EMA5001 Lecture 10
Grain Boundaries & Their Migration

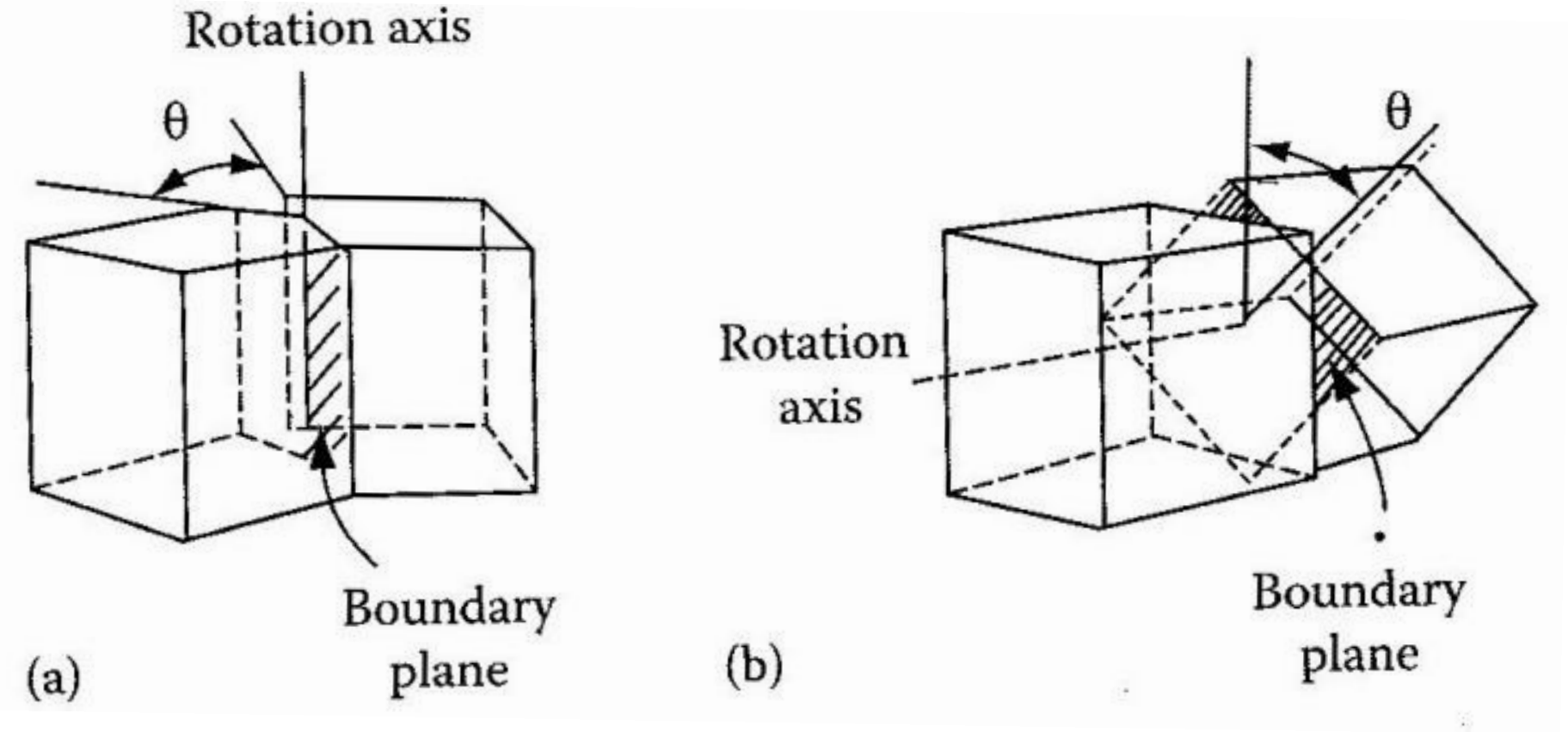
FLORIDA INTERNATIONAL UNIVERSITY

Grain Boundaries

- Two simplest Cases

Tilt boundary

Twist boundary



Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 122

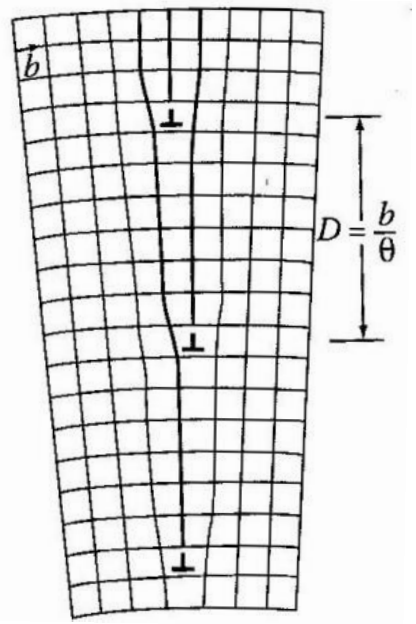
Small Angle Grain Boundaries

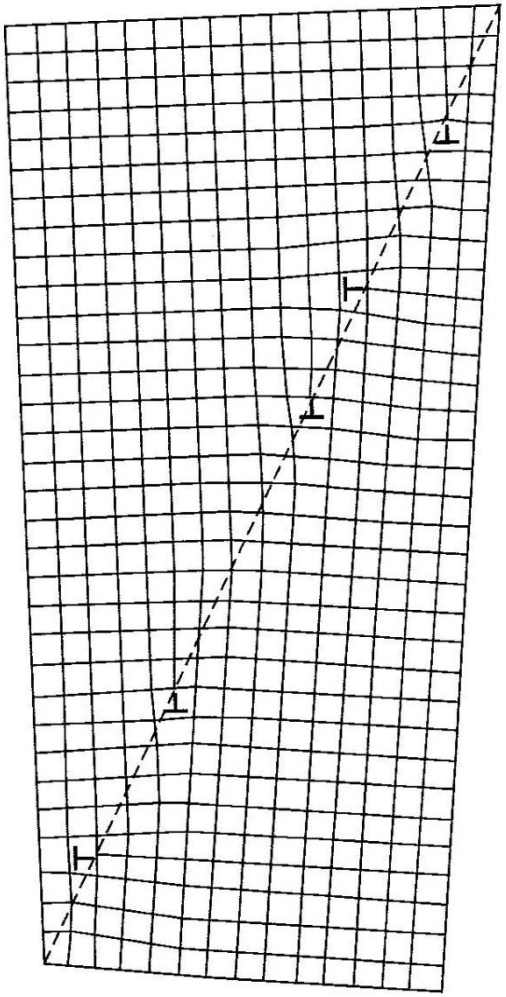
- **Low angle tilt boundary**
  - An array of parallel edge dislocations w/ Burger's vector b
