3.40J / 22.71J
Modern Physical Metallurgy

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Lecture 10 NOTES: 3D Defects I

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3D Defects:

- Grain boundaries: Nonplanar regions of dislocations, lattice mismatch
- Inclusions
- Voids
- Precipitates (2^{nd} phases)

Continued on next page.

3D Defects:

- Grains are 3D
- Grains are formed via: (1) solidification; (2) annealing after high strain
  Cover these topics in Kinetic Processes

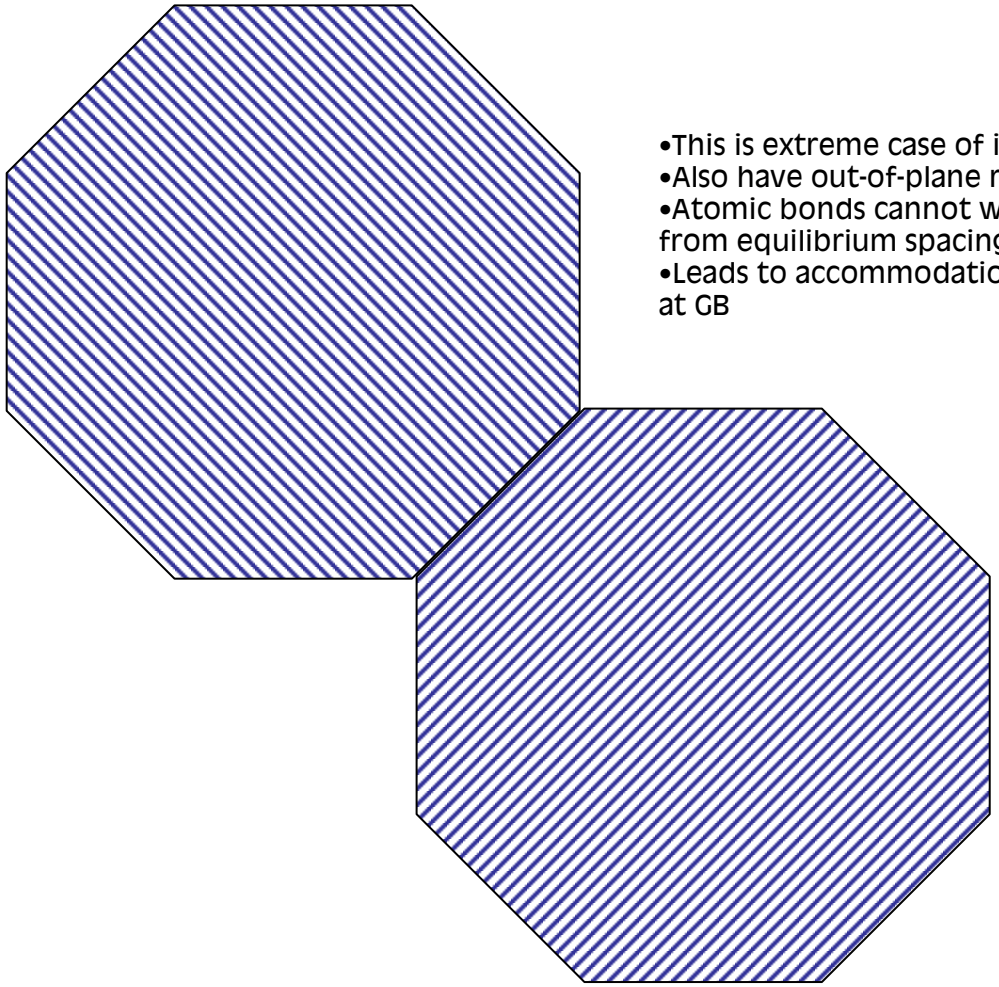
Lord Kelvin (1887):
Minimize surface area/volume
And surface tension via shape called
tetrakaidecahedron:
14 sides; 24 corners; 36 edges

Not exactly right:
Equal surface tension → 3 meeting grains form
120°, which TKDH does not.

This space-filling argument is general, and could also apply to atomic packing.

