HOMEWORK
From Dieter
6-5

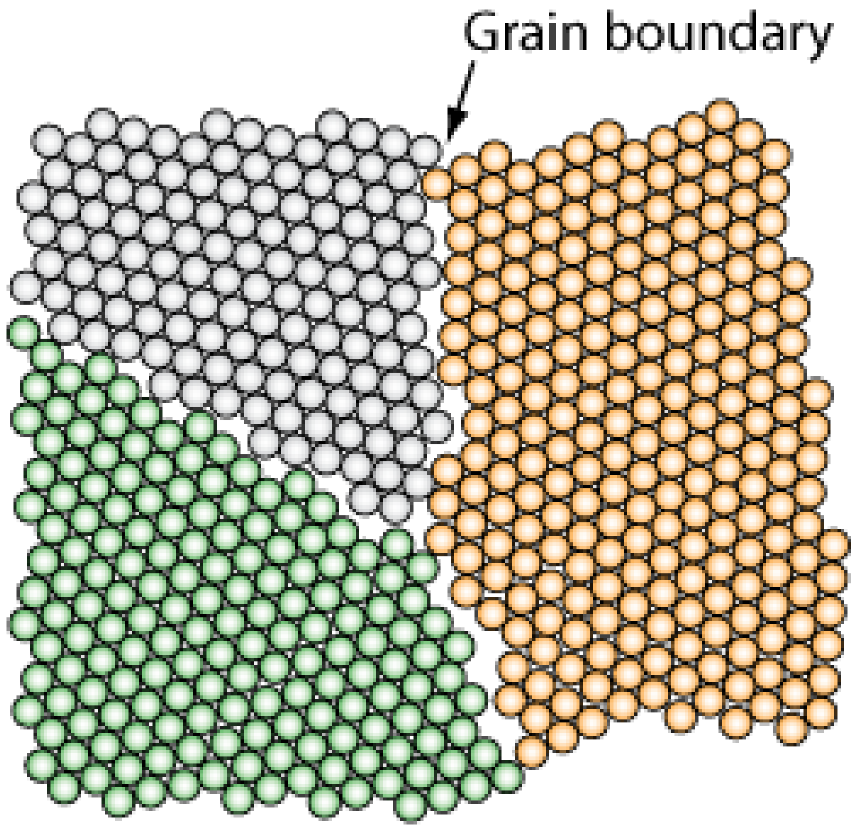
Module #18

Grain Size Hardening
("Hall-Petch Relationship")

READING LIST

►DIETER: Ch. 6, pages 188-197

- J.C.M. Li, *Trans. AIME*, v. 227 (1963) pp. 239-247.
- H. Conrad, "Work-hardening model for the effect of grain size on the flow stress of metals," in Ultrafine-Grain Metals, edited by J.J. Burke and V. Weiss, Syracuse University Press (1970) pp. 213-229.



[From Ashby, Shercliff, and Cebon, 2007, p.120]

Misorientation between grains.

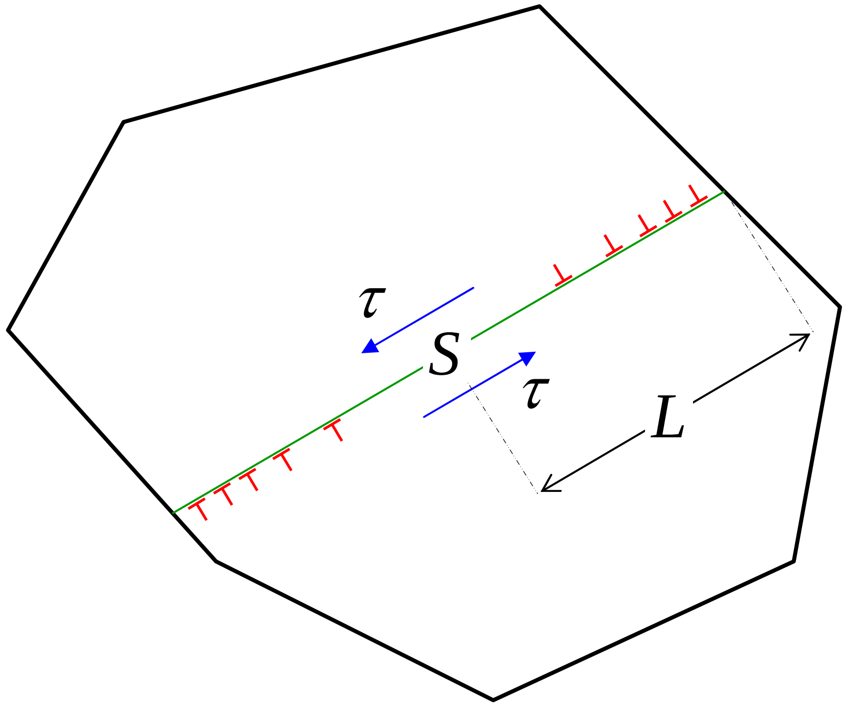
“Slip planes don’t line up.”