  - If the tilt angle is θ
  - Distance between dislocations D

$$D = \frac{b}{Sin\,\theta} \approx \frac{b}{\theta}$$

- **Low angle twist boundary**
  - Two sets of screw dislocations

- **Asymmetrical low angle grain boundaries**
  - Dislocations w/ different Burgers' vectors





Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 122-123

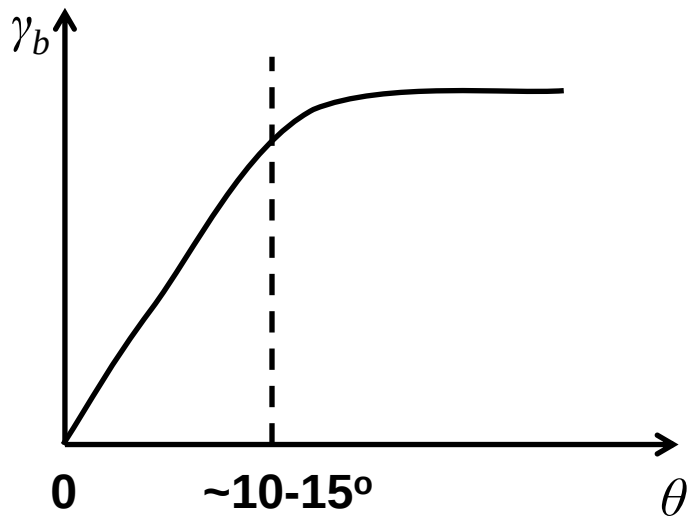
Grain Boundary Energy vs. Misorientation

