Materials Engineering 272-C
Fall 2001, Lectures 11 & 12

Dislocations and Strengthening

The strength of materials is one of the most important design parameters for engineering applications.

- One can estimate the theoretical strength of a metal from a consideration of atomic density and bonding strength.
    - (Consider what happens when a material fails by fracture; all of the atomic bonds along the fracture plane must be broken and the amount of work that must be supplied in order to make this happen is on the order of the bonding energy per atom (~ 1 eV/atom) multiplied by the atomic density (atoms/cm^2) multiplied by the total fracture area (cm^2)).
- Such estimates of the fracture strength of metals give results on the order of GPa (1000 MPa, or 10^9 N/m^2), which is orders of magnitude higher than the observed strength. Obviously, this model of the fracture process must be in error.

The discrepancy between the theoretical and observed strength of metals was resolved with the development of electron microscopic imaging, which made possible the detection of a crystalline defect known as **dislocations**. As discussed previously, the movement of dislocations allows interplanar "slip" to occur at a much lower shear stress than if all the atomic bonds in the slip plane were broken simultaneously. We now know that **dislocation motion and interaction is the primary mechanism responsible for plastic deformation in metals**.

As we shall see, the properties of dislocations can be exploited in several ways to design materials with improved strength. These approaches for strengthening include

- strain hardening,
- solid solution alloying, and
- grain size refinement.

We will discuss each method and give examples in this section.

A review of basic principles of dislocation propagation and generation:

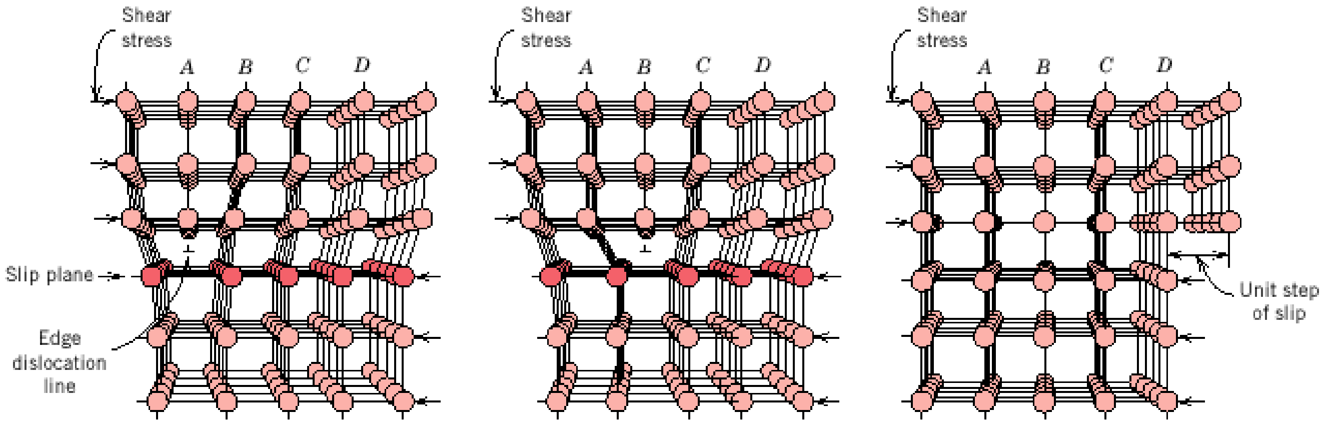
Recall that a dislocation can be thought of as an extra half plane of atoms in a crystalline lattice.

- Somewhat analogous to a driving an axe into a block of wood.
- The presence of the axe (or dislocation) results in local strain because the natural (equilibrium) spacing of the material is disrupted or distorted.

Plastic deformation corresponds to the motion of large numbers of dislocations along their respective slip planes.

- Slip only occurs in close-packed planes and only in close-packed directions. (The largest interplanar spacing between successive plane sets in a crystal corresponds to close-packed planes; this means that the net atomic force between successive close-packed planes is lowest.)