Grain boundary strengthening (1)

- Grain boundaries also impede dislocation motion. Thus, they also contribute to strengthening.
- The *magnitude of* the observed *strengthening depends upon* the *structure of the grain boundaries* and the degree of *misorientation between grains*.
- Several models describe grain boundary strengthening. Nearly all of them reduce to the form of the original Hall-Petch relationship.
  - E.O. Hall, "The deformation and ageing of mild steel III. Discussion of results," *Proceedings of the Physical Society B*, 64 (1951) p. 747.
  - N.J. Petch, "The cleavage strength of polycrystals," *J. Iron Steel Inst.*, 174 (1953), p. 25.

RECALL: Dislocation Pileups

- When dislocations generated by sources approach obstacles on slip planes, they often pile up. Suitable obstacles include:
  - ► Grain boundaries
  - – Second phases
  - – Sessile dislocations
  - – Etc…



- Lead dislocation is acted on by applied shear stress <u>and</u> interaction forces (i.e., back stress) from other dislocations.

$$\tau(\text{lead dislocation}) \cong n\tau$$

- # dislocations in pileup is:

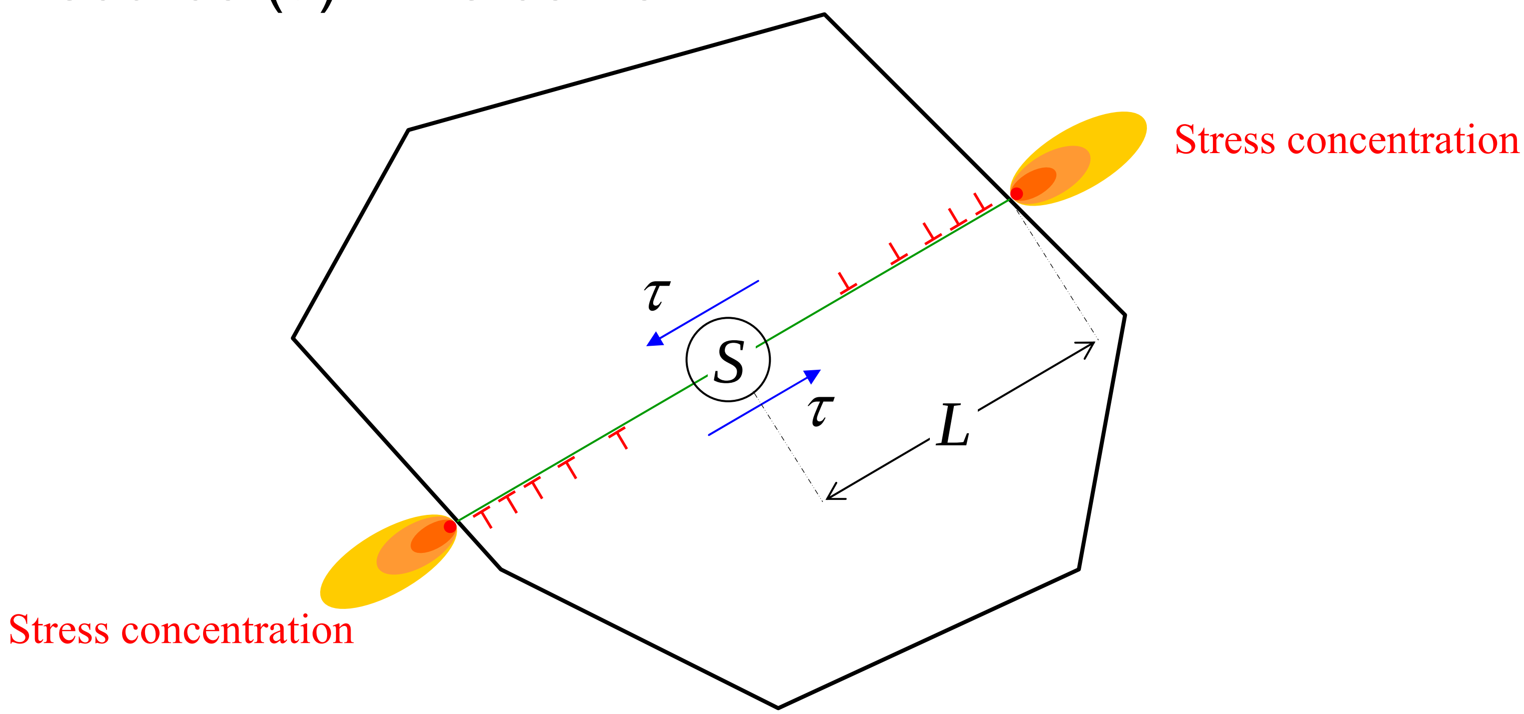
$$n = \frac{k\pi\tau L}{Gb} \quad \text{or} \quad n = \frac{k\pi\tau D}{4Gb}$$