- **Grain boundary (excess) free energy γ_b depends on misorientation (or tilt) angele θ**
  - At small angle θ < ~10-15°
    - Poor fit only occurs at dislocation cores
    - γ_b equals total energy of dislocation per unit area (per unit length normal to dislocations)

$$\gamma_b \propto \frac{1}{D} \approx \frac{\theta}{b}$$

    - We have $\gamma_b \propto \theta$
  - At angle θ > ~10-15°
    - Relatively open structure and large areas of poor fit in grain boundaries
    - Experiments found relatively constant grain boundary energy

$$\gamma_b \approx \frac{1}{3}\gamma_{SV}$$

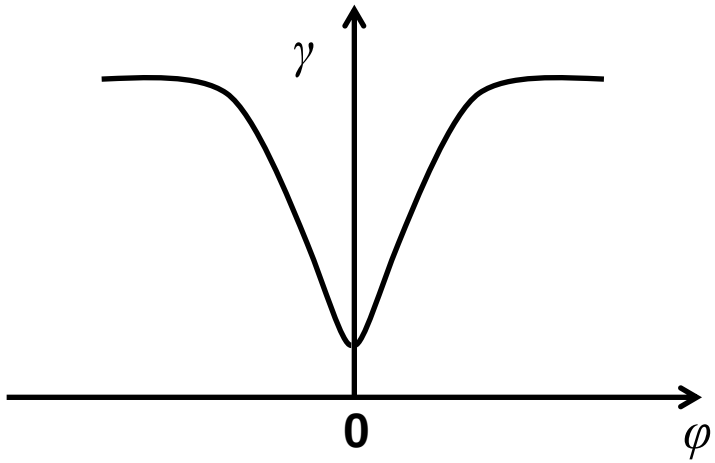


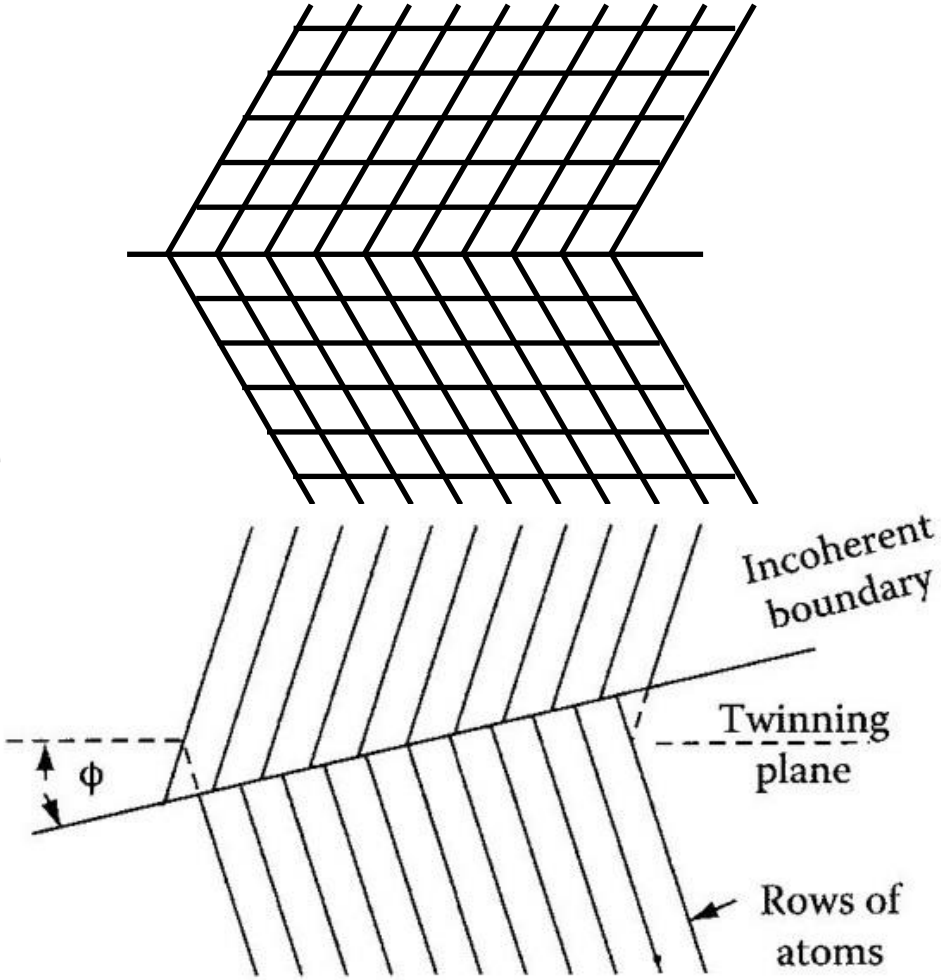
Material	γ_b (mJ/m²)	T (°C)	γ_b/γ_{SV}
Sn	164	223	0.24
Al	324	450	0.30
Cu	625	925	0.36
W	1080	2000	0.41

Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 126

Coherent & Incoherent Grain (Twin) Boundaries (1)

- **Coherent twin boundary**
  - High angle grain boundary
  - Very low (excess) energy due to very little mismatch
- **Incoherent twin boundary**
  - Twin boundary off from twinning plane
  - Energy variation has large dependenc on angle

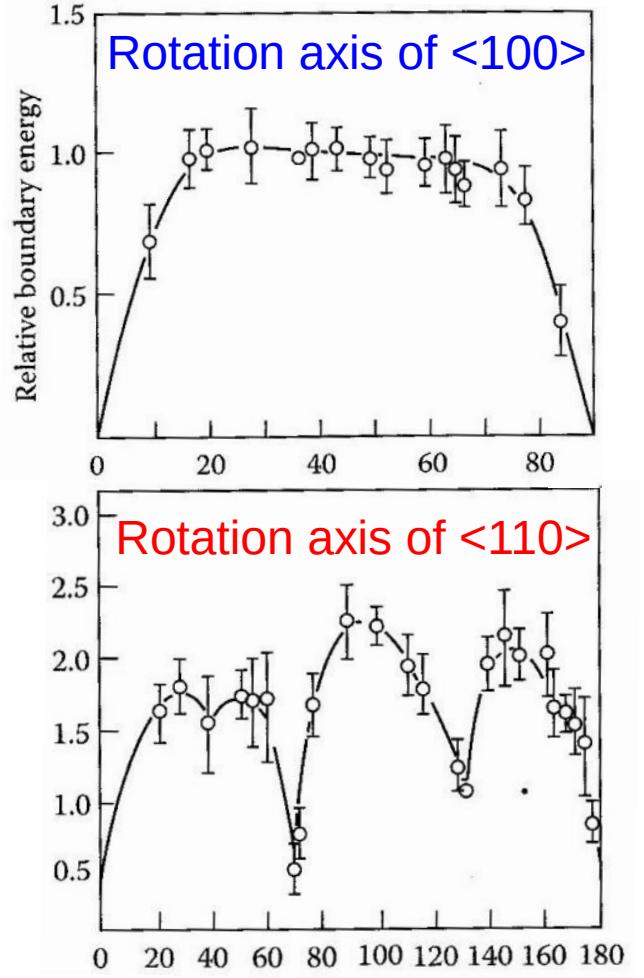


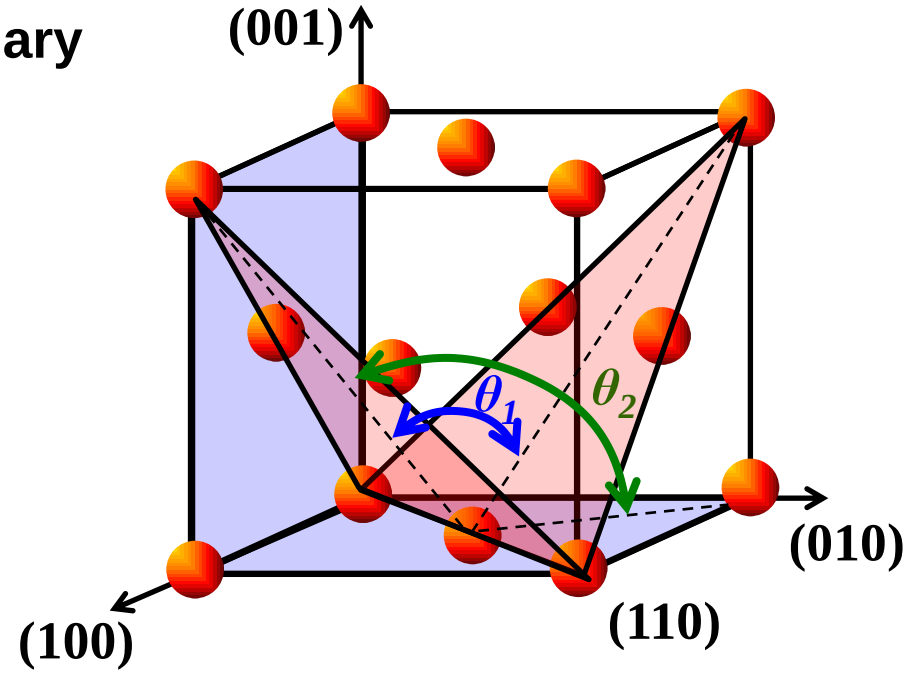


Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 122-127

Coherent & Incoherent Grain (Twin) Boundaries (2)