3D Defects:

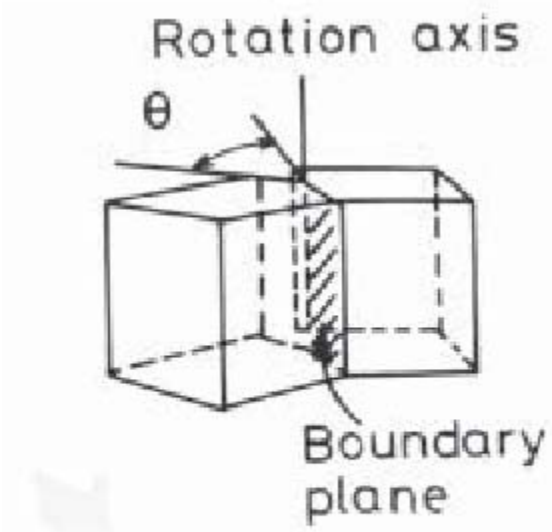
- Each grain is a single crystal
- Each single crystal contains many, many unit cells
- When 2 single crystals meet at an interface, they will be mismatched both in and out of plane



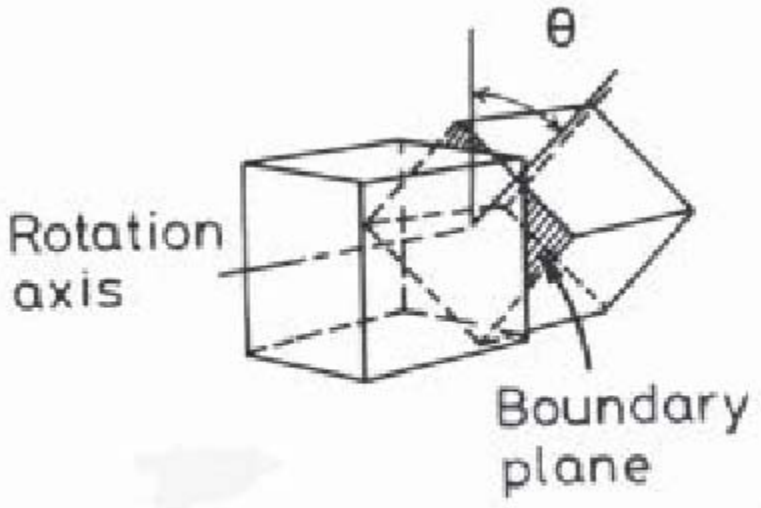
- This is extreme case of in-plane mismatch.
- Also have out-of-plane rotation.
- Atomic bonds cannot withstand such deviations from equilibrium spacing.
- Leads to accommodation, defects, and high strain at GB

3D Defects:

GBs are INTERFACE DEFECTS:
- In-plane: Tilt Boundary
- Out-of-plane: Twist Boundary
- Real GBs: Mixed



