(a) Ashby’s model of deformation of a polycrystal.

(b) Polycrystal deforms in macroscopic uniform way, produces overlap, and voids at boundaries. These can be corrected by introducing geometrically necessary dislocations at (c) and (d). Note that statistical dislocations are not shown.
where $M$ is an orientation factor (the reciprocal of the Schmid factor). For a polycrystal the orientation factor $M$ varies from grain to grain.

The best estimate for an fcc lattice is $\overline{M} = 3.1$, obtained by G. I. Taylor based on the use of the von Mises compatibility condition and assuming that all grains undergo the same deformation as the overall deformation.

$$\tau = \sigma \sin x \cos x = \frac{\sigma}{M} \quad 5-1$$

$$\sigma \, d\varepsilon = \sum_{i=1}^{n} \tau \, d\gamma_{i} \quad 5-2$$
Calculation of the Energy of a Grain Boundary

- The dislocation model of grain boundary can be used to compute the energy of low-angle boundaries ($\theta \leq 10^\circ$).

- For such boundaries the distance between dislocations in the boundary is more than a few interatomic spaces, as:

$$\frac{b}{D} \approx \theta \leq 10^\circ \approx \frac{1}{6} \text{rad} \quad \text{or} \quad D \approx 6b$$  \hspace{1cm} (16-2)
Consider a tilt boundary consisting of edge dislocations with spacing $D$. Let us isolate a small portion of dimension $D$, as in Figure 16.5, with a dislocation at its center.

The energy associated with such a portion, $E$, includes contributions from the regions marked I, II, and III in figure 16.5.
Figure 16.5. Model for the computation of grain boundary energy.
- $E_I$ is the energy due to the material inside the dislocation core of radius $r_I$.

- $E_{II}$ is the energy contribution of the region outside the radius and inside the radius $R = KD > b$, where $K$ is constant less than unity.

- In this region II, the elastic strain energy contributed by other dislocations in the boundary is very small.

- $E_{II}$ is mainly due to the plastic strain energy strain energy associated with the dislocation in the center of this portion.
• $E_{III}$, the rest of the energy in this portion, depends on the combined effects of all dislocations.

• The total strain energy per dislocation in the boundary is, then,

\[ E_{\perp} = E_I + E_{II} + E_{III} \quad (16-3) \]

• Consider now a small decrease, $d\theta$, in the boundary misorientation. The corresponding variation in the strain energy is

\[ dE_{\perp} = dE_I + dE_{II} + dE_{III} \quad (16-4) \]
The new dimensions of this crystal portion are shown in Fig. 16-6.

The region immediately around the dislocation, contributing an energy $E_I$, does not change.

This region does not change because $E_I$, the localized energy of atomic misfit in the dislocation core, is independent of the disposition of other dislocations.

\[
-\frac{d\theta}{D} = \frac{dD}{D} = \frac{dR}{R} \quad (as \ R = KD)
\]
Figure 16-6. New dimensions of a portion of crystal after a decrease $d\theta$ in the boundary misorientation.
• Thus, \( \text{d}E_I = 0 \). \( E_{\text{II}} \) increases by a quantity \( \text{d}E_{\text{II}} \), corresponding to an increase in \( R \) by \( \text{d}R \).

• \( E_{\text{III}} \), however, does not change with an increase in \( D \), because although the volume of region III increases, the number of dislocations contributing to the strain energy of this region decreases.
Role of Grain Boundaries

- Grain boundaries have very important role in plastic deformation of polycrystalline materials.

- We outline below the important aspects of the role of grain boundaries.

1. At low temperature (T<0.5T_m, where T_m is the melting point in K), the grain boundaries act as strong obstacles to dislocation motion. Mobile dislocations can pile up against the grain boundaries and thus give rise to stress concentrations that can be relaxed by initiating locally multiple slip.
2. There exists a condition of compatibility among the neighboring grains during the deformation of polycrystals; that is, if the development of voids or cracks is not permitted, the deformation in each grain must be accommodated by its neighbors.

- This accommodation is realized by multiple slip in the vicinity of the boundaries which leads to a high strain hardening rate.

- It can be shown, following von Mises, that for each grain to stay in contiguity with others during deformation, there must be operating at least five independent slip systems - Taylors Theorem.
• This condition of strain compatibility leads a polycrystalline sample to have multiple slip in the vicinity of grain boundaries.

• The smaller the grain size, the larger will be the total boundary surface area per unit volume.

• In other words, for a given deformation in the beginning of the stress-strain curve, the total volume occupied by the work-hardened material increases with the decreasing grain size.

• This implies a greater hardening due to dislocation interactions induced by multiple slip.
3. At high temperatures the grain boundaries function as sites of weakness.

- Grain boundary sliding may occur, leading to plastic flow and/or opening up of voids along the boundaries.

4. Grain boundaries can act as sources and sinks for vacancies at high temperatures, leading to diffusion currents as, for example, in the Nabarro Herring creep mechanism.

5. In polycrystalline materials, the individual grains usually have a random orientation with respect to one another.
• The term **polycrystalline** refers to any material which is composed of many individual grains.

• However, some materials are actually used in their **single crystal** state: silicon for integrated circuits and nickel alloys for aircraft engine turbine blades are two examples.

• The sizes of individual grains vary from submicrometer (for nanocrystalline structures) to millimeters and even centimeters (for materials especially processed for high-temperature creep resistance).

• Figure 16.7 shows typical equiaxed grain configurations for polycrystalline tantalum and titanium carbide.