Dislocations and grain boundaries

Dislocations:

The idea of lattice defects caused by the motion of dislocations was published in 1943 independently by Taylor, Orowan, and Polanyi.

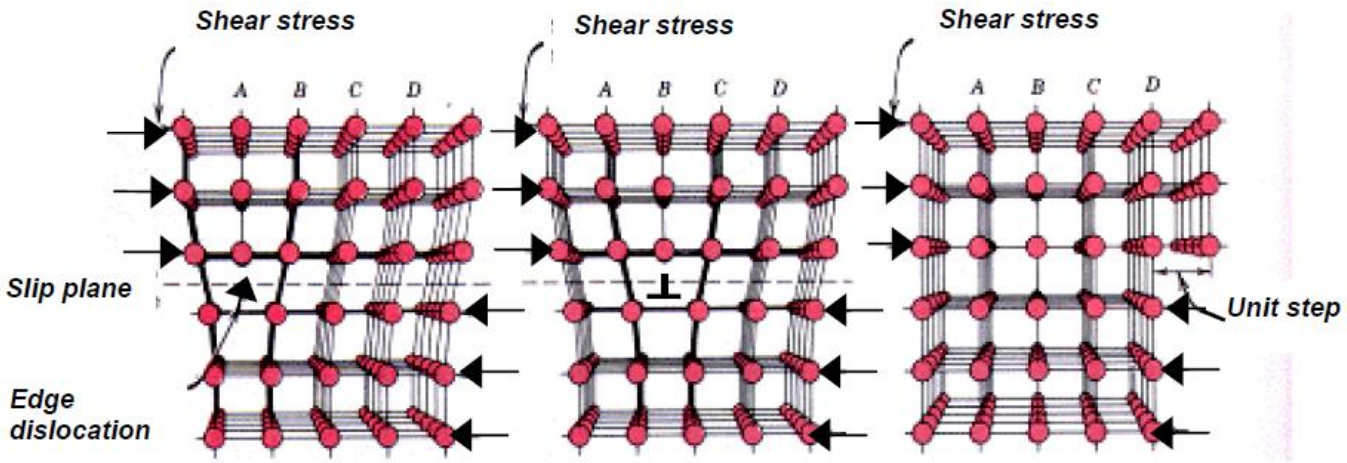
Interpretation of the plastic mechanical properties of crystalline solids in terms of theory of dislocations.

Two main types of dislocation exist: edge and screw. Dislocations found in real materials typically are *mixed*.

Edge dislocations

An edge dislocation is a defect where an extra half-plane of atoms is introduced midway through the crystal, distorting nearby planes of atoms.

When enough force is applied from one side of the crystal structure, this extra plane passes through planes of atoms breaking and joining bonds with them until it reaches the **grain boundary**.



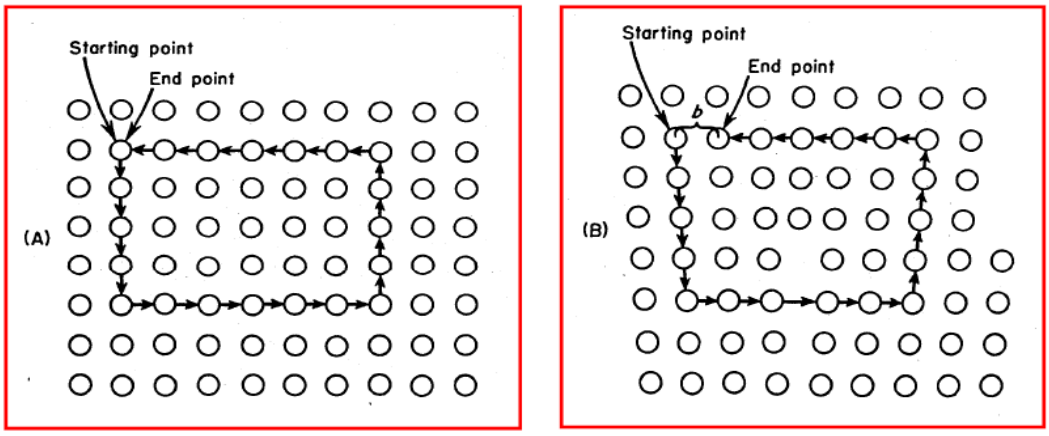
Burgers vector (b)

Vector b characterizes the magnitude and direction of a given dislocation

Determination:

1- choose, arbitrary, a positive direction
2- Draw a counterclockwise (RHS) circle of atom-to-atom steps.