The following diagram illustrates how an edge dislocation “glides” along a slip plane:



(a)

(b)

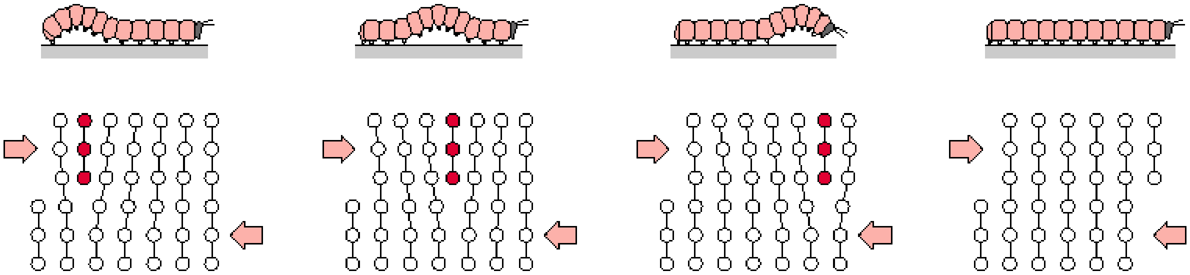
(c)

- the movement of the dislocation (to the right in this sequence) requires the breaking (and formation) of only one set of bonds per step.

<u>An analogy to edge dislocation motion:</u>

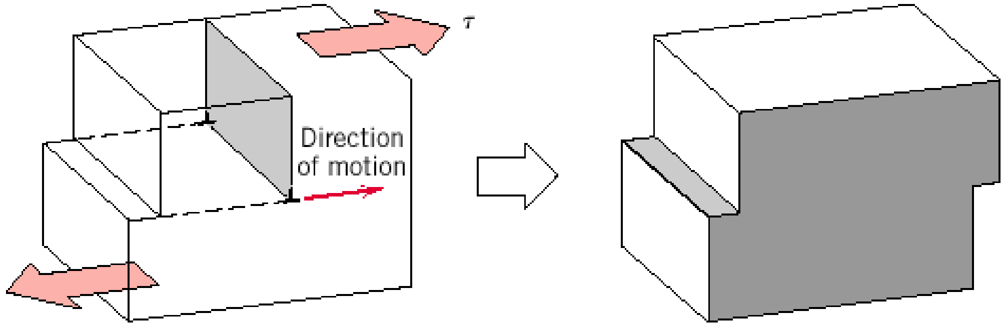
If we try to eliminate a wrinkle in a large area rug by pulling on the opposite side, we have to overcome the frictional forces of every contact point between the edge and the wrinkle. This is equivalent to shifting an entire close-packed plane of atoms at once by breaking all of the interplanar chemical bonds. On the other hand, if we work the wrinkle out of the rug by gradually working it with a toe, we only have to overcome the local frictional forces in the neighborhood of the wrinkle itself. In a step-wise manner, the wrinkle works its way to the edge and disappears. Similarly, by breaking (and reforming) only the bonds in the immediate vicinity of the dislocation, a plane of atoms can be shifted relative to another plane with comparatively little effort.

The motion of a caterpillar offers another analogy to that of an edge dislocation:

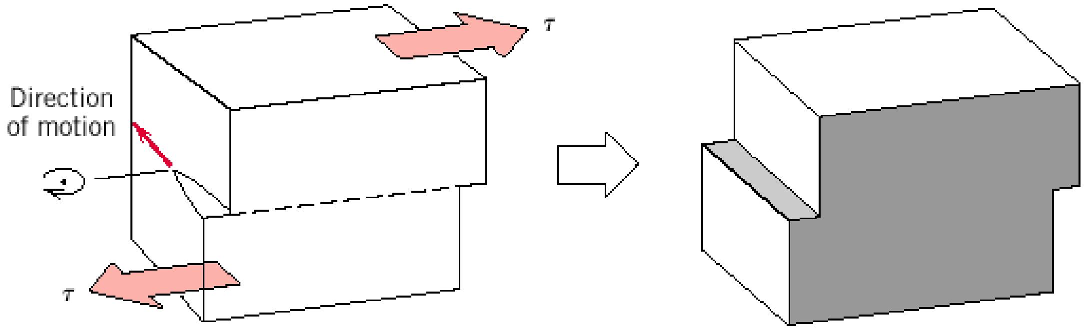


The motion of edge or screw dislocations under the action of an applied shear stress causes one atomic plane to slide over another, resulting in permanent (plastic) deformation.