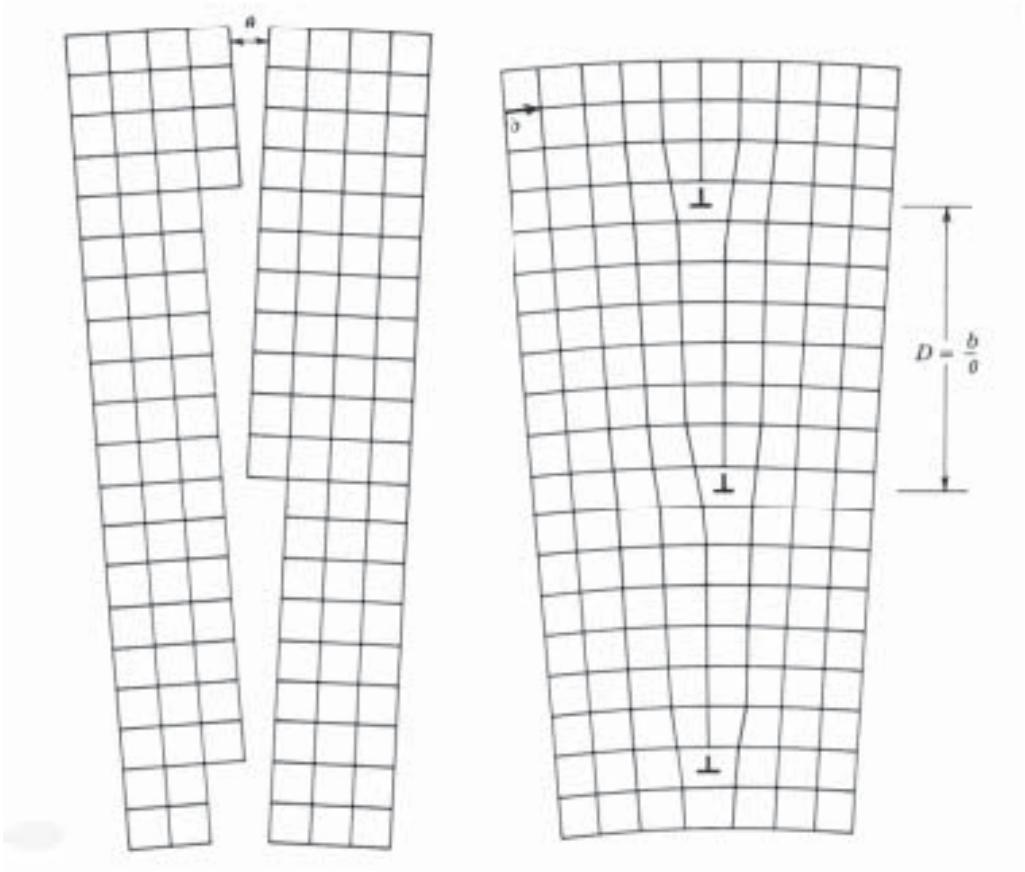
Tilt boundary



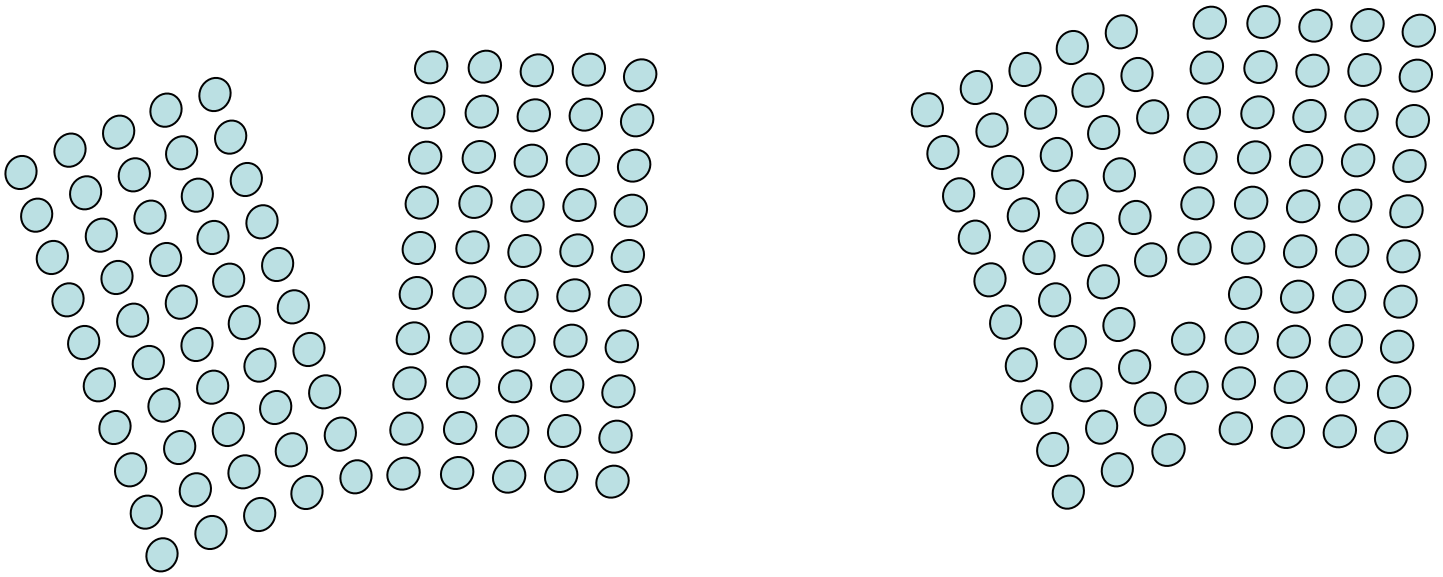
Twist boundary

GRAIN BOUNDARIES: Tilt boundary as a model

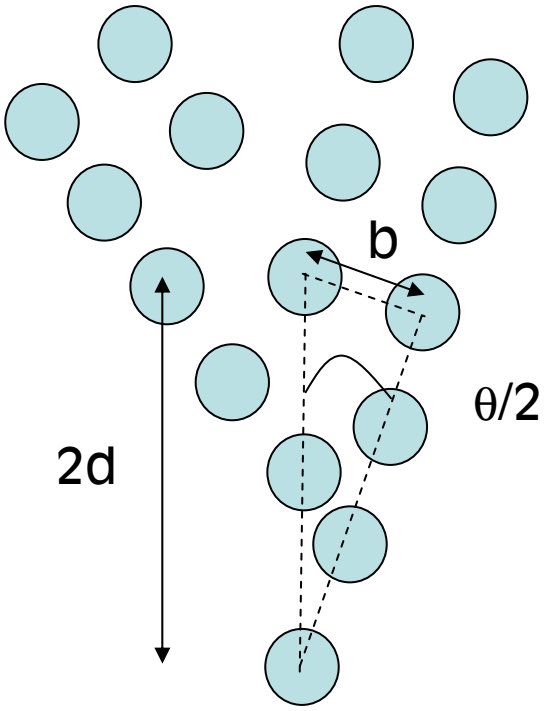
- GB as dislocation array (Bragg, Burgers – 1940)
- Stable array of dislocations formed by in-plane rotation of 2 single crystals
- Requires mismatch angle to be "small" → Small Angle GB