[For ⊥ source in center of grain]

where $k = 1$ for screw dislocations and $(1\text{-}\nu)$ for edge dislocations.

Grain boundary strengthening (2)

- Consider a grain that contains a single dislocation source (S) in its center.



- Dislocations emitted from point sources within individual grains (e.g., Frank-Read sources) encounter a *lattice friction stress* τ_o (i.e., a Peierls stress) as they move on a slip plane towards a grain boundary.

Grain boundary strengthening (2)

- The lattice friction stress opposes the *applied shear stress* $\tau_{applied}$.

- The *effective shear stress* τ_{eff} that contributes to plastic deformation (i.e., the stress to make a dislocation move) is then given by:

$$\tau_{eff} = \tau_{applied} - \tau_o$$

- Since dislocation motion is impeded by grain boundaries, dislocations will pile up at GBs until the stress is large enough for them to break through the GBs.

Grain boundary strengthening (3)

- In this model, the shear stress at the GB is given by:

$$\tau_{gb} = \tau_{eff}\sqrt{\frac{D}{4r}} = (\tau_{applied} - \tau_o)\sqrt{\frac{D}{4r}}$$

$D =$ grain size

$r =$ distance from source

- The quantity:

$$\sqrt{\frac{D}{4r}}$$

represents stress concentration on lead dislocation.

Grain boundary strengthening (3)

- For explanation only, if we assume that bulk yielding ($\tau_{applied}$ = τ_{ys}) occurs at a critical value of τ_{gb}, we can rearrange the preceding equation in terms of the applied shear stress.

$$\tau_{applied} = \tau_o + \tau_{gb}\sqrt{\frac{4r}{D}}$$

- τ_{gb} and r are essentially constant, which reduces this equation to:

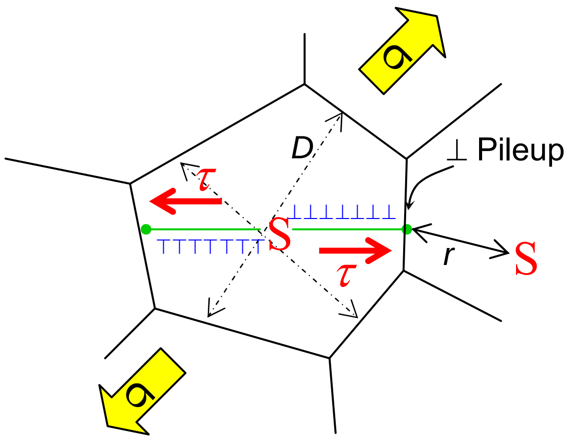
$$\tau_{ys} = \tau_o + k_y' D^{-1/2} \quad \text{or} \quad \sigma_{ys} = \sigma_o + k_y D^{-1/2}$$

This form of the HP equation is derived when we incorporate the Taylor factor, thus turning shear stress into a normal stress.