Let’s take a macroscopic view: (a shear stress shifts part of a crystal relative to the rest, resulting in a slip band)



(a)



(b)

Dislocations are produced by :

- solidification from the melt,
- mechanical work (e.g., rolling, swaging, drawing, compressive impact, tensile or shear stress), or
- thermal stresses

As a metal is plastically deformed:

- the density of dislocations increases
- they begin to interact with each other.
  This interaction is responsible for the observed increase in strength

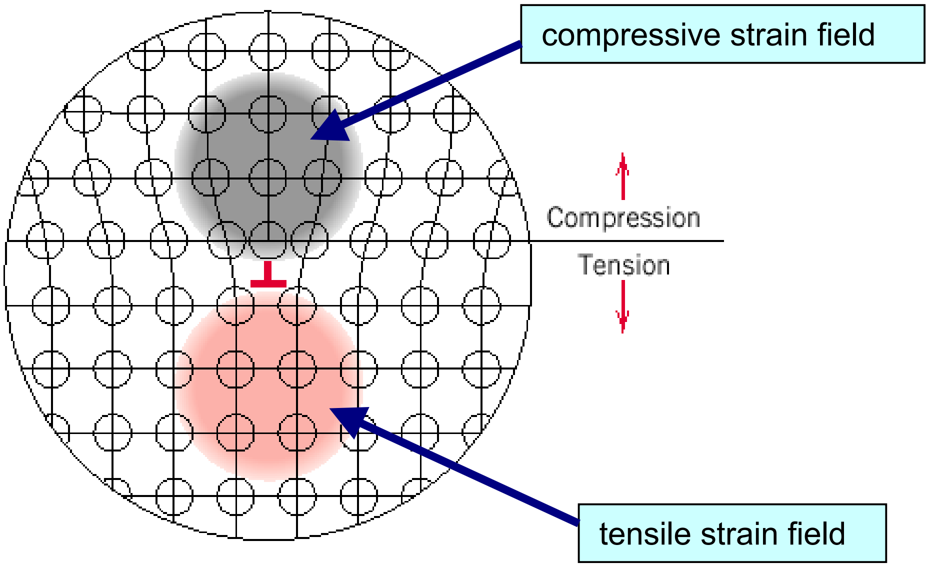
To a first approximation, the energy required to move an edge dislocation is ZERO because energy req'd to stretch a bond on one side = energy released in contracting a bond on the other side. This is why the observed strength of metals << theoretical strength

- (in reality, a finite amount of energy given by the Peierls-Nabarro force, is required to move a dislocation)

Characteristics of Dislocations:

I. Local Lattice Strains

The extra half-plane of atoms generates a "**strain field**" in the vicinity of the dislocation core:



During deformation, ~ 5% of the deformation energy is retained in the material (mostly as strain energy). (The remaining ~95% is dissipated as heat.)

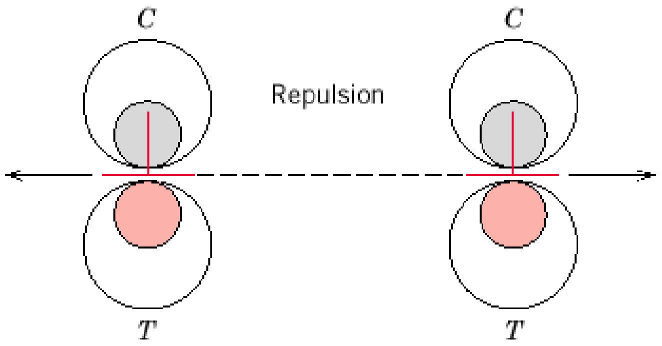
The extra half-plane of atoms (much like an axe driven into a block of wood) causes atoms above the slip plane to be crowded together (compressive strain). There is also a region just below the dislocation core in which the interatomic spacing is greater than the equilibrium value. This corresponds to a tensile strain.

The magnitude of these strain fields decreases with radial distance from the dislocation.