- Variation of measured grain boundary energy vs. misorientation





$$\theta_1 = 2 \cdot arctg\left(\frac{\sqrt{2}}{2}\right) = 2 \times 35.26^{O} = 70.5^{O}$$

$$\theta_2 = 180 - (90^{O} - \frac{\theta_1}{2}) = 90^{O} + 35.26^{O} = 125.3^{O}$$

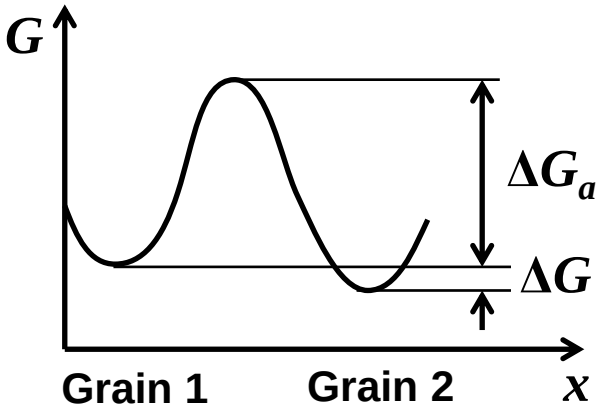
Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 128

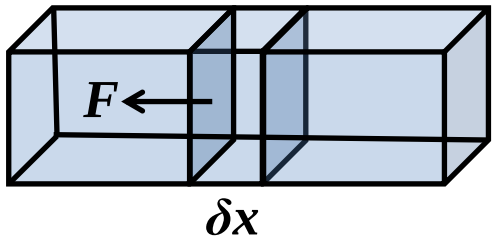
Grain Boundaries Migration & Its Driving Force

- **Grain boundaries are high energy regions (w/ excess energy)**

  Annealing may produce re-arrangement or movement of grain boundaries

- **Interface migration comes from atoms movement from higher energy state (grain/phase) to lower energy state**
  - δx Interface displacement
  - ΔG Difference in molar free energy in grain 1 vs. grain 2 per molar
  - V_m Molar volume





Unit area

Free energy change associated with movement of δx for **unit area of GB** $\Delta G \cdot \dfrac{\delta x \cdot 1}{V_m}$

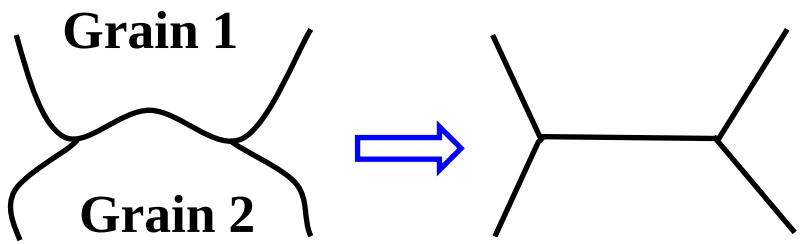
Equivalent work if F is driving force per unit area $W = F \cdot \delta x = \Delta G \dfrac{\delta x}{V_m}$

Driving force for grain boundary migration $F = \dfrac{\Delta G}{V_m}$ in the unit of N/m^2

Driving Force for Straightening of Grain Boundaries

- **Straightening of grain boundaries**

  Initial grain boundary may be curved → Total energy $A\gamma$ tends to minimize interface (grain boundary) area → Straightening of the grain boundaries



- **Driving force for straightening of interface (due to interface curvature)**

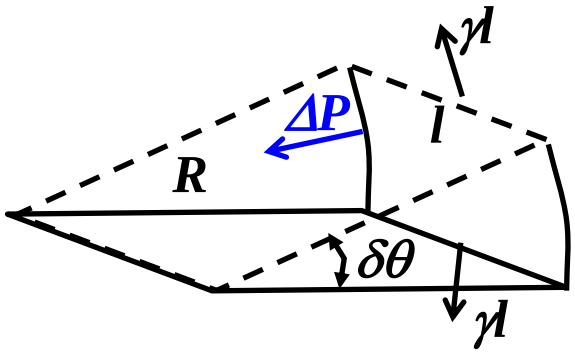
  For curved interface or GB, interface/surface tension tries to flatten it, which drives it towards the center