There are other models for GB strengthening
(I've outlined a few of them on the next 3 pages)

Grain boundary strengthening (4)

- A.H. Cottrell ("Theory of brittle fracture in steel and similar metals," *Trans. AIME*, 212, 1958, p. 192) modified the original Hall-Petch model.
- *Virtually impossible for dislocations to burst through grain boundaries*.



- Assumed that the stress concentration that produced a pileup in one grain activated a dislocation source in an adjacent grain.
- The maximum shear stress at a distance r ahead of the boundary is given by:

$$\Delta\tau = (\tau_{applied} - \tau_o)\sqrt{\frac{D}{4r}}$$

where τ is the stress required to activate the source in the adjacent grain (i.e., stress required to initiate dislocation motion); $\tau_{applied}$ is the applied shear stress at which the source becomes active; and τ_o is the Peierls stress. In this model, $r < D/2$.

- $(D/4r)^{1/2}$ represents the stress concentration arising from the pileup. It increases as the number of dislocations increases (thus it ↑ as D ↑).

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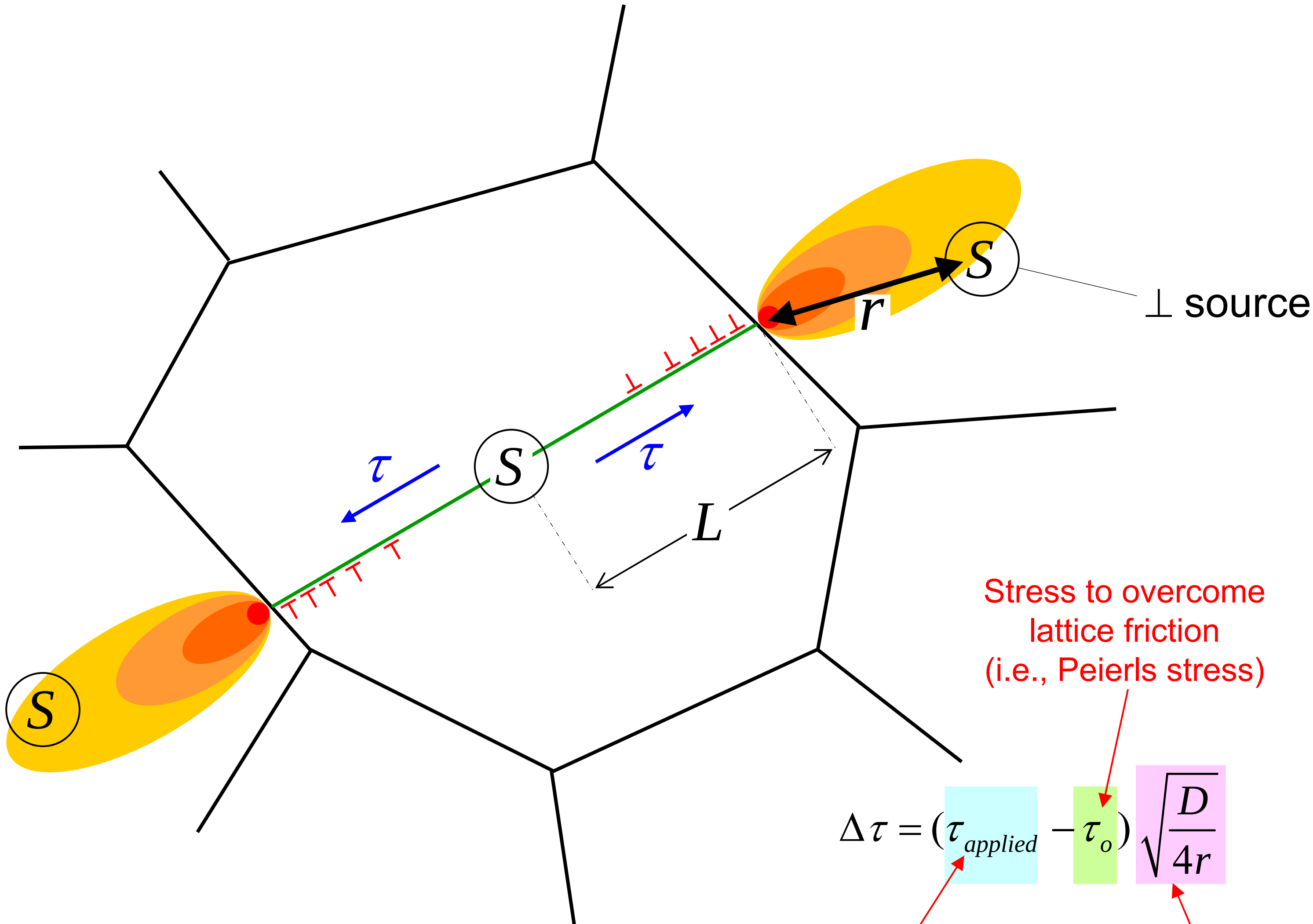
Cottrell, 1958