3- Vector b connecting the end point to the starting point is Bugers vector of the dislocation.



In an edge dislocation, the Burgers vector is perpendicular to the line direction

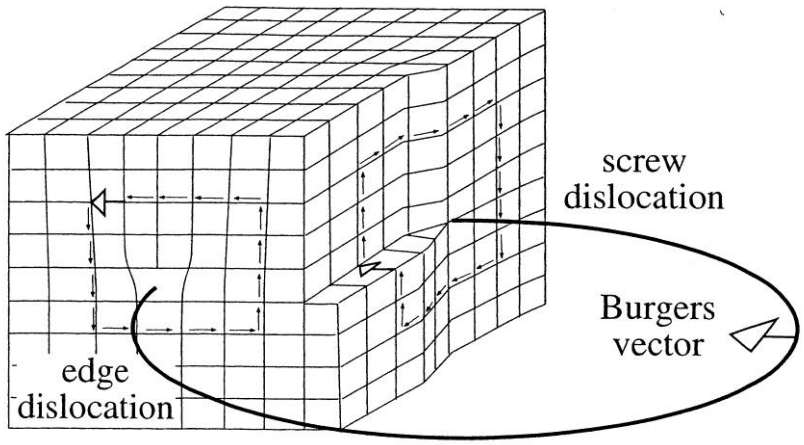
The stresses caused by an edge dislocation are complex due to its inherent asymmetry.

Screw dislocations

- Cutting a crystal along a plane and slipping one half across the other by a lattice vector, the halves fitting back together without leaving a defect.

If the cut only goes part way through the crystal, and then slipped, the boundary of the cut is a screw dislocation.

In pure screw dislocations, the Burgers vector is parallel to the line direction.



Stress field of dislocations (elastic properties of dislocations)

Screw dislocation:

The stresses caused by a screw dislocation are less complex than those of an edge dislocation.

These stresses need only one equation, as symmetry allows only one radial coordinate to be used:

The corresponding shear stress in an elastic continuum is: $\tau_{\theta z} = \mu b/2\pi r$

where μ is the shear modulus of the material (see table .1 chapter 21, Kittel, edition 8) , b is the Burgers vector, and r is a radial coordinate.

This equation suggests a long cylinder of stress radiating outward from the cylinder and decreasing with distance.

Energy of dislocations:

The total elastic energy per unit length of a screw dislocation is found on integration to be

$$E_{screw} = 1/2 \int_{r_0}^{r_1} \tau_{\theta z}\, b dr = \frac{\mu b^2}{4\pi} ln \frac{r_1}{r_0}$$

Where r_1 and r_0 are appropriate upper and lower limits for the variable r. A reasonable value of r_0 is comparable to the magnitude b of the Burgers vector or to the lattice constant; the value of r_1 cannot exceed the dimensions of the crystal.

$$E_{edge} = \frac{\mu b^2}{4\pi(1-\nu)} ln \frac{r_1}{r_0}$$

where r_1 and r_0 are appropriate upper and lower limits for the variable r. A reasonable value of r_0 is comparable to the magnitude *b* of the Burgers vector or to the lattice constant; the value of r_1 cannot exceed the dimensions of the crystal.

Crystals contain many dislocations, and dislocations tend to form configurations in which the superimposed long range stress fields cancel out!

Forces between dislocations:

The force experienced by a dislocation due to another at a distance x on the slip plane may be given by:

$$F = \frac{\mu b^2}{2\pi(1-\nu)x}$$

where μ is the shear modulus of the material, b is the Burgers vector. The poisson ratio $\nu \approx 0.3$ for most crystals.

Screw dislocations of opposite sign attract and those of the same sign repel

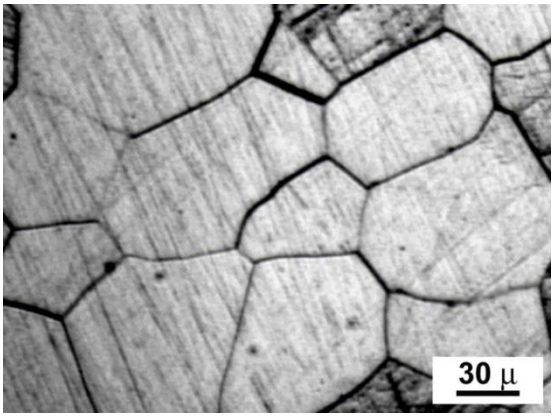
The magnitude of the attractive/repulsive force is inversely proportional to the distance between them.

