Dislocations in Crystals

Dislocations provide stepwise motion scaled to the spacing of atoms in crystals.

Line Defects: Dislocations and their Scale

Figure 4.1 Dimensional ranges of different classes of defects.
Theoretical Strength of Crystals

Once it was established that crystals deform by slip on specific crystallographic systems, physicists tried to calculate the strength of crystals. However, the agreement between their calculated strength and the experimental values were very poor (order of magnitude too high).

<table>
<thead>
<tr>
<th>Material</th>
<th>Theoretical strength, $\mu/2\pi$ (MPa)</th>
<th>Experimental strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>4200</td>
<td>0.7–0.8</td>
</tr>
<tr>
<td>Silver</td>
<td>4800</td>
<td>0.4–0.5</td>
</tr>
<tr>
<td>Copper</td>
<td>7700</td>
<td>0.5–3</td>
</tr>
<tr>
<td>Nickel</td>
<td>12,000</td>
<td>3–5</td>
</tr>
<tr>
<td>Iron</td>
<td>13,000</td>
<td>25–30</td>
</tr>
<tr>
<td>SiC*</td>
<td>23,000</td>
<td>11,000</td>
</tr>
<tr>
<td>$\text{Al}_2\text{O}_3$*</td>
<td>20,000</td>
<td>19,000</td>
</tr>
<tr>
<td>Diamond (C)*</td>
<td>46,000</td>
<td>21,000</td>
</tr>
</tbody>
</table>

*Estimated from deformation under hydrostatic compression (e.g., indentation hardness testing).
Consider the following arrangement shown and assume that the 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...). At each equilibrium position, it is assumed that $\tau = 0$. Plastic deformation will occur when the applied shear stress ($\tau_{app}$) is large enough to overcome these barriers. Atoms will 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:

$$\tau = K \sin\left(\frac{2\pi x}{b}\right)$$

Where $K$ is a constant that describes the amplitude of the shear stress (sine wave) and $b$ is the period of the sine wave. For small displacements Hooke’s Law applies:

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

Solving for $K$

$$K = G\frac{b}{2\pi a} = \tau_{Max}$$

Where $b$ is the distance between atoms on lines of contact and $a$ is the distance between planes.

Consider a face centered cubic (fcc) crystal. The relationship between the lattice parameter ($a_o$) and the interplanar spacing ($d$) is given by:

$$b = \frac{a_o}{\sqrt{2}}$$

$$d = \frac{a_o}{\sqrt{h^2 + k^2 + l^2}}$$
For FCC crystals, shear will occur in the (111) plane

\[ \tau_{\text{Max}} = G \frac{a_o \sqrt{3}}{2\pi a_o \sqrt{2}} = \frac{G}{5.13} \]

For most cubic crystals, \( a \) and \( b \) are of the same order of magnitude and

\[ \tau_{\text{Max}} \approx \frac{G}{2\pi} \]

\[ d = \frac{a_o}{\sqrt{3}} \]

Theoretical and experimental yield strengths in various Materials

<table>
<thead>
<tr>
<th>Material</th>
<th>( \frac{G}{2\pi} ) (MPa)</th>
<th>( \frac{G}{2\pi} ) (10^6 psi)</th>
<th>MPa</th>
<th>psi</th>
<th>( \tau_{\text{Max}} ) ( \text{exp.} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silver</td>
<td>12.6</td>
<td>1.83</td>
<td>0.37</td>
<td>55</td>
<td>~3 \times 10^4</td>
</tr>
<tr>
<td>Aluminum</td>
<td>11.3</td>
<td>1.64</td>
<td>0.78</td>
<td>115</td>
<td>~1 \times 10^4</td>
</tr>
<tr>
<td>Copper</td>
<td>19.6</td>
<td>2.84</td>
<td>0.49</td>
<td>70</td>
<td>~4 \times 10^4</td>
</tr>
<tr>
<td>Nickel</td>
<td>32</td>
<td>4.64</td>
<td>3.2-7.35</td>
<td>465-1,065</td>
<td>~1 \times 10^4</td>
</tr>
<tr>
<td>Iron</td>
<td>33.9</td>
<td>4.92</td>
<td>27.5</td>
<td>3,990</td>
<td>~1 \times 10^3</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>54.1</td>
<td>7.85</td>
<td>71.6</td>
<td>10,385</td>
<td>~8 \times 10^2</td>
</tr>
<tr>
<td>Niobium</td>
<td>16.6</td>
<td>2.41</td>
<td>33.3</td>
<td>4,830</td>
<td>~5 \times 10^2</td>
</tr>
<tr>
<td>Cadmium</td>
<td>9.9</td>
<td>1.44</td>
<td>0.57</td>
<td>85</td>
<td>~2 \times 10^4</td>
</tr>
<tr>
<td>Magnesium (basal slip)</td>
<td>7</td>
<td>1.02</td>
<td>39.2</td>
<td>5,685</td>
<td>~2 \times 10^4</td>
</tr>
<tr>
<td>Magnesium (prism slip)</td>
<td>7</td>
<td>1.02</td>
<td>39.2</td>
<td>5,685</td>
<td>~2 \times 10^4</td>
</tr>
<tr>
<td>Titanium (prism slip)</td>
<td>16.9</td>
<td>2.45</td>
<td>13.7</td>
<td>1,385</td>
<td>~1 \times 10^3</td>
</tr>
<tr>
<td>Beryllium (basal slip)</td>
<td>49.3</td>
<td>7.15</td>
<td>1.37</td>
<td>200</td>
<td>~4 \times 10^4</td>
</tr>
<tr>
<td>Beryllium (prism slip)</td>
<td>49.3</td>
<td>7.15</td>
<td>52</td>
<td>7,540</td>
<td>~1 \times 10^3</td>
</tr>
</tbody>
</table>
Dislocations—Linear Defects

