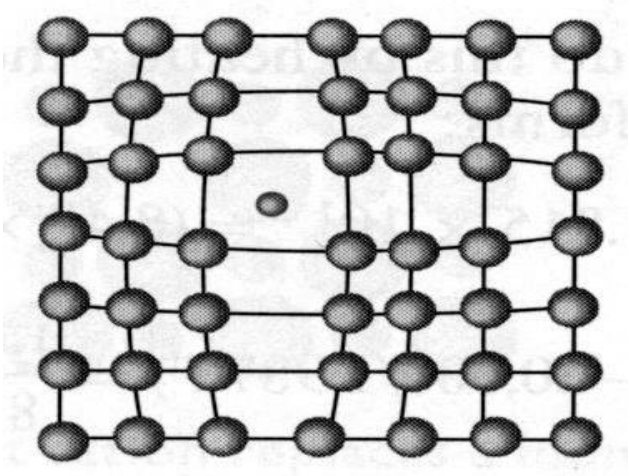
Thus, the number of vacancies at 1000°C (1273 K) is equal to

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

$$= (8.0 \times 10^{28}\ \text{atoms/m}^3) \exp\left[-\frac{(0.9\ \text{eV})}{(8.62 \times 10^{-5}\ \text{eV/K})(1273\ \text{K})}\right]$$

$$= 2.2 \times 10^{25}\ \text{vacancies/m}^3$$

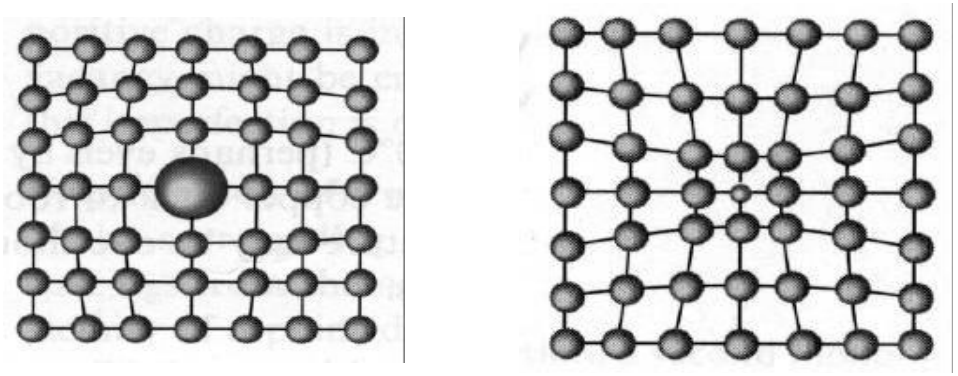
- **B- Interstitial Defects**
- An Interstitial defect is formed when an extra atom occupies a normally unoccupied site (interstitial site).
- Since the interstitial atoms are larger than the interstitial sites the surrounding lattice is in compression.



C- Substitutional Defects

Substitutional defects are produced when one atom is replaced by a different type of atom.

- If the substitutional atom is smaller than the original atom then the Lattice is in tension.
- If the substitutional atom is larger than the original atom then the lattice is in compression.