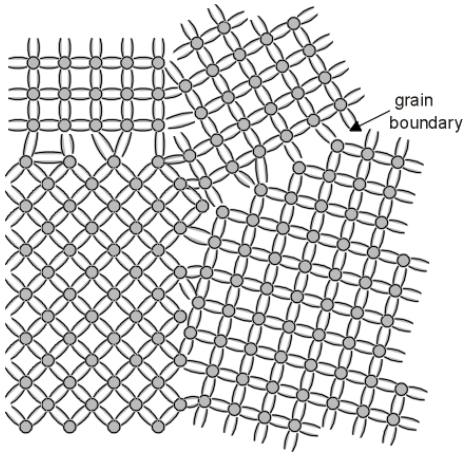
Edge dislocations: dislocations on the same slip plane attract each other if they are of opposite signs and repel if of the same sign.

Grain boundaries

Grain boundaries are the most important from the **mechanical properties point of view**.

Crystalline solids generally consist of millions of individual grains separated by boundaries, where each grain (or subgrain) is a **single crystal**.



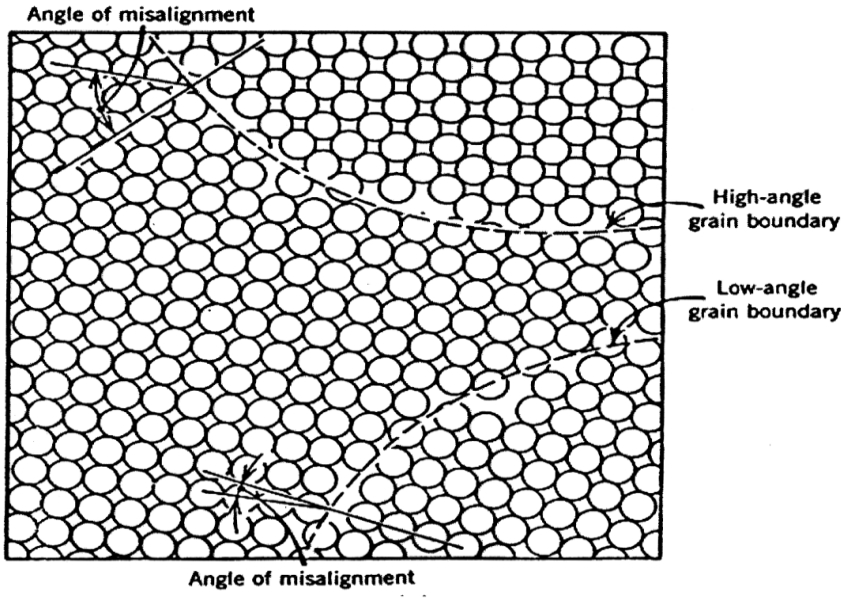


A **grain boundary** is the interface between two grains, or crystallites, in a polycrystalline material

Within each individual grain there is a **systematic packing of atoms**. Therefore each grain has **different orientation** and is separated from the neighboring grain by grain boundary.

When the **misorientation between two grains is small**, the grain boundary can be described by a relatively simple configuration of dislocations (e.g., an edge dislocation wall) and is called a **low-angle boundary**.

When the misorientation is large (high-angle grain boundary), more complicated structures are involved.



These **transition regions** (grain boundaries) may consist of various kinds of **dislocation arrangements**.

Tilt and Twist Boundaries

The simplest grain boundary consists of a configuration of edge dislocations between two grains.

The misfit in the orientation of the two grains is accommodated by a perturbation of the regular arrangement of crystals in the boundary region.