  The driving force (i.e., change in pressure) $\Delta P = \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right)$

  If $R_1 = R_2 = r$ → $\Delta P = \frac{2\gamma}{r}$

  The equivalent driving force for straightening of grain boundaries per unit area will be

$$F = \frac{\Delta G}{V_m} = \Delta P = \frac{2\gamma}{r}$$

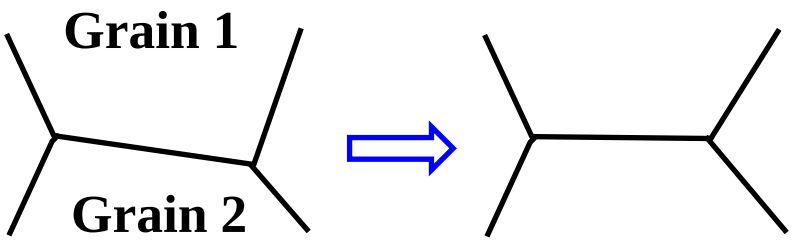


$$2\gamma \cdot l \cdot Sin\frac{\delta\theta}{2} = \Delta P \cdot (R \cdot \delta\theta) \cdot l$$

Driving Force for Rotation of Grain Boundaries

❑ Rotation of grain boundaries

Initial grain boundaries may not be at the lowest orientation between different grains → Rotation of grain boundaries



❑ Driving force for rotation of grain boundaries

For boundary length l and unit length width

If a grain boundary rotates by θ

Free energy change due to GB rotation

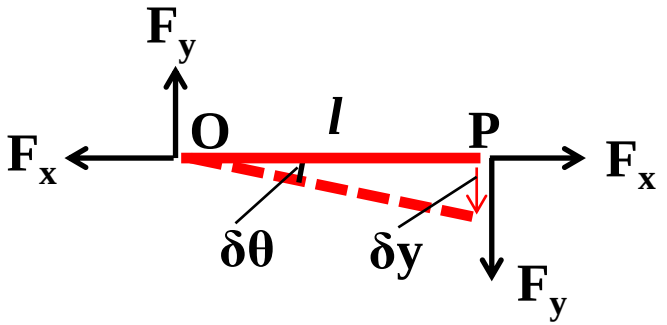
$$\delta\gamma = l \cdot \frac{d\gamma}{d\theta} \cdot \delta\theta$$

Assume force F_y on GB, equivalent work done in the rotation process

$$W = F_y \delta y = l \cdot \frac{d\gamma}{d\theta} \cdot \delta\theta = \delta\gamma$$

Because $\delta y = l \cdot \delta\theta$, we have

$$F = \frac{\Delta G}{V_m} = F_y = \frac{d\gamma}{d\theta}$$



F_y tends to drive the boundary rotating towards a low energy position (cusp)

Examples of Shape of Grain Boundaries (1)

- **Three grains come together in equilibrium**

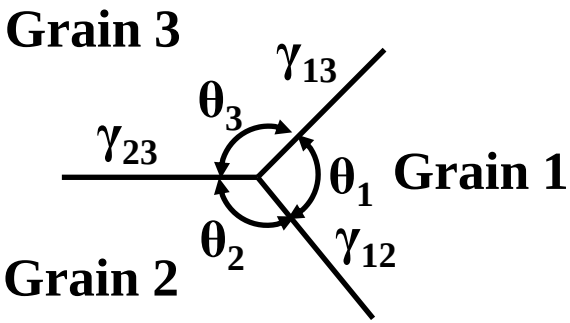
  If interface energy is independent of orientation $\frac{d\gamma}{d\theta}=0$

  Equilibrium requires: $\frac{\gamma_{23}}{Sin\theta_1}=\frac{\gamma_{13}}{Sin\theta_2}=\frac{\gamma_{12}}{Sin\theta_3}$

  If in the same phase $\theta_1+\theta_2+\theta_3=2\pi$

  We have $\gamma_{23}=\gamma_{13}=\gamma_{12}$

  $$\theta=\frac{2}{3}\pi=120^\circ$$

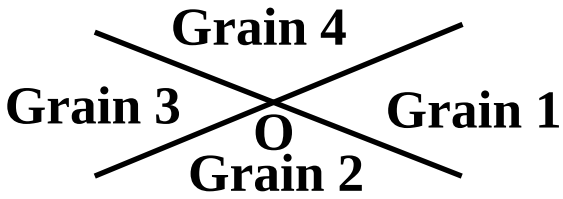


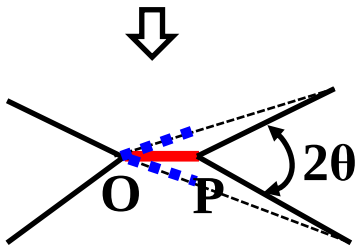
- **There will NOT be four (4) grains meeting in the same edge**

