Phase Transformation of Materials

Nong-Moon Hwang

Oct. 28, 2008

3.3 Boundaries in Single-Phase Solids

Consider an orientation relation between two grains in contact.
The grain boundary structure depends on this orientation relation.

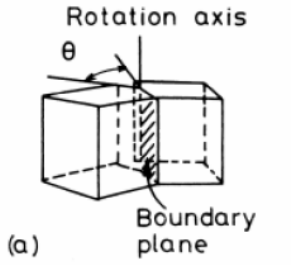
3 degrees of freedom in misorientations between two grains in contact
2 degrees of freedom in orientations of the boundary plane
→ 5 degrees of freedom

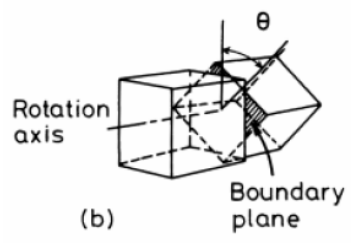
The lattices of any two grains can be made to coincide by rotating one of them through a suitable angle about a single axis.
→ misorientation (θ)

A tilt boundary → the axis of rotation is parallel to the plane of the boundary

A twist boundary → the axis is perpendicular to the boundary

3.3 Boundaries in Single-Phase Solids





tilt boundary

θ → misorientation
→ tilt angle

twist boundary

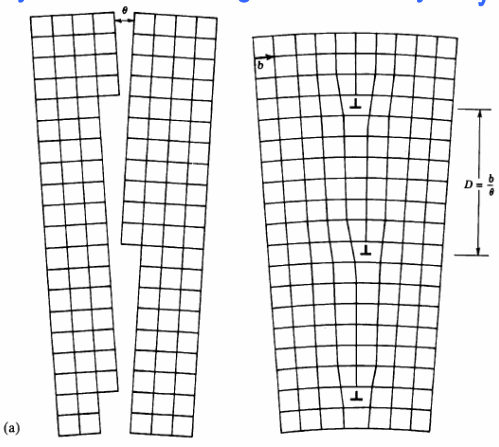
θ → misorientation
→ twist angle

- symmetric tilt or twist boundary
- non-symmetric tilt or twist boundary

3.3.1 Low-Angle and High-Angle Boundaries

Low-Angle Boundaries

Symmetrical low-angle tilt boundary



Symmetrical low-angle twist boundary

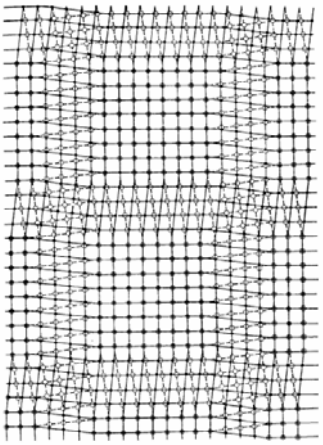


Fig. 3.7 (b)

Fig. 3. 7 (a) Low-angle tilt boundary, (b) low-angle twist boundary: ○ atoms in crystal below, ● atoms in crystal above boundary. (After W.T. Read Jr., *Dislocations in crystals*, McGraw-Hill, New York, 1953.)

Unsymmetric Tilt Boundary

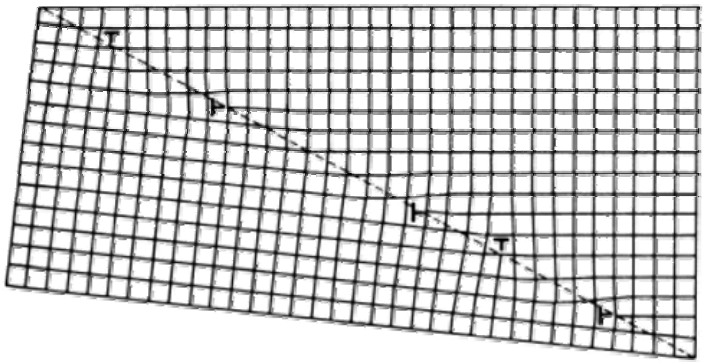


Fig. 3.8 An unsymmetric tilt boundary. Dislocations with two different Burgers vectors are present. (After W.T. Read Jr., Dislocations in Crystals, McGraw-Hill, New York, 1953.)