Figure shows some vertical atomic planes termination in the boundary and each termination is represented by an edge dislocation.

a) b)

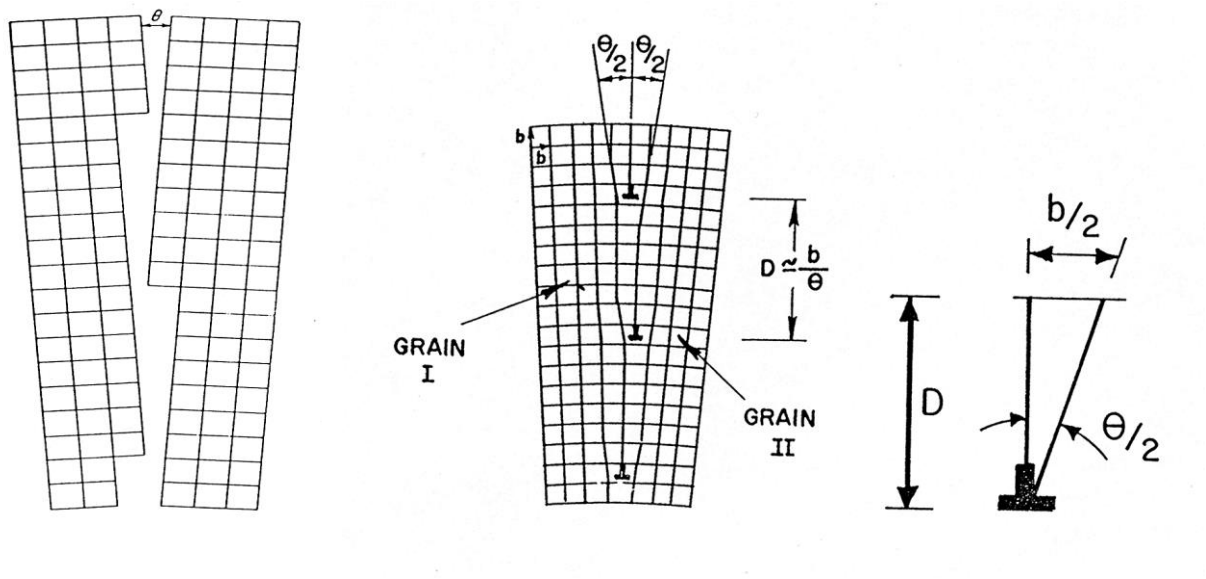


Diagram of low-angle grain boundary. (a) Two grains having a common [001] axis and angular difference in orientation (b) two grains joined together to form a low-angle grain boundary made up of an array of edge dislocations.

The misorientation at the boundary is related to spacing between dislocations, *D*, by the following relation:

$$D = \frac{b}{2\sin\left(\frac{\theta}{2}\right)} \approx \frac{b}{\theta} \quad \text{(for } q \text{ very small)}$$

where b is the Burgers vector.

A more precise expression for energy of low angle-grain boundary over range of $0 < \theta < 10°$ may be given by:

$$E = \frac{\mu b}{4\pi(1-\upsilon)}\theta(A - ln\theta)$$

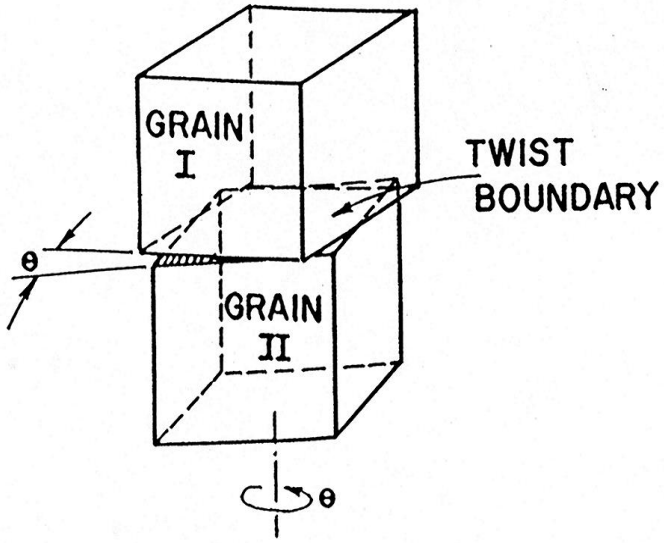
where A is a constant. This is valid over range $0 < \theta < 10°$.

As the misorientation θ increases, the spacing between dislocations is reduced, until, at large angles; the description of the boundary in terms of simple dislocation arrangements does not make sense.

A boundary consisting entirely of **screw dislocations** is called **twist boundary**, because the misorientation can be described by a relative rotation of two grains about an axis.

Figure shows a twist boundary consisting of two groups of screw dislocations.

It is possible to produce misorientations between grains by combined tilt and twist boundaries. In such a case, the grain boundary structure will consist of a network of edge and screw dislocations.



Low-angle twist boundary