Lattice Defects
Theoretical Strength of a Crystal

• The theoretical strength of a material with a perfect lattice is very high and of great importance.

• Theoretical strength is determined by the nature of:
  – inter-atomic forces
  – temperature (causes atoms to vibrate)
  – stress state of the material. We shall make calculations of two states of stresses: *uniaxial normal stress* and *shear stress*

• The stresses required for failure under the two situations will be calculated, and the theoretical strength should be the lower of the two values.
Theoretical Normal Strength

- The Failure type due to normal stress is **cleavage**
- The fracture path is perpendicular to the applied stress.
- The process involves the separation of the atoms along the direction of the applied stress.
- Orowan developed a simple method for obtaining the theoretical tensile strength of a crystal. It is assumed that all atoms separate simultaneously once their separation reaches a critical value. See Figure 10.1
Figure 10-1. Stress required to separate two atomic layers. The stress will vary as a function of the distance between planes.
• The distance is initially equal to $a_o$.
• Naturally, $\sigma = 0$ for $a = a_o$; $\sigma$ will also be zero when the separation is infinite. The exact form of the curve of $\sigma$ versus $a$ depends on the nature of the inter-atomic forces.
• In Orowan’s model, the curve is simply assumed to be a sine function, hence the generality of the model.
• The area under the curve is the work required to cleave the crystal.
• The stress dependence on plane separation is then given by the following equation:

$$\sigma = K \sin \frac{2\pi}{2d} (a - a_o) \quad (10.1)$$
K can be determined from the differentiation of equation 10.1, and it is given as:

$$K = \frac{E\ d}{\pi\ a_o}$$  \hspace{1cm} (10.2)

- Following a rigorous calculation, we obtain:

$$\sigma_{\text{max}} = \sqrt{\frac{E\ \gamma}{a_o}}$$  \hspace{1cm} (10.3)

where E is the Young’s modulus and γ is the surface energy per unit volume.
According to Orowan’s model, the surface energy is given by:

\[ \gamma = \frac{Kd}{\pi} = \frac{E(d)}{a_0(\pi)} \]  

(10.4)

It has been experimentally determined that \( d \) is approximately equal to \( a_0 \). Hence,

\[ \gamma = \frac{Ea_0}{10} \quad \text{and} \quad \sigma_{\text{max}} = \frac{E}{\pi} \]  

(10.5)

We can conclude from Eq. 10.3 that, in order to have a high theoretical cleavage strength, a material must have a high Young’s modulus and surface energy and a small distance \( a_0 \) between atomic planes.
Theoretical Shear Stress

- Frenkel performed a simple calculation of the theoretical shear strength of crystals by considering two adjacent and parallel lines of atoms subjected to a shear stress as shown in Figure 10.2.

- “b” is the inter-atomic distance or the distance between atoms in the slip directions

- “a” is the separation between adjacent planes or the spacing between adjacent lattice planes.

- Under the action of the stress $\tau$, the top line will move in relation to the bottom line; the atoms will pass through successive equilibrium positions A, B, C, for which $\tau$ is zero.
Figure 10-2. Stress required to shear a crystal.
Figure 10.1 (b). Variation of shearing stress with displacement in slip direction.
As a first approximation, the relationship between shear stress and displacement can be expressed by a sine function.

\[ \tau = \tau_m \sin \frac{2\pi x}{b} \]  \hspace{1cm} (10.6)

Where \( \tau_m \) is the amplitude of the sine wave and \( b \) is the period. At small values of displacement, Hooke’s law should apply.

\[ \tau = G \gamma = \frac{Gx}{a} \]  \hspace{1cm} (10.7)

For small values of \( x/b \), Eqs. (10-6) can be written

\[ \tau = \tau_m \frac{2\pi x}{b} \]  \hspace{1cm} (10.8)
Combining Eqs. (10-7) and (10-8) provides an expression for the maximum shear stress at which slip should occur.

\[ \tau_m = \frac{G}{2 \pi} \frac{b}{a} \]  \hspace{1cm} (11.9)

As a rough approximation, \( b \) can be taken equal to \( a \), with the result that the theoretical shear strength of a perfect crystal is approximately equal to the shear modulus divided by \( 2 \pi \).

\[ \tau_m = \frac{G}{2 \pi} \]  \hspace{1cm} (10.10)
• The shear modulus for metals is in the range 20 to 150 GPa.

• Therefore, Eq. (10-10) predicts that the theoretical shear stress will be in the range (3 to 30 GPa).

• However, the actual values of the shear stress required to produce plastic deformation in metal single crystals are in the range 0.5 to 10 MPa.

\[ \text{This means that: } \sigma_{th} \gg \sigma_{exp} \]

• Since the theoretical shear strength of metal crystals is at least 100 times greater than the observed shear strength, it must be concluded that a mechanism other than bodily shearing of planes of atoms is responsible for slip.

• This is the \textbf{Holy Grail} of materials science
• If materials were perfect, those high values would have been reached. Real crystals deviate from the perfect periodically that was assumed in the previous section because they contain imperfections.

• **Point imperfection:** When the deviation from the periodic arrangement of the lattice is localized to the vicinity of only a few atoms it is called a *point defect*.

• **Lattice imperfection:** If the defect extends through microscopic regions of the crystal. These may be divided into:
  
  – *line* (*one-dimensional*) *defects*
  
  – *surface or area* (*two-dimensional*) *defects*
  
  – *plane or volume* (*three-dimensional*) *defects*
Surface defects arise from the clustering of line defects into a plane. Low-angle boundaries and grain boundaries are surface defects (see Chap 5).

The stacking fault between two close-packed regions of the crystal that have alternate stacking sequences (Sec. 4-11) and twinned region of a crystal (Sec. 4-10) are other examples of surface defects.
Figure 10-3. Dimensional ranges of different classes of defects.