Phase Transformation of Materials

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Equilibrium in Polycrystalline Materials

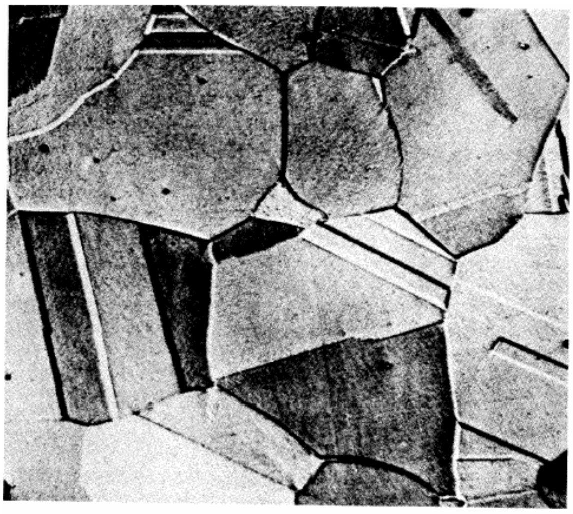
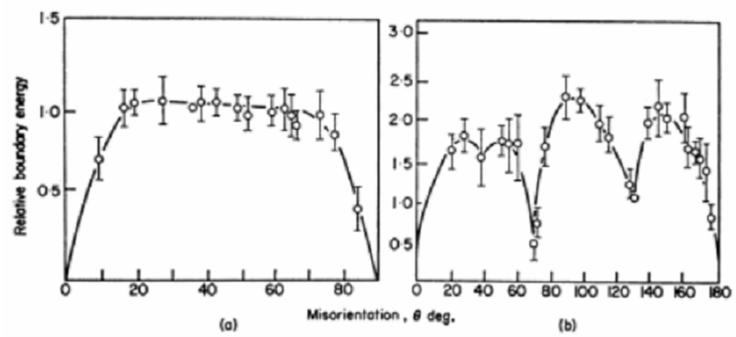
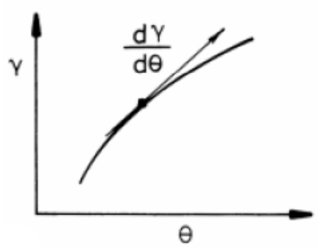


Fig. 3.15 Microstructure of an annealed crystal of austenitic stainless steel. (After P.G. Shewmon, Transformations in Metals, McGraw-Hill, New York, 1969)

Torque term





$$F = \frac{d\gamma}{d\theta} \quad \rightarrow \text{torque}$$

Torque term

γ: Energy/area = Force/length
– Surface Tension

$F_x = \gamma$ → **surface tension in x direction**

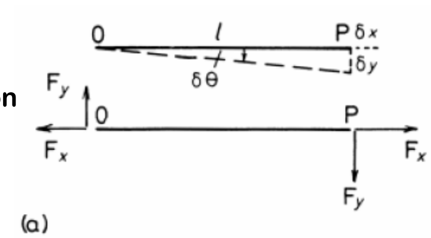
the work done for
the displacement of $\delta y \rightarrow F_y \delta y$

the increase in boundary energy
caused by the change in orientation δθ:

$$\rightarrow \ell \frac{d\gamma}{d\theta}\delta\theta \qquad F_y \delta y = \ell \frac{d\gamma}{d\theta}\delta\theta$$

Since $\delta y = \ell \delta\theta$, $\quad F_y = \dfrac{d\gamma}{d\theta}$

→ torque



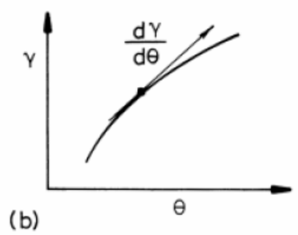


Fig. 3. 16 (a) Equilibrium forces F_x and F_y supporting a length l of boundary **OP**. (b) The origin of F_y.

Torque term

If the grain-boundary energy is dependent on the orientation of the boundary, a force dγ/dθ must be applied to the ends of the boundary to prevent it rotating into a lower energy orientation.

If γ_b is independent of orientation $\quad \dfrac{d\gamma}{d\theta} = 0$

Since the segment OP must be supported by forces F_x and F_y the boundary exerts equal but opposite forces $-F_x$ and $-F_y$ on the ends of the segment which can be junctions with other grain boundaries.

→ force balance at the triple junction or at the four grain corner

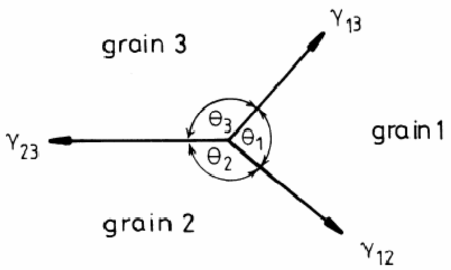


Fig. 3. 17 The balance of grain boundary tensions for a grain boundary intersection in metastable equilibrium.