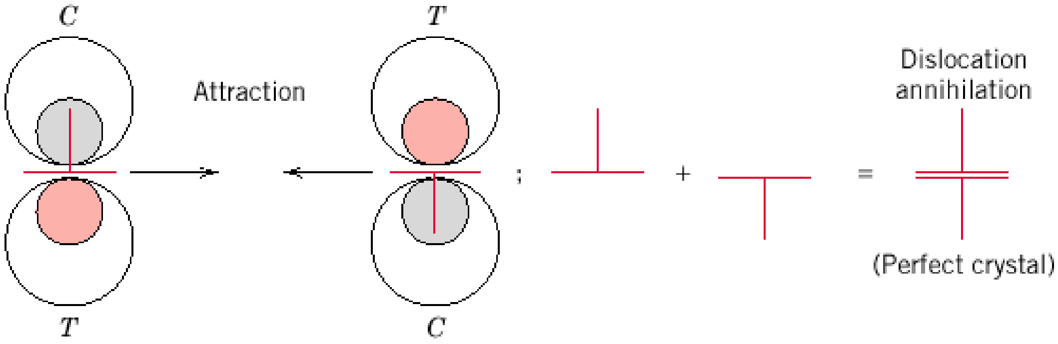
Strain fields in a crystal can interact with one another, in a manner roughly similar to that of charged particles (although the mechanism is quite different in these two cases.)

- Dislocations of the same "sign" experience a repulsive force
- Dislocations of the opposite "sign" experience an attractive force

("Sign" refers to which side of the slip plane the dislocation is on)



(a)



As the density of dislocations increases, the material retains an increasing number of dislocations of the same sign. **Not only does the total strain energy increase but also the tensile strength, which is a measure of the stress required to produce slip.**

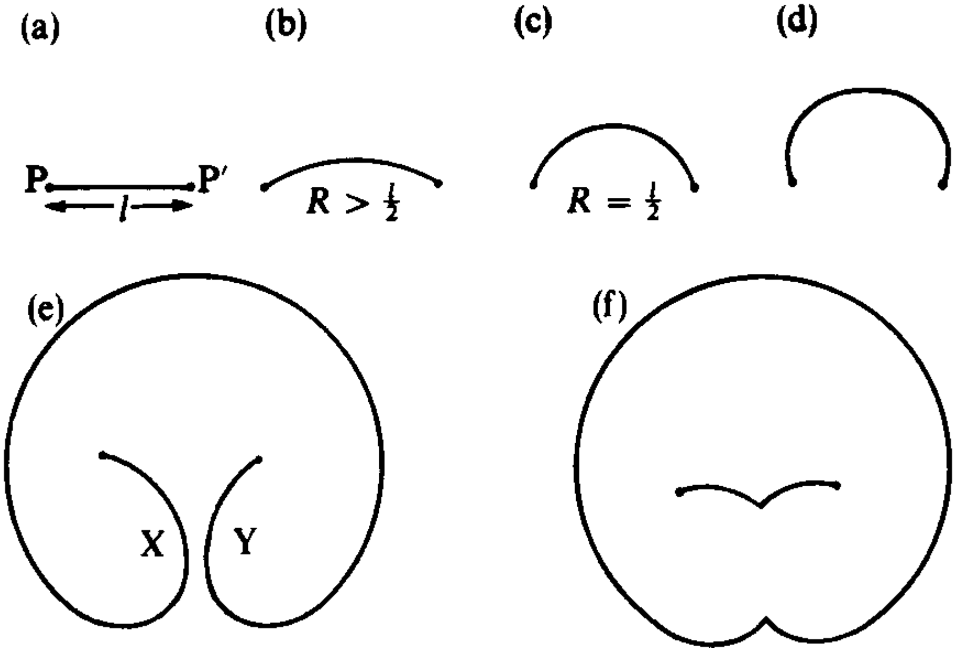
II. Dislocation multiplication

- Dislocations have the ability to reproduce themselves;
- under an applied stress, a single dislocation can multiply and produce thousands more.

Suppose that a dislocation is pinned at two points, P and P.' Under the action of an applied stress, the dislocation will bow out, the radius of curvature being related to the stress. Increasing the stress causes more bowing. The dislocation expands into a loop until the back-loop segments meet and annihilate each other, forming a complete loop and reforming the original pinned dislocation. The loop expands away from the initial segment and the pinned dislocation continues to multiply.