GRAIN BOUNDARIES: Tilt boundary as a model



GRAIN BOUNDARIES: Tilt boundary as a model

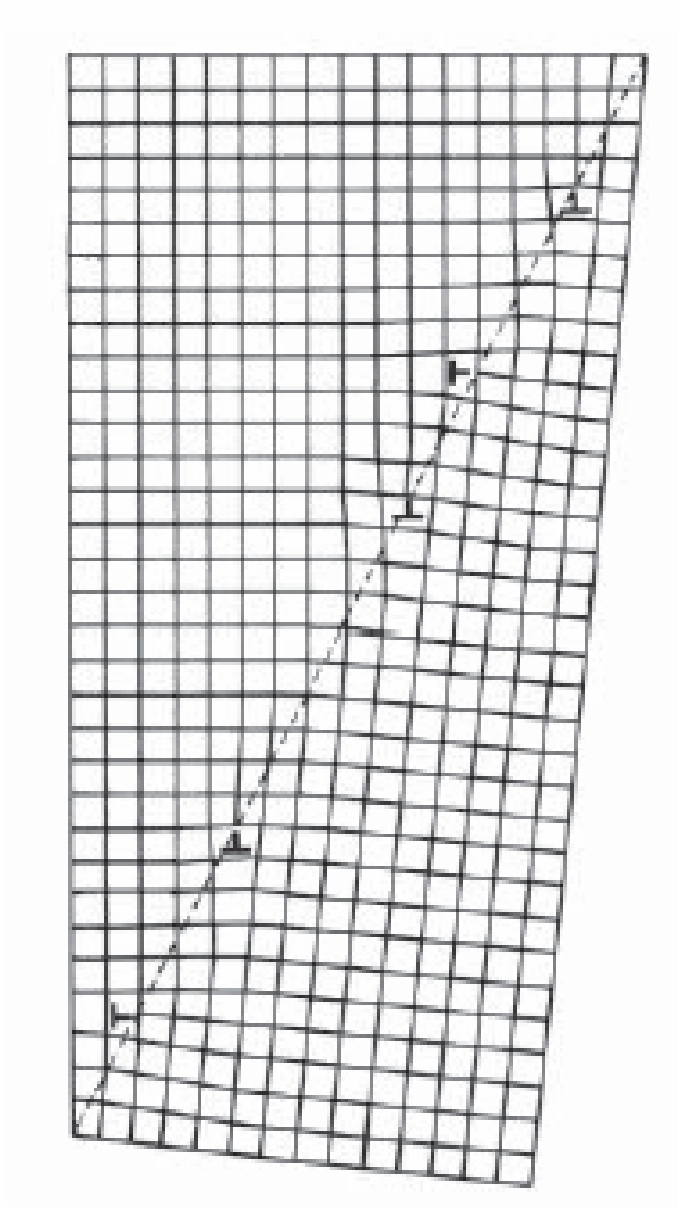


$\sin \theta/2 = b/2d$

$\sin x = x$ for small x

$\theta/2 = b/2d \rightarrow \underline{\theta = b/d}$

GRAIN BOUNDARIES: Tilt boundary as a model

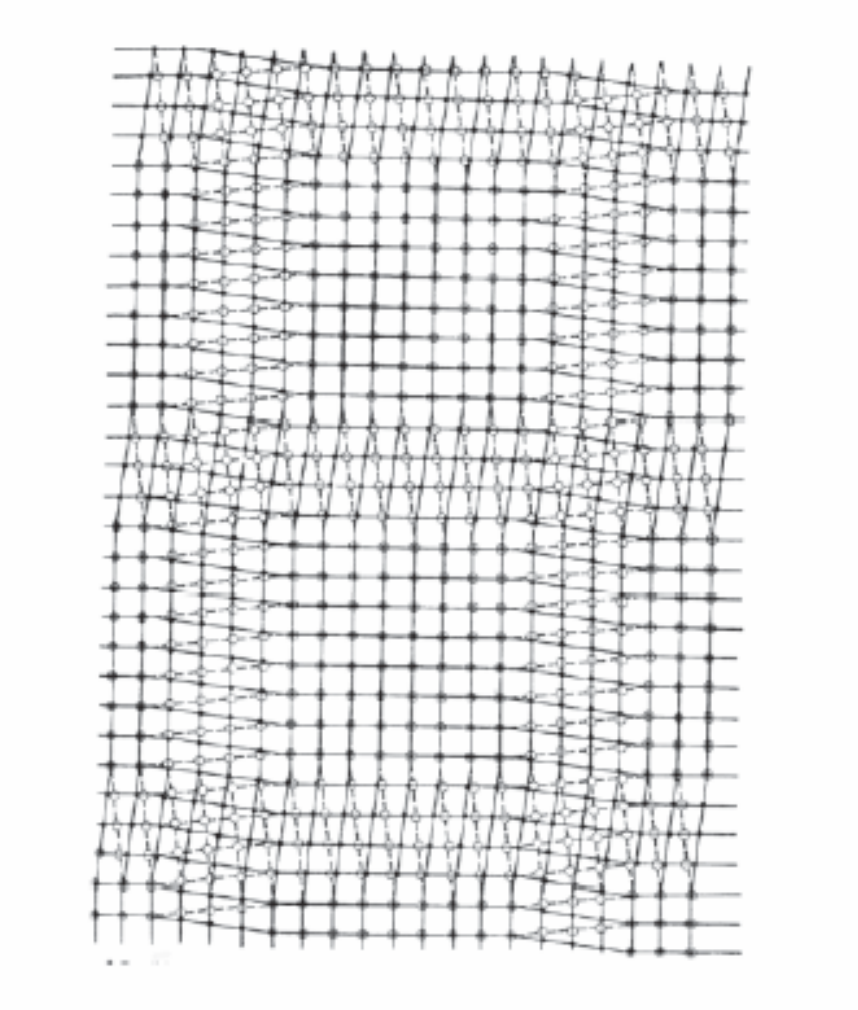


