Lecture#10

Defects in metals:
- Theoretical Strength of Crystal
- Defects in Crystals
- Point defects

References:
2- Hosford W.F, (2005), Mechanical Behavior of Materials, Cambridge
4- Dieter G.E., (1986), Mechanical Metallurgy, McGraw-Hill

Theoretical Strength of Crystal:
Materials, when exposed to external forces, will deform or fail. This may occur by:-

Cleavage: When a material breaks under a perpendicular (i.e., normal) stress and the fracture path is perpendicular to the applied stress. Consumes little energy and produces a brittle fracture. Cleavage involves the separation of atomic bonds perpendicular to an applied load/stress.

Shear: When a material breaks under a “parallel” stress and the fracture path is parallel to the applied stress. It consumes more energy as shear distorts specimens. Bond breakage is sequential.

It is possible to estimate the theoretical strength of a “perfect” material (i.e., a material that contains no defects). Theoretical strengths are related to interatomic forces, temperature, state of stress.

The theoretical cleavage strength, \( \sigma_{\text{max}} = \frac{E}{\pi} \) (will be illustrated later)

In order to have high theoretical cleavage strength, materials must have high E and surface energy and small distance between atomic planes.
**Theoretical shear stress:**  
Frenkel has devised a simple method to estimate the theoretical shear strength of a perfect crystal.

- Consider the arrangement shown (two neighboring planes within a crystal with a separation distance $a$ and an interatomic distance $b$).
- Assume that individual planes do not distort when a shear stress is applied. Under an applied stress, atoms will pass sequentially through equilibrium positions (i.e., A, B, C, etc…). Plastic deformation will occur when atoms move until the planes separate (i.e., fracture occurs). Between equilibrium positions, $\tau$ varies cyclically. Assuming the variation is sinusoidal, we can express it as:

\[ \tau = k \sin \frac{2\pi x}{b} \]

and for small displacement

\[ \tau = k \frac{2\pi x}{b} \]

the material will be deformed elastically, so

\[ \tau = G \frac{x}{a} \]

where $\frac{x}{a}$ is the shear strain.

\[ k = \frac{Gb}{2\pi a}, \quad \text{so} \quad \tau = \frac{Gb}{2\pi a} \text{sin} \frac{2\pi x}{b} \]

The max.shear occur for $x = b/4$, So

\[ \tau_{\text{max}} = \frac{G b}{2\pi a} \]

Consider a face centered cubic (fcc) crystal, where

\[ b = a_o / \sqrt{2} \]
The relationship between the lattice parameter \(a_0\) and the interplanar spacing is given by:

\[
\text{and for (111)} \quad d_{111} = a_0 / \sqrt{3}
\]

For FCC crystals, the close packed plane, which is the most likely plane where shear will occur is (111).

The spacing \(d_{111}\) is equivalent to \(a\), the planar spacing in our original. If we substitute the values of \(b\) and \(a\) for the fcc crystal structure into the expression for \(\tau_{\text{max}}\), we get:

\[
\tau_{\text{max}} = G / 5.1
\]

The theoretical strength derived above is on the order of gigapascals; but, the actual strength of materials is orders of magnitude below that.

*Experimental shear stress \(<\) theoretical shear stress. Dislocations prevent ductile materials from obtaining their theoretical shear stress.*

Also \(\sigma_{\text{experimental}} \ll \sigma_{\text{theoretical}}. \) Cracks prevents brittle materials from obtaining their theoretical cleavage stress.

The equations of theoretical cleavage and shear strengths predict exceedingly high strengths (on the order of GPa), and few materials reach such strengths. If materials were perfect, those values could be reached. However, all materials contain imperfections, either by design or inadvertently produced during processing. They are classified, according to their dimensions, into four kinds as follows:

- Point (atomic or electronic) defects
- Line (or one-dimensional) defects
- Interfacial (or two-dimensional) defects
- Volume defects

**Point defects:**

![Diagram of point defects](image-url)
These defects exist on an atomic scale. These defects can have a diameter of approximately $10^{-10}$ m. Although relatively small compared to other imperfections, atomic defects do generate a stress field in the crystal lattice and affect the properties of the material.

**Production of Point Defects**

1- Vacancies or self-interstitials point defects exist in well-established equilibrium concentrations. The equilibrium concentration of defects, given by the ratio of the number of defects to the number of atomic sites, $(n/N)$ corresponding to the condition of minimum free energy is

$$n/N = \exp(-E_f/kT)$$

where $n$ is the equilibrium number of vacancies per unit volume of the material at an absolute temperature, $T$(in deg K), $N$ is the total number of atomic sites per unit volume (which depends upon the crystal structure), $E_f$ is the activation energy to form the vacancy (related to the energy barrier that must be surmounted to dislodge an atom from its normal position and create a vacancy), and $k$ is the Boltzmann’s constant $(13.81 \times 10^{-24}$ J/K).

For the vacancy, the formation energy, $E_f$, is that required to remove one atom from its lattice site to a place on the surface of the crystal. The rate at which a point defect moves from site to site in the lattice is proportional to $\exp(-E_m/kT)$, where $E_m$ is the defect migration energy. The rate decreases exponentially with decreasing temperature and consequently in many metals it is possible to retain a high vacancy concentration at room temperature by rapidly quenching from a high equilibrating temperature.

The concentration of these defects can be increased by quenching, or ultra-high-speed cooling. The concentration of vacancies in BCC, FCC, and HCP metals is greatly superior to that of interstitials and on the order of $10^{-3}$ when the metal is at a temperature close to the melting point; it is only $10^{-6}$ when the metal is at a temperature of about half the melting point.

2- By plastic deformation. The movement of dislocations generates point defects. (**will be explained later**)

3- Irradiation of the metal by high-energy particles. The radiation displaces the electrons, or ionizes, displaces atoms by elastic collisions. The displacement of atoms is produced by the elastic collision of the bombarding particles with the lattice atoms, transferring the kinetic energy
of the particles to the atoms. This may cause the atoms to travel through the lattice. Consequently, a vacancy is produced, together with a self-interstitial.

4- Ion Implantation
Charged ions are accelerated in an electric field to very high energies and allowed to strike the target solid in a moderate vacuum and implanted into the target surface. The technique is used to enhance the structure of surfaces for better corrosion and oxidation resistance, tribological properties, and superconductivity.

**Effect of Point Defects on Mechanical Properties**

1- Increasing yield strength  
2- Sometimes embrittlement.

The strengthening by quenching is due to the interaction of dislocations and vacancies or groups thereof.

Properties change because point defects distort the crystal lattice locally. **Impurity atoms** (substitutional or interstitial) in a crystal can be considered as **extrinsic** point defects and they play a very important role in the physical and mechanical properties of all materials. All the point defects mentioned produce a local distortion in the otherwise perfect lattice depends on the amount of 'space' between the atoms in the lattice and the 'size' of the atoms introduced.

The interstice sites between atoms generally have volumes of less than one atomic volume, and the interstitial atoms therefore tend to produce large distortions among the surrounding atoms. This can result in crystal volume increases.