Grain Boundaries
In the last four lectures, we dealt with point defects (e.g. vacancy, interstitials, etc.) and line defects (dislocations).

There is another class of defects called interfacial or planar defects:

- They occupy an area or surface and are therefore bidimensional.
- They are of great importance in mechanical metallurgy.

Examples of these form of defects include:

- grain boundaries
- twin boundaries
- anti-phase boundaries
- free surface of materials

Of all these, the grain boundaries are the most important from the mechanical properties point of view.
• Crystalline solids (most materials) generally consist of millions of individual grains separated by boundaries.

• Each grain (or subgrain) is a single crystal.

• Within each individual grain there is a systematic packing of atoms. Therefore each grain has different orientation (see Figure 16-1) and is separated from the neighboring grain by a 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, fittingly, called a low-angle boundary.
Figure 16.1. Grains in a metal or ceramic; the cube depicted in each grain indicates the crystallographic orientation of the grain in schematic fashion.
• When the misorientation is large (high-angle grain boundary), more complicated structures are involved (as in a configuration of soap bubbles simulating the atomic planes in crystal lattices).

• The grain boundaries are therefore:
  – where grains meet in a solid.
  – transition regions between the neighboring crystals.
  – Where there is a disturbance in the atomic packing, as shown in Figure 16-2.

• These transition regions (grain boundaries) may consist of various kinds of dislocation arrangements.
Figure 16.2. At the grain boundary, there is a disturbance in the atomic packing.
• In general, a grain boundary has five degrees of freedom.

• We need **three degrees** to specify the **orientation of one grain with respect to the other**, and

• We need the other **two degrees** to specify the **orientation of the boundary** with respect to one of the grains.

• Grain structure is usually specified by giving the average diameter or using a procedure due to ASTM according to which grains size is specified by a number $n$ in the expression $N = 2^{n-1}$, where $N$ is the number of grains per square inch when the sample is examined at 100x.
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 (one on each side of the boundary) is accommodated by a perturbation of the regular arrangement of crystals in the boundary region.
- Figure 16.3 shows some vertical atomic planes termination in the boundary and each termination is represented by an edge dislocation.
Figure 16.3. Low-angle tile boundary.
Figure 16-3(b). Diagram of low-angle grain boundary. (a) Two grains having a common [001] axis and angular difference in orientation of $\theta$ (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:

$$D = \frac{b}{2 \sin \left( \frac{\theta}{2} \right)} \approx \frac{b}{\theta} \quad \text{(for $\theta$ very small)} \quad (16-1)$$

where $b$ is the Burgers vector.

• As the misorientation $\theta$ 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.
• For such a case, $\theta$ becomes so large that the dislocations are separated by one or two atomic spacing;
  – the dislocation core energy becomes important and the linear elasticity does not hold.
  – Therefore, the grain boundary becomes a region of severe localized disorder.

• Boundaries consisting entirely of edge dislocations are called tilt boundaries, because the misorientation, as can be seen in Figure 16.3, can be described in terms of a rotation about an axis normal to the plane of the paper and contained in the plane of dislocations.
The example shown in figure 16.3 is called the symmetrical tilt wall as the two grains are symmetrically located with respect to the boundary.
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 16.4 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.
Figure 16.4. Low-angle twist boundary.
Grain Boundaries and Deformation

Figure 5.5. (a) Schematic atomic model of a grain boundary. (b) Dislocation model of a grain boundary.