• Unsymmetric tilt:
Edge dislocations at varying orientations

•Edges will interact with one another depending on orientation, spacing

GRAIN BOUNDARIES: Twist boundary

- Mesh of 2 sets of screw dislocations



GB ENERGY

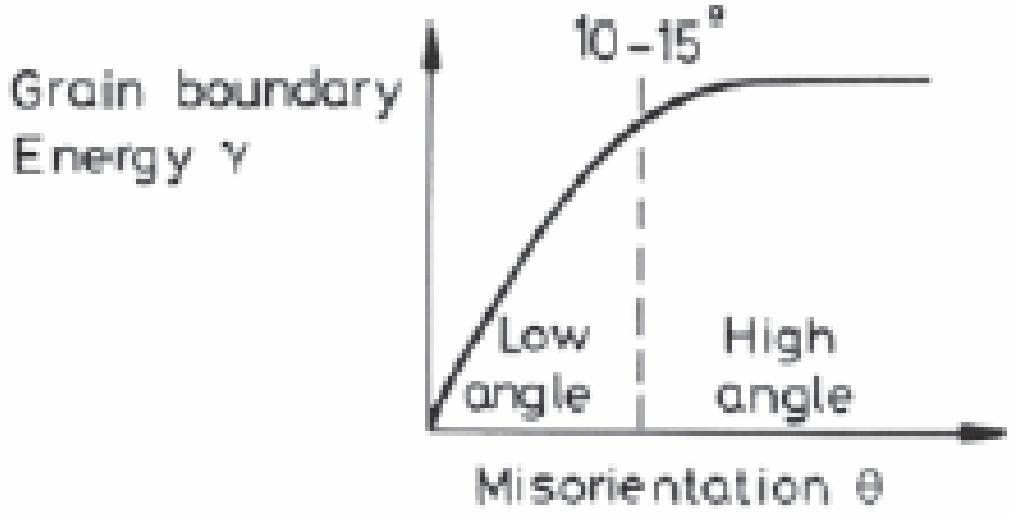