Dislocations are abrupt changes in the regular ordering of atoms, along a line (dislocation line) in the solid. They occur in high density and are very important in mechanical properties of material. They are characterized by the Burgers vector, found by doing a loop around the dislocation line and noticing the extra interatomic spacing needed to close the loop. The Burgers vector in metals points in a close packed direction.

Edge dislocations occur when an extra plane is inserted. The dislocation line is at the end of the plane. In an edge dislocation, the Burgers vector is perpendicular to the dislocation line.

Screw dislocations result when displacing planes relative to each other through shear. In this case, the Burgers vector is parallel to the dislocation line.
**Edge Dislocations**

It can be visualized as an extra half-plane.

\[ b \perp \zeta \]

\[ \hat{\zeta} \times \vec{b} \]

Points in direction of extra half plane
Motion of an Edge Dislocation

Shear stress

Burger’s Vector = \( b \)
The arrow joining the starting and ending atoms following this circuit is the Burgers vector, denoted by $\vec{b}$. 

Two other directional quantities characterize a dislocation: the direction of movement $\vec{\xi}$ and the direction of the line $\vec{M}$. 

For edge dislocations:

$$\vec{b} \perp \vec{\xi}, \quad \vec{M} \parallel \vec{b}, \quad \vec{M} \perp \vec{\xi}$$
The shear stress to maintain motion of an isolated dislocation in an absolutely pure crystal with no nearby dislocations is called the **Peierls stress**.

Its value is estimated at $\sim 10^{-8}G$, which is several orders of magnitude lower than the measured stress need to sustain slip in annealed metals. The presence of other dislocations and of impurities ranging from atoms to large agglomerates is responsible for the actual stress required to cause slip in real crystals.
Screw Dislocations

For a screw dislocation:

\[ \vec{b} \parallel \hat{\xi} \quad \vec{M} \perp \vec{b} \quad \vec{M} \parallel \hat{\xi} \]
Burger's Vector
Direction of screw dislocation
screw moves this way
"line"
Burger's Vector
Of screw
The magnitude of the Burgers vector, $b$, for the simple cubic lattice, whether screw or edge, is equal to the lattice parameter $a_o$, the slip direction is $[100]$, and the slip plane in which it moves is $(100)$. The notation for this Burgers vector is:

$$\vec{b}_{SC} = a_o [100] (100)$$

where the first term on the right is the magnitude of $b$, the second is the direction of $b$ and the last term designates the slip plane.
Mixed Dislocations

The exact structure of dislocations in real crystals is usually more complicated than the ones shown. Edge and screw dislocations are just extreme forms of the possible dislocation structures. Most dislocations have mixed edge/screw character.

To add to the complexity of real defect structures, dislocation are often split in "partial“ dislocations that have their cores spread out over a larger area.
The Burgers vector for the mixed dislocation is neither perpendicular nor parallel to the dislocation line but retains a fixed orientation in space consistent with the previous definitions for the pure edge and screw dislocations. The atomic arrangement around a mixed dislocation is difficult to visualize but the Burgers vector provides a convenient and useful description.
**Dislocation Loops**

Loops are closed curves whose periphery consists of a dislocation. The loop may or may not be planar. There are two varieties. In one type, the interior of the loop consists of atoms that have been shifted by one Burgers vector. The crystal structure at the interior plane of the loop is perfect.

The distortion caused by the shift of atoms is accommodated by the peripheral dislocation. This type of loop is called a *shear loop* because it is produced by the action of a shear stress on the slip plane.
The dislocation that forms the periphery of the shear loop is most easily understood by considering the loop to be a square rather than a circle on the slip plane. The magnitude of the shift is one atomic spacing in a simple cubic structure or the magnitude of the Burgers vector for other crystal types.