- Assumed that the stress concentration is large enough to activate a dislocation source in an adjacent grain.



$$\Delta\tau = (\tau_{applied} - \tau_o)\sqrt{\frac{D}{4r}}$$

Stress to overcome lattice friction (i.e., Peierls stress) → τ_o

Stress to activate dislocation source → $\tau_{applied}$

Stress concentration from pileup → $\sqrt{\frac{D}{4r}}$

Grain boundary strengthening (5)

$$\tau = (\tau_a - \tau_o)\sqrt{\frac{D}{4r}}$$

- Assuming that $\tau_a = \tau_{ys}$, this equation can now be rewritten as:

$$\tau_{ys} = \tau_o + \tau\sqrt{\frac{4r}{D}} = \boxed{\tau_{ys} = \tau_o + k_y' D^{-1/2}}$$

or

$$\boxed{\sigma_{ys} = \sigma_o + k_y D^{-1/2}}$$

- The Hall-Petch and Cottrell models have physical appeal. However, very few investigators have observed dislocation pileups at boundaries.

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Grain boundary strengthening (6)

- Li ("Petch relation and grain boundary sources," *Trans. TMS-AIME*, 227, 1963, p. 239) considered that grain size effects were caused by dislocation emission from grain boundary ledges.

- In this model, the ability of a grain boundary to emit dislocation is characterized by new parameter μ.

$$\mu = \frac{\text{total length of } \perp \text{ line emitted}}{\text{unit area of grain boundary}}$$

- The parameter μ is also related to the dislocation density at yielding, $\rho_\perp$, by the relation:

$$\rho_\perp = \frac{3\mu}{D}$$

- Recall from our lectures on work hardening the following:

$$\tau = \tau_o + \alpha G b \sqrt{\rho_\perp}$$

- Combining terms, we obtain:

$$\tau_y = \tau_o + \alpha G b \sqrt{\frac{3\mu}{D}} = \tau_o + k_y' D^{-1/2} \text{ or } \boxed{\sigma_y = \sigma_o + k_y D^{-1/2}}$$

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Grain boundary strengthening (7)

$\sigma_y = \sigma_o + k_y D^{-1/2}$ or $\Delta\sigma_{gb} = k_y D^{-1/2}$

A FEW IMPORTANT THINGS TO CONSIDER:

- k_y increases when the Schmid factor *m* increases.
- Higher values of k_y correlate with increasing strength.
- In metals it is “usually” necessary to produce grains that are smaller than 5 μm in diameter to gain appreciable strengthening.
- However, there are some notable exceptions…