- This mechanism of dislocation generation is referred to as a **Frank-Read source**, after the originators.

The following is a schematic representation of how a Frank-Read source operates under the action of an applied stress:



Important points:

- **the number of dislocations increases in response to an applied stress.**
- **The movement of these dislocations is what enables plastic flow (or slip) to occur in materials.**

How do dislocations move throughout a crystal?

- Dislocations move in close-packed directions within close-packed planes.
- The combination of C-P plane (the slip plane) and C-P direction (the slip direction) is called a **slip system**.

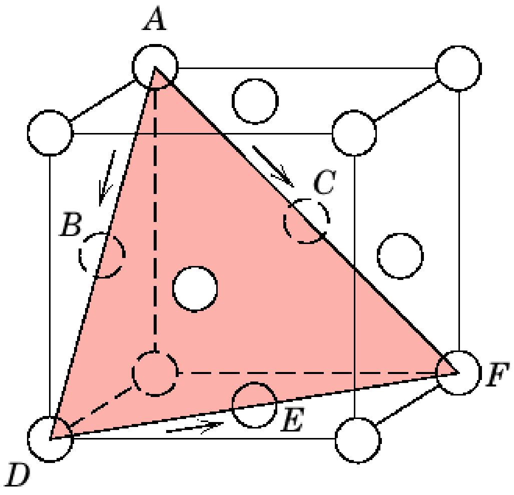
SLIP SYSTEMS DEPEND ON THE CRYSTAL STRUCTURE OF THE MATERIAL!

The following table lists close-packed planes and close-packed directions for FCC, BCC, and HCP metals:

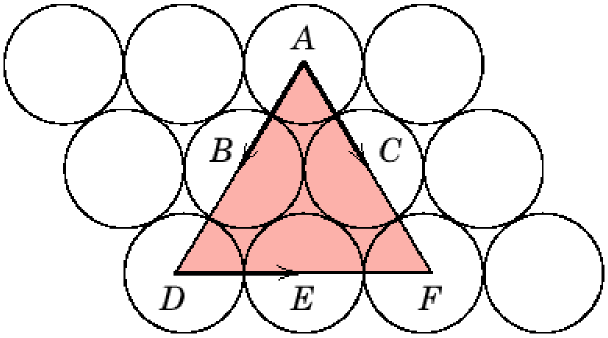
Metals	*Slip Plane*	*Slip Direction*	*Number of Slip Systems*
Face-Centered Cubic			
Cu, Al, Ni, Ag, Au	$\{111\}$	$\langle 1\bar{1}0\rangle$	12
Body-Centered Cubic			
α-Fe, W, Mo	$\{110\}$	$\langle \bar{1}11\rangle$	12
α-Fe, W	$\{211\}$	$\langle \bar{1}11\rangle$	12
α-Fe, K	$\{321\}$	$\langle \bar{1}11\rangle$	24
Hexagonal Close-Packed			
Cd, Zn, Mg, Ti, Be	$\{0001\}$	$\langle 11\bar{2}0\rangle$	3
Ti, Mg, Zr	$\{10\bar{1}0\}$	$\langle 11\bar{2}0\rangle$	3

- The more slip systems available, the easier it is for dislocations to move, which is why (on the average) FCC and BCC metals are more ductile than HCP metals.
- For any given tensile axis, there is a greater probability in FCC and BCC metals that some slip systems are favorably oriented for slip to occur.

Let’s look at an example of a slip system in a **FCC metal** such as Ag, Au, Cu, Ni, or Al:



(a)



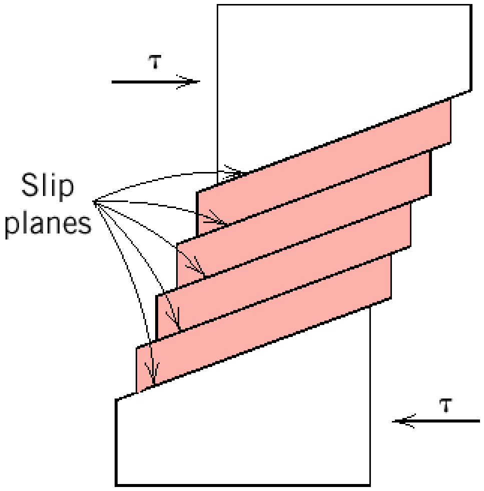
(b)