A remarkable feature of the loop, whether it be square or circular, planar or non-planar, is that it is characterized by a single Burgers vector. The Burgers vector is perpendicular to the pure edge portions of the loop and parallel to the pure screw components. Only the directions of $b$ are reversed between the negative and positive edge portions and the right-hand and left-hand parts. When a shear stress is applied to the slip plane, the loop expands outward on all sides.

*Fig. 6.5 Dislocations in a square loop (top) and in a circular loop (bottom)*
The other type, the loop is formed by the removal/addition of a disk of atoms from/between close-packed atomic planes. The periphery of these loops are also dislocations. This type of loop is called a **prismatic loop**. This type is fundamentally different from the shear loop; the only features the two types have in common is their circular shape and their ability to expand or contract radially.

The interstitial loop consists of a disk-shaped layer (seen end-on in the figure) of atoms formed by assembling free interstitial atoms from the bulk solid. The atom-layer agglomeration is thermodynamically more stable than the same number of atoms dispersed in the lattice as self-interstitials.

![Fig. 6.6 The two types of prismatic loops](image)
Vacancy loops are formed by the collapse of a disk of vacancies on a close-packed plane. In common with the interstitial loop, the periphery of the vacancy loop is a circular edge dislocation with a Burgers vector perpendicular to the plane of the loop. However, the Burgers vectors of the two types are of opposite sign.

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Shear loop</th>
<th>Prismatic loop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Location</td>
<td>On slip plane</td>
<td>Between close-packed planes</td>
</tr>
<tr>
<td>Peripheral dislocation type</td>
<td>Mixed</td>
<td>Edge</td>
</tr>
<tr>
<td>Central portion of loop</td>
<td>Perfect crystal lattice</td>
<td>Stacking fault</td>
</tr>
<tr>
<td>Mechanism of growth</td>
<td>Shear stress</td>
<td>Absorption of point defects</td>
</tr>
<tr>
<td>Orientation of Burgers vector</td>
<td>Parallel to loop</td>
<td>Perpendicular to loop</td>
</tr>
</tbody>
</table>
Dislocations can annihilate one another!

Non-overlapping edges create vacancies.
Overlapping edges create interstitials.
Climb and Cross Slips of dislocations

Dislocations are capable of leave its slip plane via two mechanisms: a dislocation climb (for edge dislocations) and cross slip (for screw dislocations.

The presence of obstacles in the solid such as precipitates, voids, grain boundaries and others, can effectively halt dislocation glide (or slip). If a mobile dislocation is pushed by a shear stress into one of these obstructions, one of three events occur:
1. The mobile dislocation is stopped
2. The mobile dislocation literally “cuts through” the obstacle
3. The mobile dislocation moves to another slip plane that is parallel to the original slip plane, on which it can continue to glide.

The ability of a dislocation to evade the obstacles in its path is crucial to plastic deformation; if dislocations did not possess this flexibility, they would quickly become immobile.
Figure 7.12  Dislocation motion past a particle either (a) without or (b), (c), (d) with cross slip. The Burgers vector in (b), (c), (d) is denoted by b. (After Hirsch and Humphreys (1969). Physics of Strength and Plasticity p 189 M. I. T. Press.)

From Hall and Bacon 4th Ed
For an edge dislocation, movement from one slip plane to a parallel one requires movement call *climb*. In this mechanism, the extra half plane of atoms that constitutes the dislocation literally grows or shrinks. It does so by absorbing vacancies or interstitials from the bulk solid.

![Diagram showing dislocation movement](image)

Because climb requires mobility of vacancies in the lattice, it is active only at high temperatures (say 1/3 of the melting point and higher) while slip has no temperature dependence and is the sole mechanism of edge dislocation movement at room temperature.
Dislocation Density

To define the quantity of dislocations within a material, the dislocation density is given as:

\[
\rho_\perp = \frac{\text{Total Length of the dislocations}}{\text{Volume}} = \frac{L_\perp}{V} = \frac{\text{Number of Dislocations}}{\text{Area}} = \frac{N_\perp}{A}
\]

Consider the TEM showing 20 dislocations taken from a foil 200nm thick. The total area of the micrograph is 1.5μm and 1.25μm and the total length of the dislocations is about 15μm.

\[
\rho_\perp = \frac{L_\perp}{V} = \frac{15 \times 10^{-6}}{1.5 \times 10^{-6} \times 1.25 \times 10^{-6} \times 200 \times 10^{-9}} = 4 \times 10^{13} \text{ m}^{-2}
\]

\[
\rho_\perp = \frac{N_\perp}{A} = \frac{20}{1.5 \times 10^{-6} \times 1.25 \times 10^{-6}} = 1.1 \times 10^{13} \text{ m}^{-2}
\]