If the boundary is unsymmetrical, dislocations with different Burgers vectors are required to accommodate the misfit.

In general boundaries of a mixture of the tilt and twist type,
→ several sets of different edges and screw dislocations.

3.3.1 Low-Angle and High-Angle Boundaries

Low-Angle Boundaries

Tilt Boundary

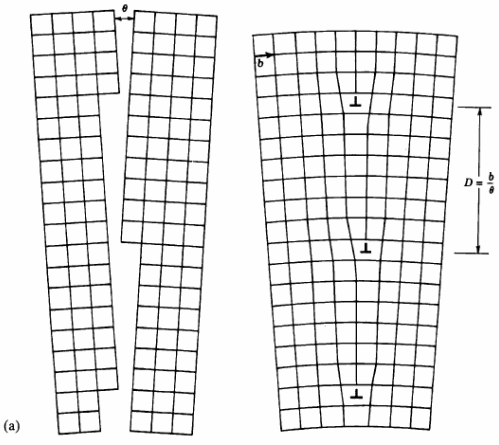
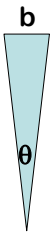


Fig. 3. 7 (a) Low-angle tilt boundary, (b) low-angle twist boundary: ○ atoms in crystal below, ● atoms in crystal above boundary. (After W.T. Read Jr., *Dislocations in crystals*, McGraw-Hill, New York, 1953.)



$$\sin\frac{\theta}{2} = \frac{b/2}{D}$$

$$\sin\frac{\theta}{2} \approx \frac{\theta}{2}$$

$$D \cong \frac{b}{\theta}$$

relation between D and γ ?

Density of dislocation in the boundary: 1/D

$$\gamma \propto 1/D = \frac{\theta}{b}$$

$$\gamma \propto \theta$$

Low-angle grain boundary : the total energy of the dislocations within unit area of boundary.

Grain boundary energy γ is approximately proportional to the density of dislocations in the boundary.

$$\gamma \propto \theta \propto 1/D, \quad D = b/\theta$$

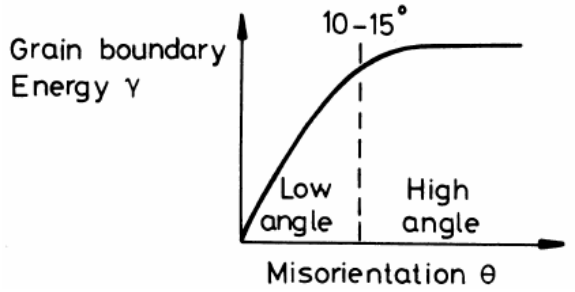


Fig. 3.9 Variation of grain boundary energy with misorientation (schematic).

High Angle Grain Boundary

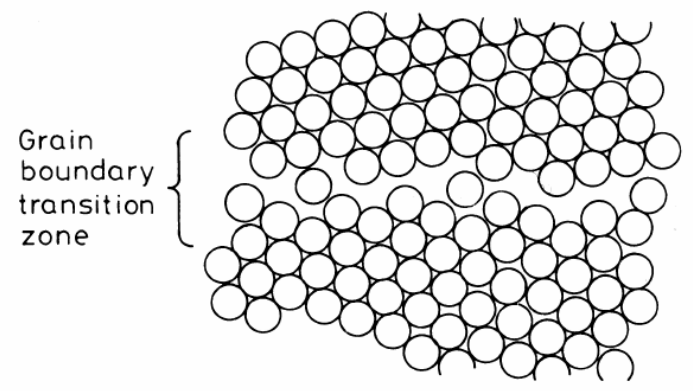


Fig. 3.10 Disordered grain boundary structure (schematic).