GBE = γ = Total dislocation energy/boundary area

$\gamma \alpha$ 1/2d → $\gamma \alpha \theta$

100 mJ/m^2 < γ < 1000 mJ/m^2 for metals

As θ increases, dislocation spacing decreases → P-K effects cancel and dislocations become indistinct

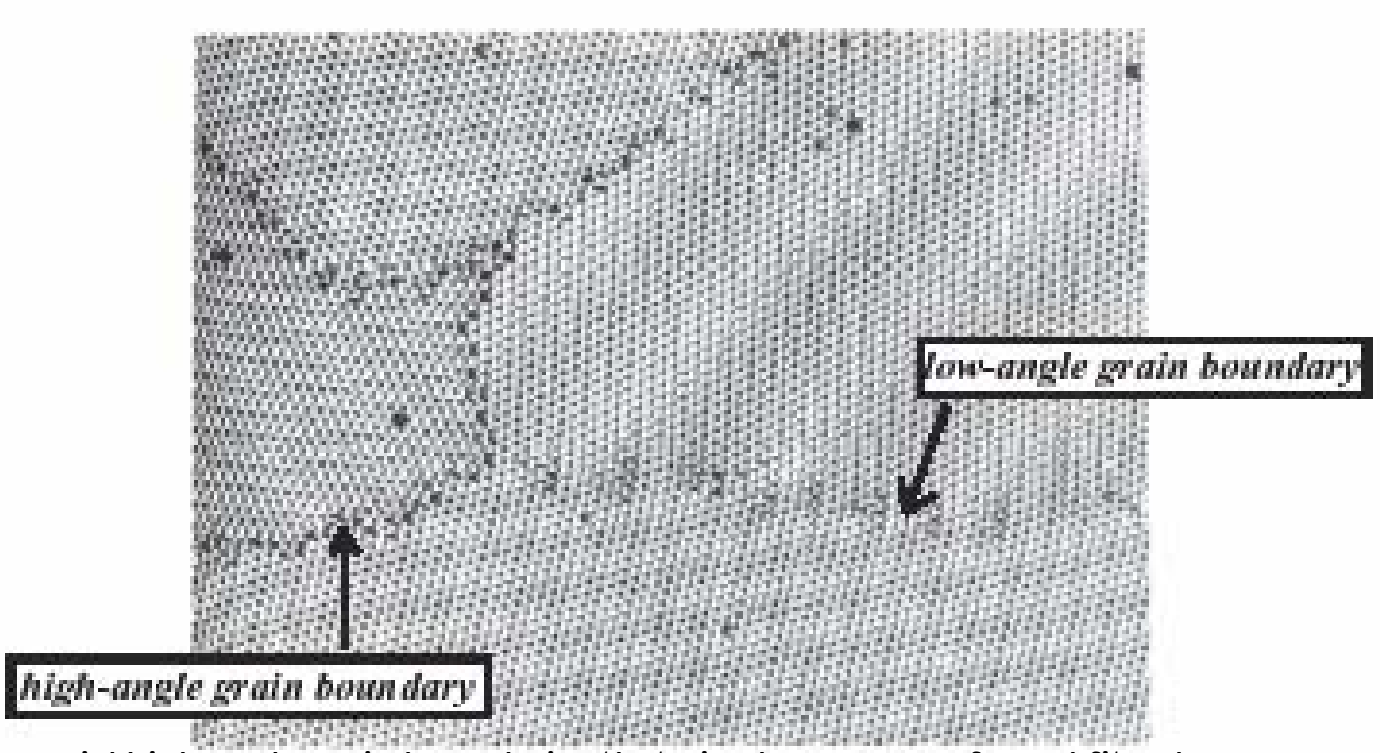
Thus, there is a limit to θ for a low angle GB