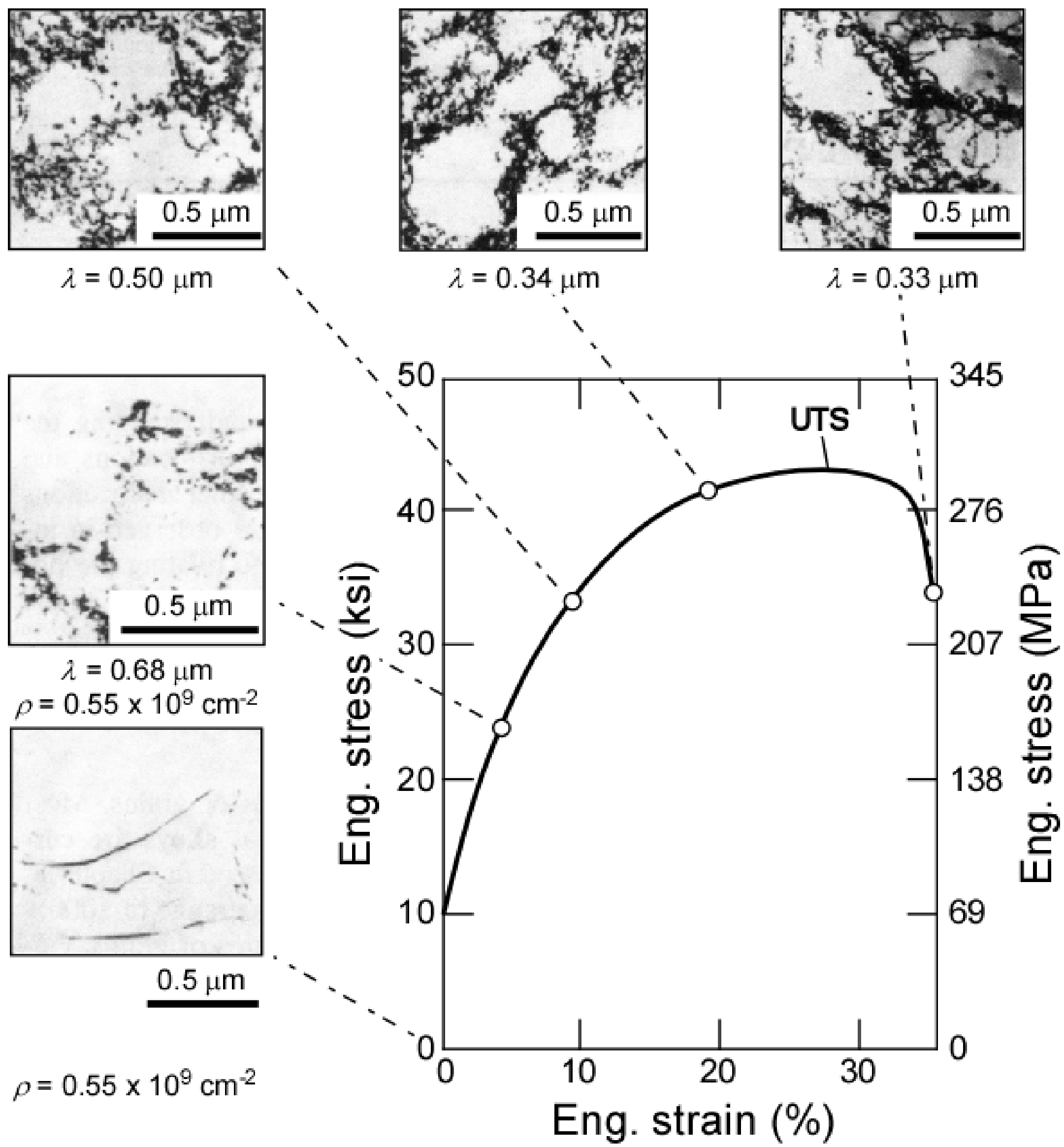
Ex.: Nanocrystalline materials

  - These are materials with grain sizes that are less than 100 nm (generally with GS near 10 nm).
  - They can be viewed as composites consisting of small dislocation-free crystals in an amorphous matrix. Grain boundaries are on the order of 5 nm in width.

Grain boundary strengthening (8)

<u>MORE IMPORTANT THINGS TO CONSIDER:</u>

- The Hall-Petch relationship has been reported in a large number of crystalline materials.
- The degree to which grain boundary (i.e., grain size) strengthening can be effectively used depends on the material's Hall-Petch coefficient and the degree of grain-size refinement possible in the material.
- Example:
  - Engineered ceramics generally have finer grain sizes than metals and are thus much stronger. Of course this is also related to their complex crystal structures.
  - Fine grained ceramics are stronger and more fracture resistant than their coarse grained counterparts.
  - Nanocrystals?