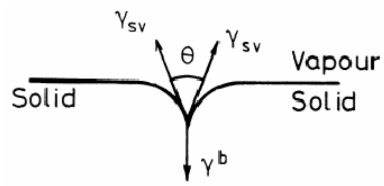


Fig. 3. 18 The balance of surface and grain boundary tensions at the intersection of a grain boundary with a free surface.

$$\frac{\gamma_{23}}{\sin\theta_1} = \frac{\gamma_{31}}{\sin\theta_2} = \frac{\gamma_{12}}{\sin\theta_3}$$

$$2\gamma_{SV}\cos\frac{\theta}{2} = \gamma_b$$

3.3.4. Thermally Activated Migration of Grain Boundaries

If the boundary is curved in the shape of cylinder, Fig. 3.20a, it is acted on by a force of magnitude γ/r towards its center of curvature.

Therefore the only way the boundary tension forces can balance in three dimensions is if the boundary is planar ($r = \infty$) or if it is curved with equal radii in opposite directions, Fig. 3.20b and c.

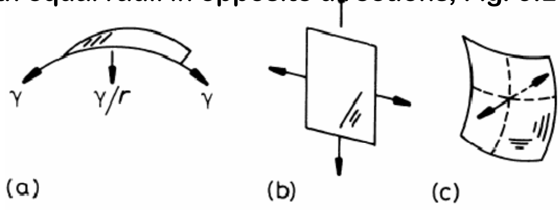


Fig. 3.20 (a) A cylindrical boundary with a radius of curvature r is acted on by a force γ/r. (b) A planar boundary with no net force. (c) A doubly curved boundary with no net force.

Direction of Grain Boundary Migration during Grain Growth

For isotropic grain boundary energy in two dimensions

Equilibrium angle at each boundary junction? →120°

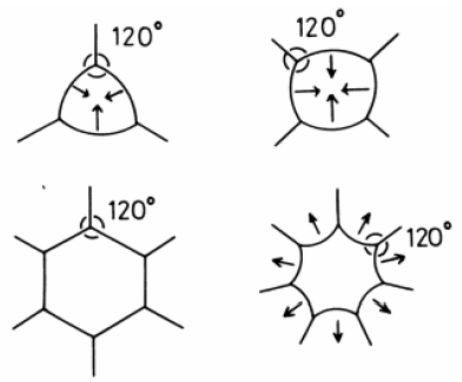


Fig. 3.21 Two-dimensional grain boundary configurations. The arrows in

Equilibrium angle at each boundary junction in 3D? →109°28'

Grain Growth (Soap Bubble Model)

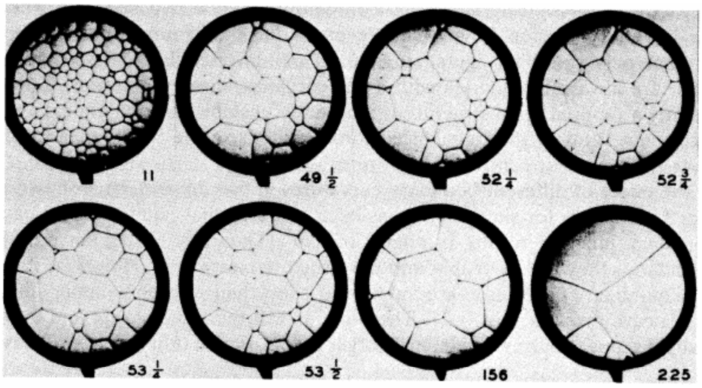


Fig. 3.22 Two-dimensional cells of a soap solution illustration the process of grain growth. Numbers are time in minutes. (After C.S. Smith, Metal Interfaces, American Society for Metals, 1952, p. 81.)

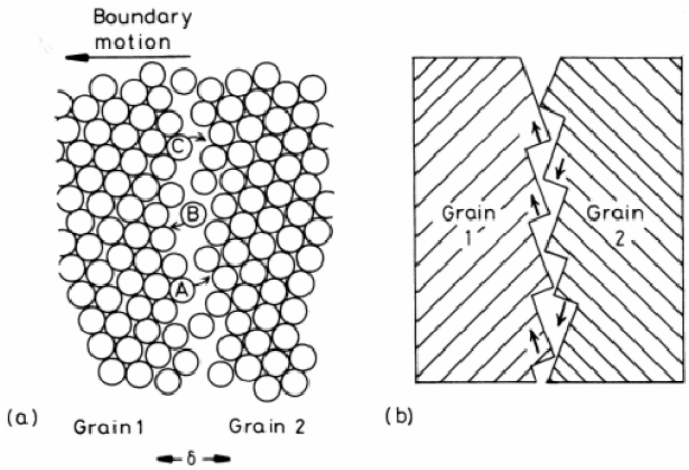


Fig. 3.23 (a) The atomic mechanism of boundary migration. The boundary migrates to the left if the jump rate from grain 1→ 2 is greater than 2 → 1. Note that the free volume within the boundary has been exaggerated for clarity. (b) Step –like structure where close-packed planes protrude into the boundary.