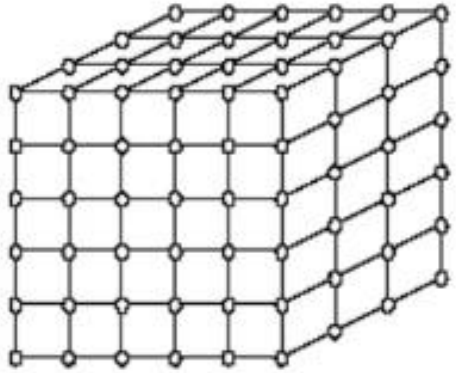


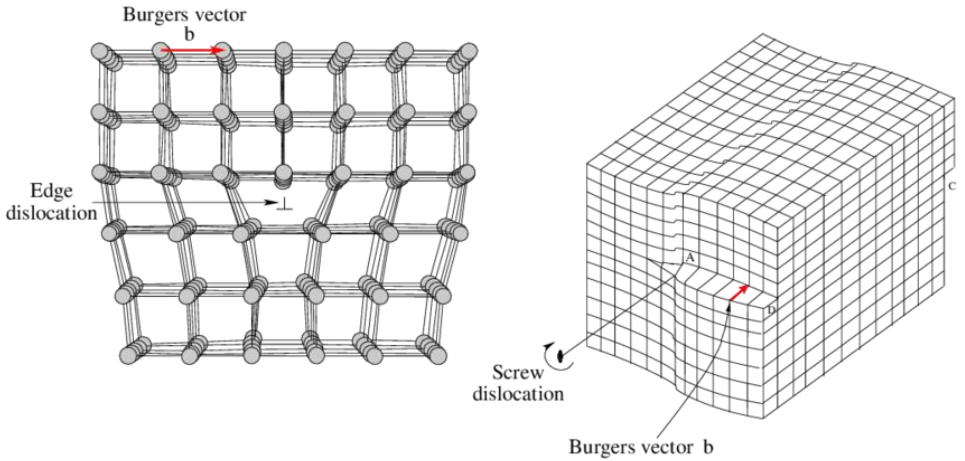
2- Line defect

- There are two type

1. **Edge dislocation**: is a type of line defect in crystal lattices in which the defect occurs either due to the presence of an extra plane of atoms or due to the loss of a half of a plane of atoms in the middle of the lattice. This defect causes the nearby planes of atoms to bend towards the dislocation. Therefore, the adjacent planes of atoms are not straight. The region in which the defect occurs is the dislocation core or area. When we apply stress on a crystal having this defect, the dislocation area moves parallel to the direction of stress.

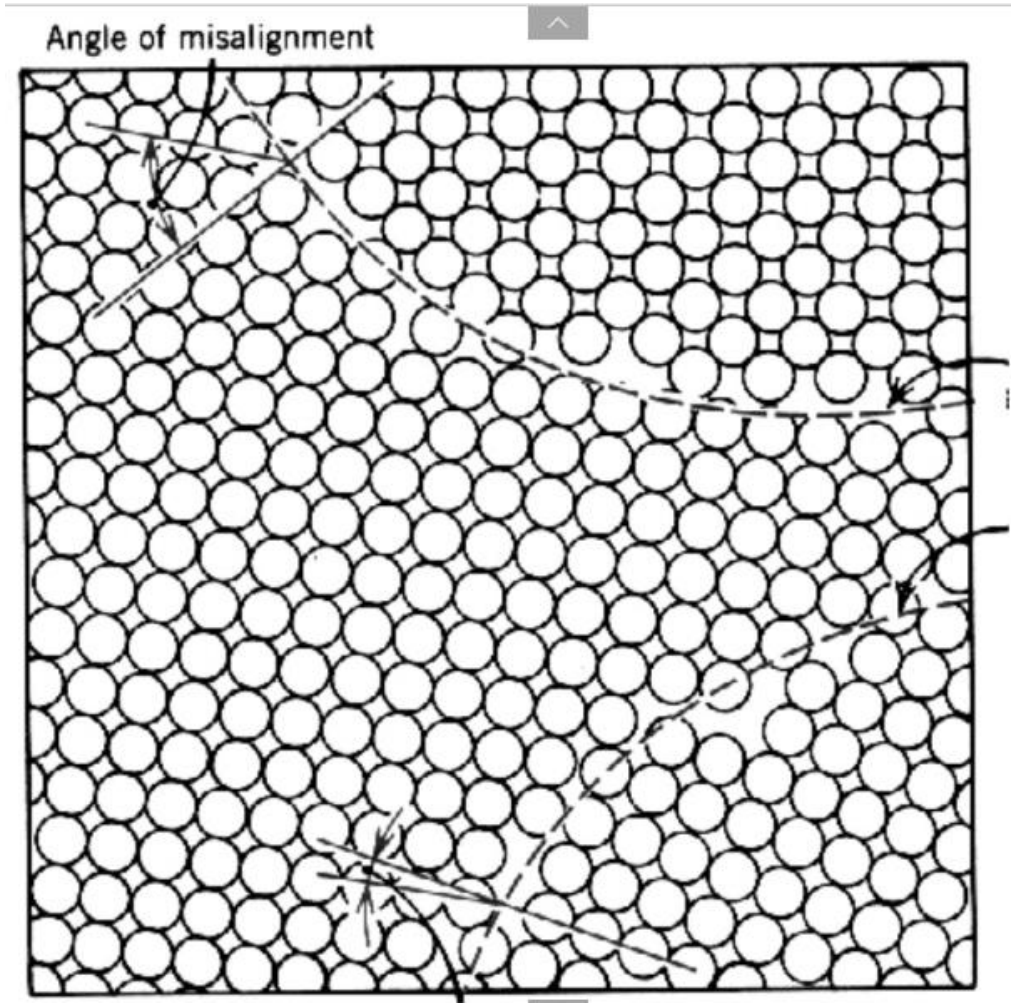
2. **Screw dislocation**: is another type of line defect in which the defect occurs when the planes of atoms in the crystal lattice trace a helical path around the dislocation line. Visualizing this type of defects in crystals is difficult. **Unlike** in edge dislocation, when we apply stress on a crystal having this defect, the dislocation area moves perpendicular to the direction of stress