  If O moves by a small distance l_{OP} to P,

  $$\Delta E=\gamma l_{OP}-2\gamma\left(l_{OP}Cos\theta\right)$$

  $$\Delta E=\gamma l_{OP}\left(1-2Cos\theta\right)$$

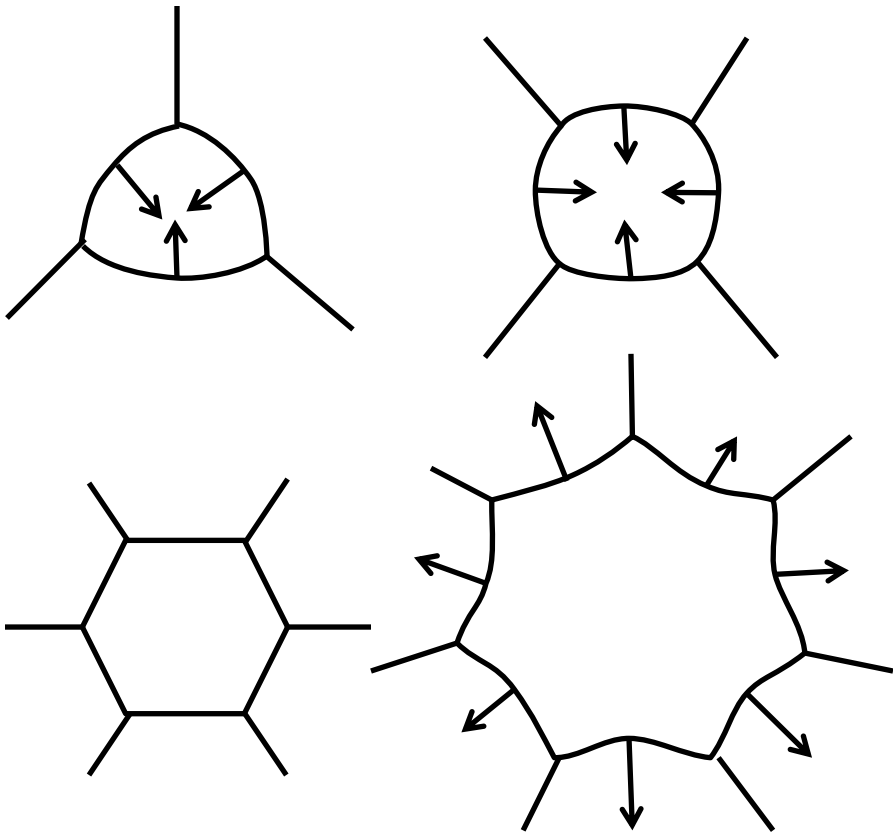




When $\theta<60^o$, $\Delta E<0$ → four grain edge will disappear

Examples of Shape of Grain Boundaries (2)

- **For single phase polycrystalline material, to reach equilibrium:**
  - Angle at three grains to reach 120^o → Curved grain boundaries for some grains
  - Minimize interface area → Straightening of the grain boundaries



- **Consequences**
  - Grains with <6 interfaces tend to shrink
  - Grains with >6 interfaces tend to grow

- **Thermal activation**
  - Grain boundary migration is also a thermal activated process

Example of Grain Growth Kinetics

- **For growth of grains**

  Assuming mean radius of curvature equals average grain diameter $r = \overline{D}$

  M is mobility of grain boundary motion

  F is driving force for grain boundary movement

  Grain growth velocity

$$v = \frac{d\overline{D}}{dt} = M \cdot F = M \cdot \frac{2\gamma}{\overline{D}}$$

  Integrate and consider $\overline{D} = \overline{D}_0$ when t = 0, we have $\overline{D}^2 = \overline{D}_0^2 + kt$