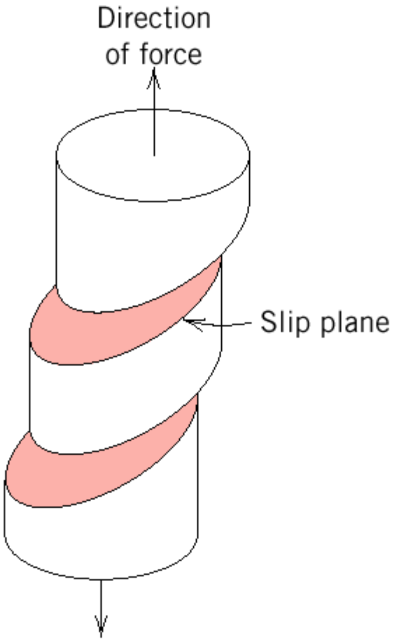
One of the (111) planes is shaded in the unit cell above. If we looked straight down on this plane of atoms, we would see something like the diagram in (b). From this perspective, the core of an edge dislocation would run parallel to the surface of the paper (or screen). It would move in only one of three possible directions: along the line connecting atoms A-D, A-F, or D-F; these constitute the three close-packed directions within this plane. (You should recall (or be able to figure out) that these are the **<110>** family of directions.)

All materials are either polycrystalline (like the pieces of aluminum passed around in class) or single crystalline. (We will neglect *amorphous* materials for the moment.) While the vast majority of engineered materials are polycrystalline, the overall response to an applied stress ultimately depends on how each grain (a single crystal) responds.

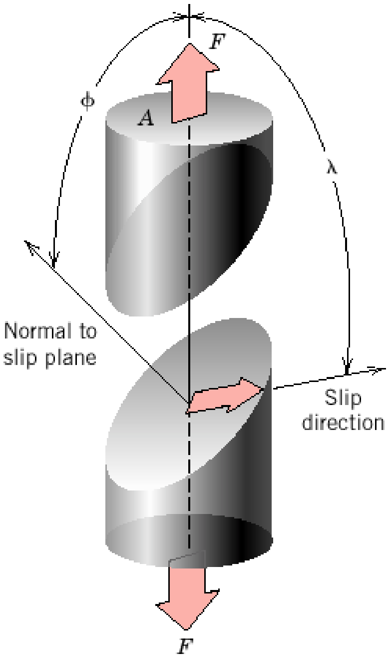
Therefore, we need to understand how a single crystal responds to an applied load.

What does slip look like in the case of a tensile axis oriented at some arbitrary angle to the slip planes in a single crystal?





If the applied load (tensile, for the sake of argument) is parallel to one of the C-P planes and oriented along a C-P direction, slip will occur when some critical magnitude of the stress is reached. In general, however, the tensile axis will lie at some arbitrary angle with respect to the slip plane, as shown in the following figure:



Two angles are important here:

1. The angle between the tensile axis and the normal to the C-P plane (ϕ)
2. The angle between the tensile axis and the slip direction (λ)

Each crystallographic plane (other than those that happen to be aligned parallel or perpendicular to the tensile axis) has a shear component, even though the applied load may be pure tensile. Recall, we showed earlier how a shear deformation is responsible for slip; it is the magnitude of this shear component that is responsible for the slip in any given plane.

- The larger the shear component, the more likely slip will occur in that plane.

- The important parameter is the resolved shear stress, τ_r, or the component of the applied load:

$$\tau_r = \sigma \cos(\phi)\cos(\lambda)$$

τ_r is known as the resolved shear stress.

τ_r will differ with the orientation of each slip system. There will be (at least) one slip system possessing the largest value of τ_r compared with all others. As soon as the τ_r reaches some critical value (critical resolved shear stress, or CRSS), slip will occur on the given slip system.