3- Surface defect

- These defects are named because they arise from a combination of many linear defects consisting of a surface of defects.
- Grain boundary
- Some solid materials do not consist of crystalline structure of one crystalline but of many small crystals, which are called **grain** and that each grain within the structure of the solid matter vary in direction, size, shape and distance from neighbor. And therefore have to be separated from each other delineated boundary called the grain boundaries

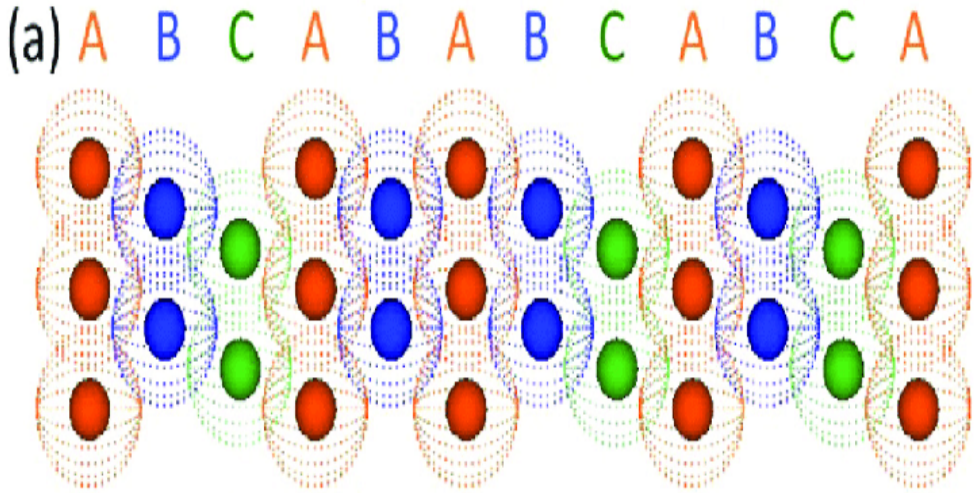


3- Surface defect

Stacking fault

These occur in FCC metals and represent an error in the stacking sequence of close-packed planes. Normally, a stacking sequence of *ABCABCABC* is produced in a perfect FCC lattice. But, suppose the sequence ***ABCABABCABC*** occurs. In the portion *ABAB*, a type *A* plane is shown where a type *C* plane should be located.

This small region, which has a HCP stacking sequence instead of the FCC stacking sequence, represents a stacking fault. Stacking faults interfere with the slip process.



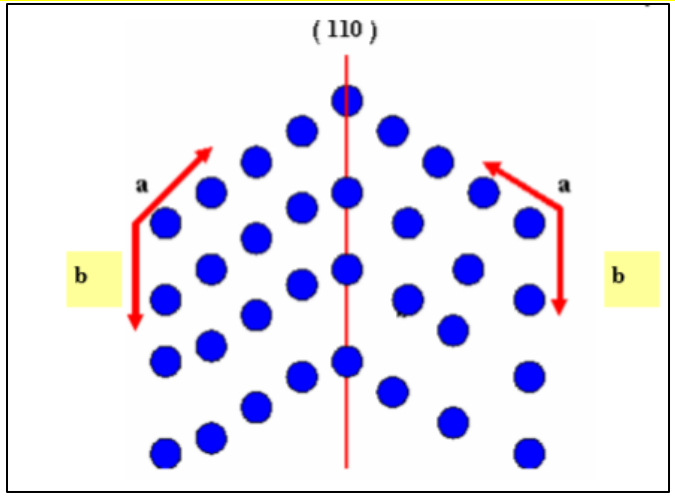
3- Surface defect

Twin Boundaries

- **A twin boundary** is a plane across which there is a special mirror image misorientation of the lattice structure as shown:

- Twins can be produced when a shear force, acting along the twin boundary, causes the atoms to shift out of position. Twinning occurs during deformation or heat treatment of certain metals. The twin boundaries interfere with the slip process and increase the strength of a metal. Movement of twin boundaries can also cause a metal to deform. The following figure shows that the formation of a twin has changed the shape of the metal.

when two identical regions of a crystal grow in a mirror-image way.



Thank you for your Kind Attention