  Or

$$\boxed{\overline{D}^2 - \overline{D}_0^2 = kt}$$

  Typical grain growth $\overline{D}^n - \overline{D}_0^n = kt \qquad n < 2$

Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 122

Grain Boundary Segregation

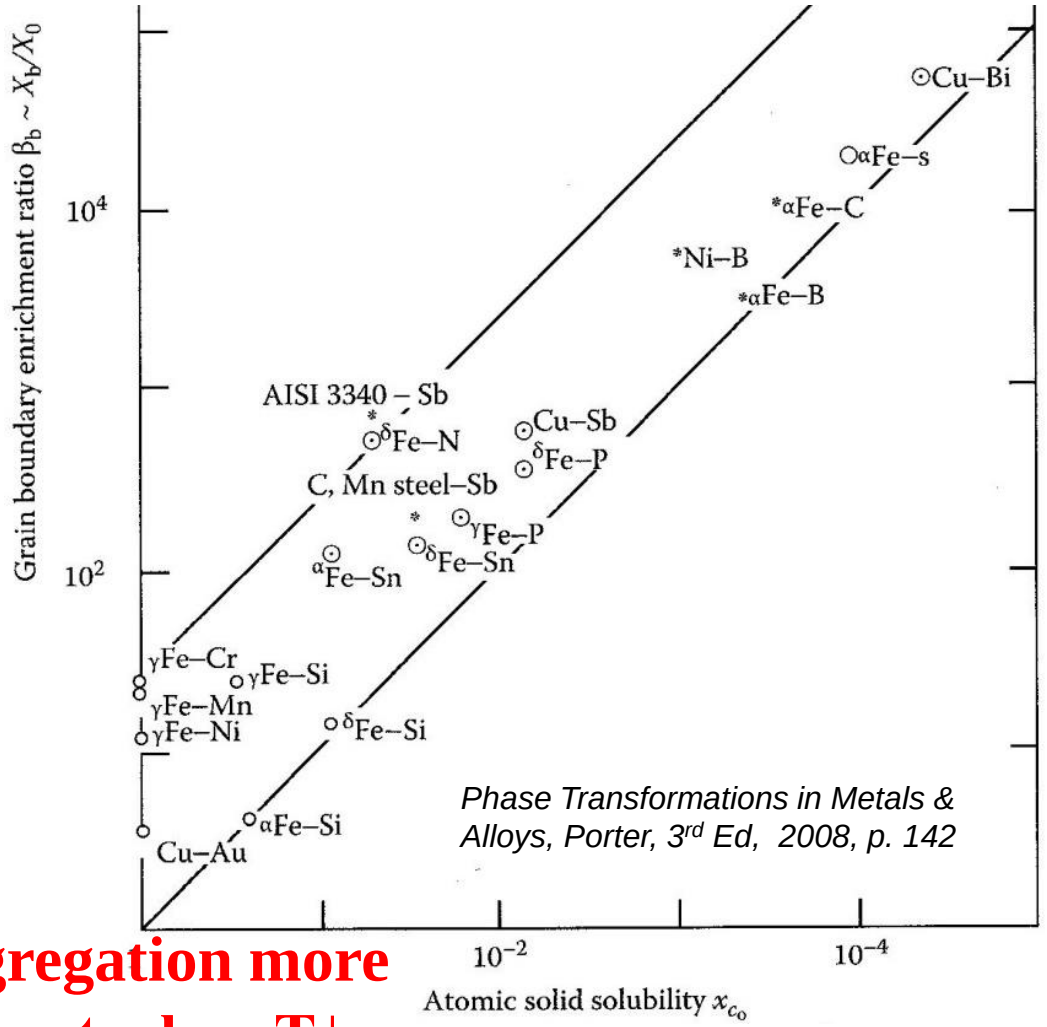
- **Grain boundary energy is <u>often</u> reduced in alloying**

  Solute atoms cause lattice strain → solute atoms move to grain boundaries w/ more open structure, lowering strain energy

  - X_b atom fraction in grain boundary
  - X_0 atom fraction in grain
  - ΔG_b molar free energy <u>released</u> when <u>solute</u> atoms move from grain to grain boundary (typically >0)
  - β_b GB segregation coefficient

  For dilute solution (alloy)

$$\beta_b = \frac{X_b}{X_0} = \exp\left(\frac{\Delta G_b}{RT}\right)$$



Phase Transformations in Metals & Alloys, Porter, 3rd Ed, 2008, p. 142

GB segregation more significant when T↓ or solubility↓

Homework

- Porter 3rd Exercise 3.1, 3.3, 3.7