High angle boundaries contain large areas of poor fit and have a relatively open structure.

→ high energy, high diffusivity, high mobility (?) (cf. segregated gb)

Soap Bubble Model

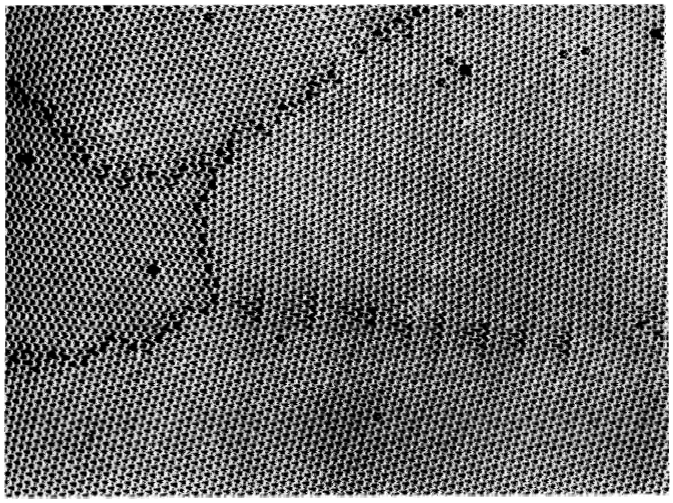


Fig. 3.11 Rafts of soap bubbles showing several grains of varying misorientation. Note that the boundary with the smallest misorientation is made up of a row of dislocations, whereas the high-angle boundaries have a disordered structure in which individual dislocations cannot be identified. (After P.G. Shewmon, *Transformations in Metals*, McGraw-Hill, New York, 1969, from C.S. Smith.)

Measured high-angle grain boundary energies

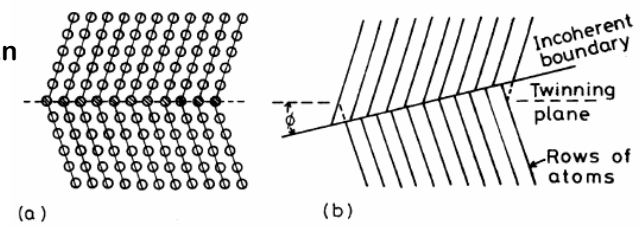
$$\gamma_b \simeq \frac{1}{3}\gamma_{sv}$$

Crystal	γ_b/mJ m^{-2}	T/°C	γ_b/γ_{sv}
Sn	164	223	0.24
Al	324	450	0.30
Ag	375	950	0.33
Au	378	1000	0.27
Cu	625	925	0.36
γ-Fe	756	1350	0.40
δ-Fe	468	1450	0.23
Pt	660	1300	0.29
W	1080	2000	0.41

Special High-Angle Grain Boundaries

Twin Boundary (Σ3)

Not all high-angle boundaries have an open disordered structure.



Special High-Angle Boundaries
→ significantly lower energies than the random boundaries

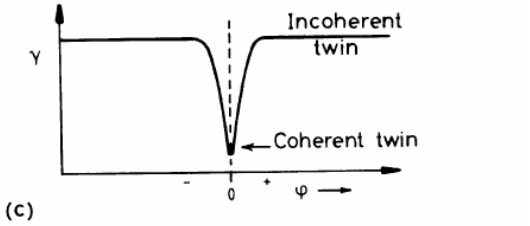


Fig. 3.12 (a) A coherent twin boundary. (b) An incoherent twin boundary. (c) Twin-boundary energy as a function of the grain boundary orientation.