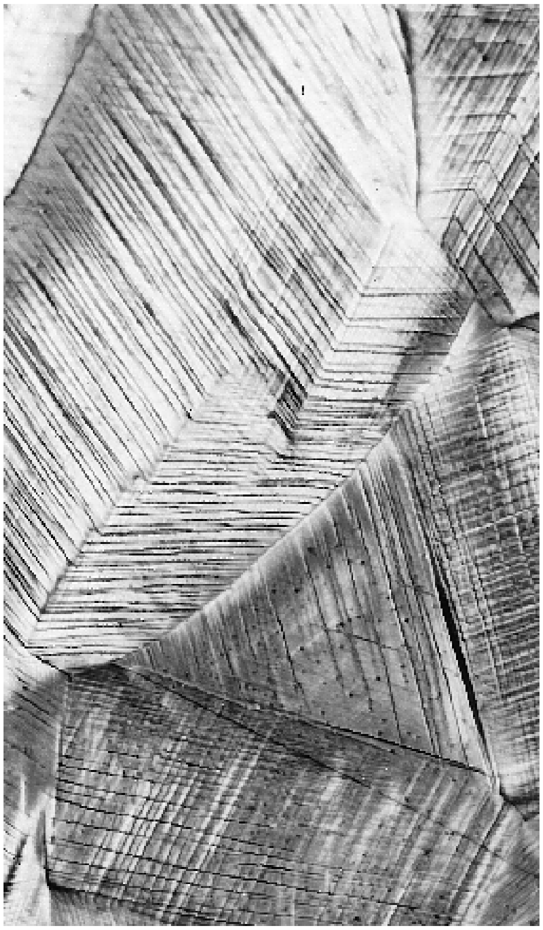
In other words,

plastic deformation occurs when

$$\tau_r = \tau_{CRSS}$$

τ_{CRSS} is a material property that determines the onset of plastic deformation.

Plastic deformation in polycrystalline materials:



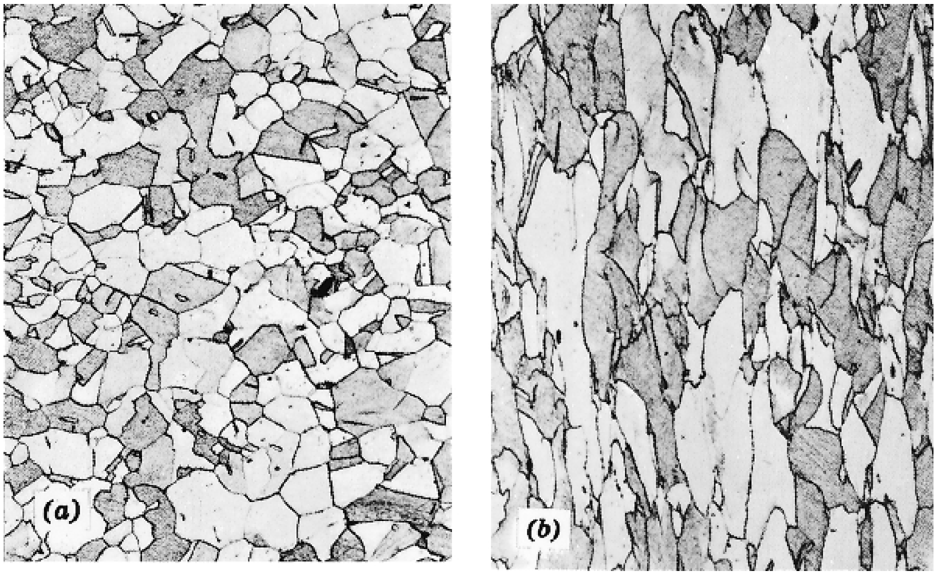
A surface of copper after plastic deformation.

Note the set of parallel lines within each grain.

These lines are slip bands; they show where dislocation motion has resulted in large-scale sliding of distinct crystallographic planes and formation of ledges or steps at the surface

Each slip line corresponds to planes that were most favorably oriented for slip (highest resolved shear stress)

An example of plastic deformation resulting in elongation of grains:



Before deformation:

Grains are **equiaxed”**

After deformation:

