Module-3

Imperfections in Solids
Contents

1) Theoretical yield strength, Point defects and Line defects or Dislocations

2) Interfacial defects, Bulk or Volume defects and Atomic vibrations
Theoretical yield strength

- Ideal solids are made of atoms arranged in an orderly way.

Diagram showing a shear stress, \( \tau \), versus displacement, \( x \), with a periodic structure denoted by \( a \) and \( b \).
Theoretical yield strength (contd…)

- Using a $sin$ function to represent the variation in shear stress

$$\tau = \tau_m \sin \frac{2\Pi x}{b} \quad \tau \approx \tau_m \frac{2\Pi x}{b}$$

$$\tau = G\gamma = \frac{Gx}{a}$$

(Hooke’s law)

$G \approx 20-150$ GPa

Shear strength $\approx 3-30$ GPa

(ideal)

Real strength values $\approx 0.5-10$ MPa

$$\tau_m = \frac{G}{2\Pi} \frac{b}{a}$$

If $b \approx a$
Theoretical yield strength (contd…)

- Theoretical strength of solids shall possess an ideal value in the range of 3-30 GPa.

- Real values observed in practice are 0.5-10 MPa.

- The assumption of perfectly arranged atoms in a solid may not be valid…i.e. atomic order must have been disturbed.

- Disordered atomic region is called *defect* or *imperfection*.

- Based on geometry, defects are: Point defects (zero-D), Line defects (1-D) or Dislocations, Interfacial defects (2-D) and Bulk or Volume defects (3-D).
Point defects

- Point defects are of zero-dimensional i.e. atomic disorder is restricted to point-like regions.

- Thermodynamically stable compared with other kind of defects.
Point defects (contd…)

- Fraction of vacancy sites can be given as follows:

\[
\frac{n}{N} = e^{-\frac{Q}{kT}}
\]

- In ionic crystals, defects can form on the condition of charge neutrality. Two possibilities are:

![Diagram of Frenkel and Schottky defects]
Line defects

- Line defects or Dislocations are abrupt change in atomic order along a line.

- They occur if an incomplete plane inserted between perfect planes of atoms or when vacancies are aligned in a line.

- A dislocation is the defect responsible for the phenomenon of slip, by which most metals deform plastically.

- Dislocations occur in high densities \((10^8-10^{10} \text{ m}^{-2})\), and are intimately connected to almost all mechanical properties which are in fact structure-sensitive.

- Dislocation form during plastic deformation, solidification or due to thermal stresses arising from rapid cooling.
Line defects – Burger’s vector

- A dislocation in characterized by Burger’s vector, $b$.

- It is unique to a dislocation, and usually have the direction of close packed lattice direction. It is also the slip direction of a dislocation.

- *It represents the magnitude and direction of distortion associated with that particular dislocation.*

- Two limiting cases of dislocations, edge and screw, are characterized by Burger’s vector perpendicular to the dislocation line ($t$) and Burger’s vector parallel to the dislocation line respectively. Ordinary dislocation is of mixed character of edge and screw type.
Line defects – Edge dislocation

- It is also called as *Taylor-Orowan dislocation*.

- It will have regions of compressive and tensile stresses on either side of the plane containing dislocation.
Line defects – Screw dislocation

- It is also called as *Burger’s dislocation*.
- It will have regions of shear stress around the dislocation line.
- For positive screw dislocation, dislocation line direction is parallel to Burger’s vector, and vice versa.
Line defects – Dislocation motion

- Dislocations move under applied stresses, and thus causes plastic deformation in solids.

- Dislocations can move in three ways – glide/slip, cross-slip and climb – depending on their character. Slip is conservative in nature, while the climb is non-conservative, and is diffusion-controlled.

- Any dislocation can slip, but in the direction of its burger’s vector.

- Edge dislocation moves by slip and climb.

- Screw dislocation moves by slip / cross-slip. Possibility for cross-slip arises as screw dislocation does not have a preferred slip plane as edge dislocation have.
Line defects – Dislocation characteristics

- A dislocation line cannot end at abruptly inside a crystal. It can close-on itself as a loop, either end at a node or surface.

- *Burger’s vector for a dislocation line is invariant* i.e. it will have same magnitude and direction all along the dislocation line.

- Energy associated with a dislocation because of presence of stresses is proportional to square of Burger’s vector length. Thus dislocations, at least of same nature, tend to stay away from each other.

- Dislocations are, thus, two types – full and partial dislocations. For *full dislocation*, Burger’s vector is integral multiple of inter-atomic distance while for *partial dislocation*, it is fraction of lattice translation.


**Interfacial defects**

- An interfacial defect is a 2-D imperfection in crystalline solids, and have different crystallographic orientations on either side of it.

- Region of distortion is about few atomic distances.

- They usually arise from clustering of line defects into a plane.

- These imperfections are not thermodynamically stable, but meta-stable in nature.

E.g.: External surface, Grain boundaries, Stacking faults, Twin boundaries, Phase boundaries.
Interfacial defects (contd…)

Grain boundaries

Twin boundaries
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 particles

- These defects act like stress raisers, thus deleterious to mechanical properties of parent solids.

- In some instances, foreign particles are added to strengthen the solid – dispersion hardening. Particles added are hindrances to movement of dislocations which have to cut through or bypass the particles thus increasing the strength.
Atomic vibrations

- Atoms are orderly arranged, but they are expected to vibrate about their positions where the amplitude of vibration increases with the temperature.

- After reaching certain temperature, vibrations are vigorous enough to rupture the inter-atomic forces casing melting of solids.

- Average amplitude of vibration at room temperature is about $10^{-12}\text{m}$ i.e. thousandth of a nanometer.

- Frequency of vibrations is the range of $10^{13}\text{ Hz}$.

- Temperature of a solid body is actually a measure of vibrational activity of atoms and/or molecules.