Table 3.3 Measured Boundary Free Energies for Crystals in Twin Relationships (Units mJ m^{-2})

Crystal	Coherent twin boundary energy	Incoherent twin boundary energy	Grain boundary energy
Cu	21	498	623
Ag	8	126	377
Fe-Cr-Ni (stainless steel type 304)	19	209	835

Special High-Angle Grain Boundaries

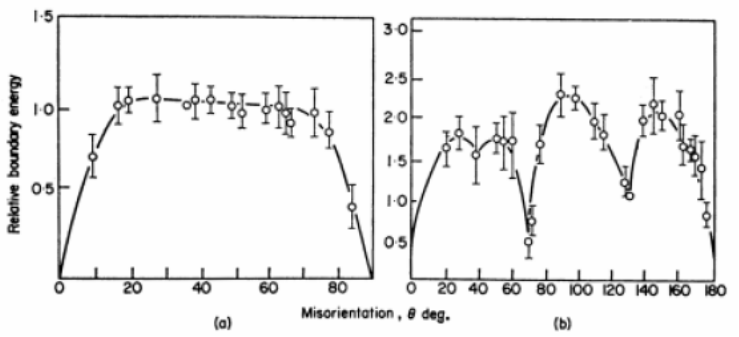


Fig. 3.13 Measured grain boundary energies for symmetric tilt boundaries in Al (a) When the rotation axis is parallel to <100>, (b) when the rotation axis is parallel to <110>. (After G. Hasson and C. Goux, Scripta Metallurgica, 5 (1971) 889.)

Why are there cusps in Fig. 3.13 (b)?

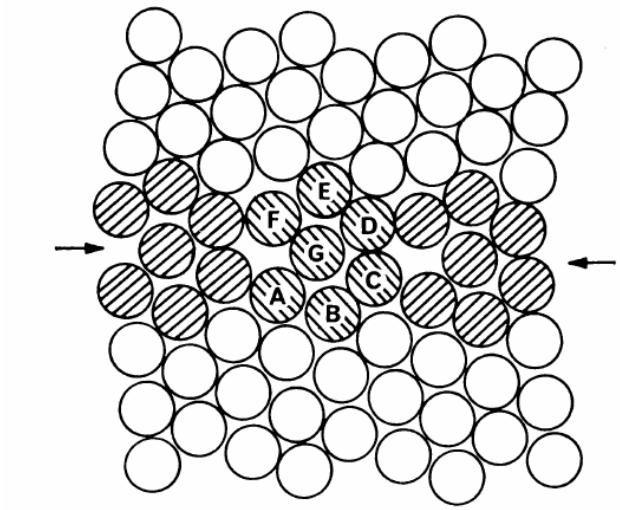


Fig. 3. 14 Special grain boundary. (After H. Gleiter, Physica Status Solidi (b) 45 (1971) 9.)

Equilibrium in Polycrystalline Materials

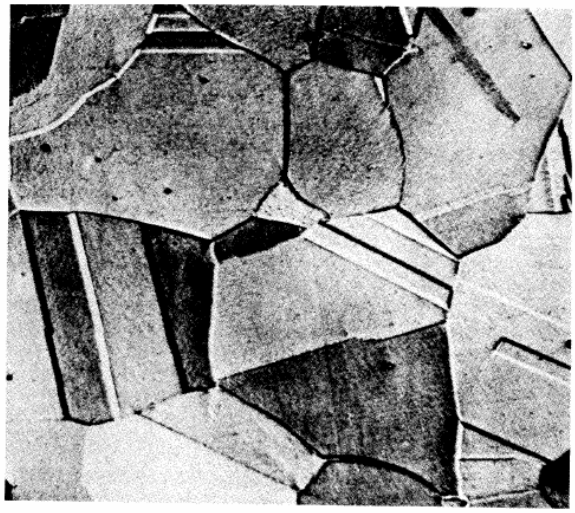


Fig. 3.15 Microstructure of an annealed crystal of austenitic stainless steel. (After P.G. Shewmon, Transformations in Metals, McGraw-Hill, New York, 1969)