RECALL

$\rho_\perp$ increases as ε_p increases.

Dislocation tangles and cells (i.e., subgrains) form.

Stress-strain behavior of 304 stainless steel at 650°C. Strain rate = $3.17 \times 10^{-4}\ s^{-1}$. Figure adapted from J.R. Foulds, A.M. Ermi, and J. Moteff, *Materials Science and Engineering*, **45** (1980) 137-141.

What is the impact of a change in ε_p and $\rho_\perp$?

- Subgrains are analogous to small grains. However, they are not really grains as we typically think of them.

- This leads to a mild "grain boundary effect". Similar to the Hall-Petch effect, which we will discuss next.

- It is easier to move $\perp$'s across cell boundaries than across GBs because the misorientations between the different cells are very small in comparison to the misorientations between regular grains.

$$\Delta\sigma'_\perp = \frac{k'_\perp}{\sqrt{s}}$$

$k'_\perp$ is the dislocation strengthening coefficient for the cell structure. It is smaller than the Hall-Petch constant.

In this equation s is the average cell diameter.

- Similar expressions exist for lamellar structures. Why could this be?

$$\Delta\sigma_\lambda \propto \frac{\text{const.}}{\sqrt{\lambda}}$$

Summary of hardening/strengthening mechanisms for crystalline solids

Hardening Mechanism	Nature of Obstacle	Strong or Weak	Hardening Law
Work hardening	Other dislocations	Strong	$\Delta\tau = \alpha G b \sqrt{\rho}$ (see [1])
Grain size / Hall-Petch	Grain boundaries	Strong	$\Delta\tau = k_y' \big/ \sqrt{d}$ (see [2])
Solid solution	Solute atoms	Weak (see [3])	$\Delta\tau = G\varepsilon_s^{3/2} c^{1/2} / 700$ (see [4])
Deforming particles	Small, coherent particles	Weak (see [5])	$\Delta\tau = CG\varepsilon^{3/2}\sqrt{\frac{fr}{b}}$ (see [6])
Non-deforming particles	Large, incoherent particles	Strong (see [7])	$\Delta\tau = \frac{Gb}{(L-2r)}$

[1] α equals about 0.2 for FCC metals and about 0.4 for BCC metals.

[2] k_y' scales with inherent flow stress and/or shear modulus; therefore k_y' is generally greater for BCC metals than for FCC metals.

[3] Exception to weak hardening occurs for interstitials in BCC metals; the shear distortion interacts with screw dislocations leading to strong hardening.

[4] Equation apropos to substitutional atoms; parameter ε_s is empirical, reflecting a combination of size and modulus hardening.

[5] Coherent particles can be "strong" in optimally aged materials.

[6] Constant C depends on specific mechanism of hardening; parameter ε relates to hardening mechanism(s). Equation shown applies to early stage precipitation. Late stage precipitation results in saturation hardening.

[7] Highly overaged alloys can represent "weak" hardening.

SYMBOLS : G = shear modulus; b = Burgers vector; ρ = dislocation density ; d = grain size; c = solute atom concentration (at.%); f = precipitate volume fraction; r = precipitate radius; L = spacing between precipitates on slip plane.

Table adapted from Courtney, *Mechanical Behavior of Materials*, 2nd edition, p. 232.

Combination of Strengthening Mechanisms
(up to this point)

MORE IMPORTANT THINGS TO CONSIDER:

- For a single phase polycrystalline alloy with a dislocation density of $\rho_\perp$, the strength increase due to work hardening and grain size hardening can be crudely estimated by superimposing some of the terms that we have derived thus far.

$$\Delta\sigma = \Delta\sigma_\perp + \Delta\sigma_{gb} + \Delta\sigma'_\perp = k_\perp\sqrt{\rho_\perp} + \frac{k_y}{\sqrt{D}} + \frac{k'_\perp}{\sqrt{s}}$$

- This of course neglects the possibility of other strengthening mechanisms and any potential interactions between them.
- Keep in mind, other things do occur which significantly complicate our ability to develop generally applicable descriptions of strengthening.