GB LOW VS. HIGH ANGLE

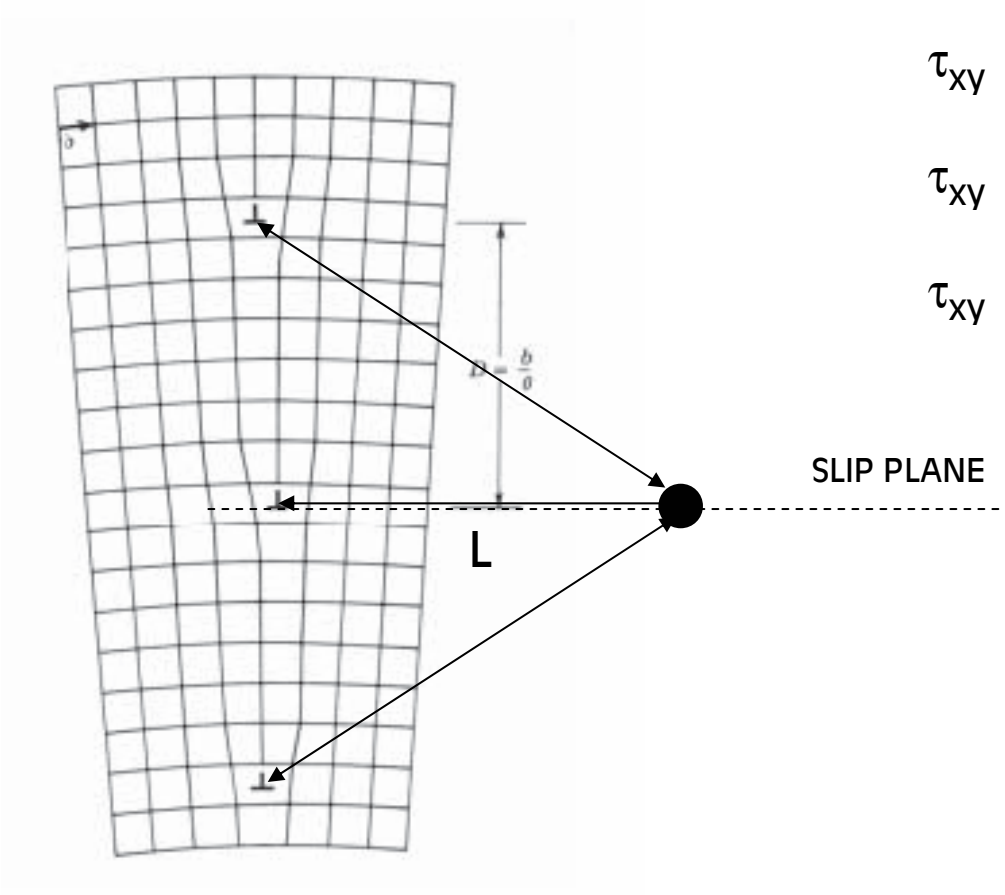
Low: large areas of good fit
separated by misfit dislocations

High: large areas of poor fit
large interatomic distortions → high strain
large free volumes (open spaces along boundary)



**There are special high angle grain boundaries that give large areas of good fit → lower energy

GB ENERGY VIA P-K



$$\tau_{xy} = Gb/[2\pi(1-\nu)] * x(x^2-y^2)/(x^2+y^2)^2$$

$$\tau_{xy} = \Sigma\,(x,\, y(d))$$

$$\tau_{xy} = Gb/[2\pi(1-\nu)]\ \pi x/[d^2 \sinh^2(\pi x/d)]$$