Pulling Force

Free energy released : $\Delta G \cdot \dfrac{\delta x}{V_m}$

$$\textit{Free Energy Released} = \Delta G \cdot \delta x / V_m = F \delta x$$

Pulling force per unit area of boundary : $F = \dfrac{\Delta G}{V_m} \quad (N\, m^{-2})$

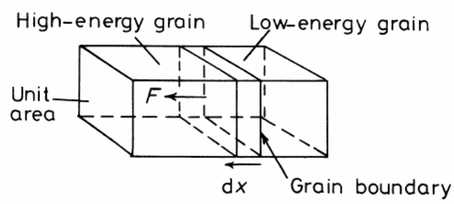


Fig. 3.25 A boundary separating grains with different free energies is subjected to a pulling force *F*.

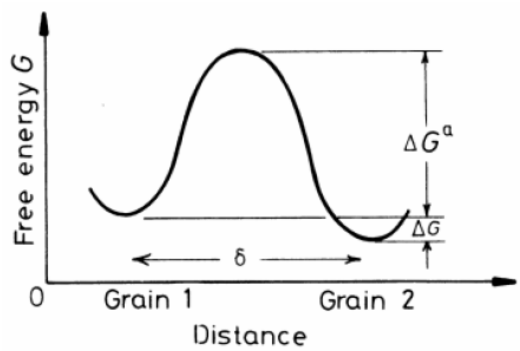


Fig. 3.24 The free energy of an atom during the process of jumping from one grain to the other.

Kinetics of Boundary Migration

From 1 to 2 : $A_2 n_1 v_1 \ \exp(-\Delta G^a / RT) \quad m^{-2} s^{-1}$

From 2 to 1 : $A_1 n_2 v_2 \ \exp -(\Delta G^a + \Delta G)/RT \quad m^{-2} s^{-1}$

Kinetics of Boundary Migration

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Effective Flux?

When $\Delta G = 0$, **there is no net boundary movement.**

$$A_1 n_2 v_2 = A_2 n_1 v_1$$

When $\Delta G \succ 0$, **there will be a net flux from grain 1 to 2.**

$$J_{net} = A_2 n_1 v_1 \ \exp\left(-\frac{\Delta G^a}{RT}\right)\left\{1 - \exp\left(-\frac{\Delta G}{RT}\right)\right\}$$

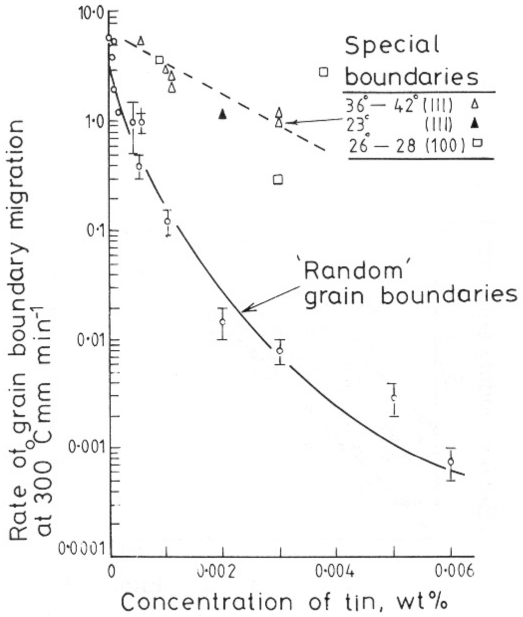
What is the velocity of the boundary?

If the boundary is moving with a velocity v, the above flux must also be equal to ? $J = C \cdot v \ \rightarrow v/(V_m/N_a)$

$$v = \frac{A_2 n_1 v_1 V_m{}^2}{N_a RT} \exp\left(-\frac{\Delta G^a}{RT}\right)\frac{\Delta G}{V_m}$$

$$or \quad v = M \cdot \Delta G / V_m$$

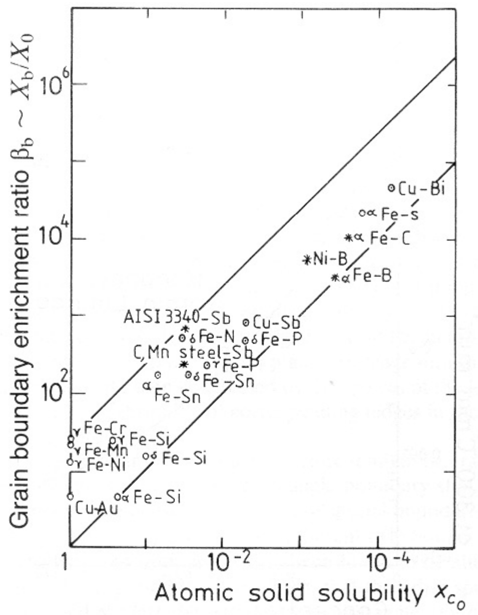
$$where \ M = \left\{\frac{A_2 n_1 v_1 V_m{}^2}{N_a RT} \exp\left(\frac{\Delta S^a}{R}\right)\right\} \exp\left(\frac{-\Delta H^a}{RT}\right)$$



ΔG_b: the free energy released per mole when a solute atom is moved from the matrix to the boundary

Grain Boundary Segregation

$$X_b = X_0 \exp\frac{\Delta G_b}{RT}$$



Phase Transformations in Metals and Alloys NRL of Charged Nanoparticles