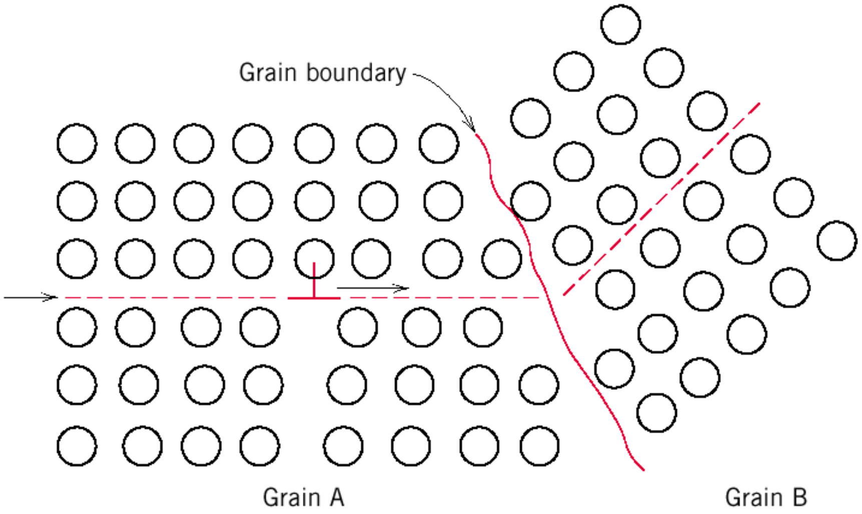
Grains have become elongated along the direction of deformation

Gross deformation of one grain requires deformation in neighboring grains. **Can you see why fine-grained materials are stronger than their coarse-grained counterparts?**

Methods of Strengthening in Metals:

If we understand the fundamental mechanism(s) responsible for the strength of metals, can we exploit this knowledge to design improved (engineered) materials with higher strengths?

Consider what happens when a dislocation encounters a grain boundary:



The grain boundary separates two single crystals of different orientation.

The slip plane in grain A assumes a different orientation in grain B

The dislocation must change directions if it is to continue moving.

Any change in direction requires additional energy

The degree of difficulty in changing direction increases with the angle of mismatch between grains

- Atomic disorder within grain boundaries → discontinuity in slip planes

Grain boundaries act as a barrier to dislocation motion.

Stating this another way:

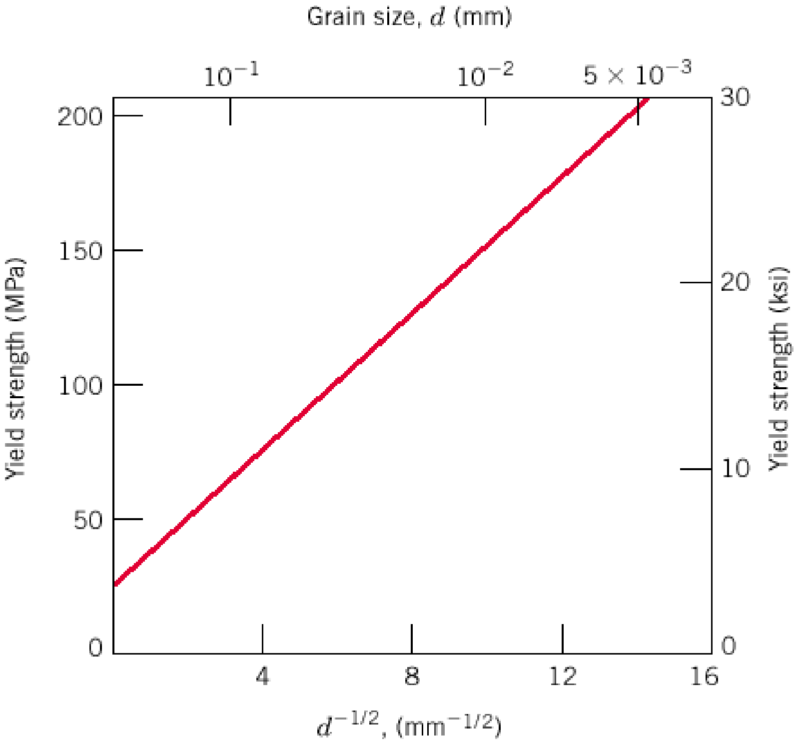
The strength of a material is inversely proportional to grain size

Quantitatively we can express this relationship as,

$$\sigma_y = \sigma_o + k_y d^{-\frac{1}{2}}$$

This is known as the **Hall-Petch equation**.

where σ_y is the yield stress, d is the average grain size, and σ_o and k_y are constants.



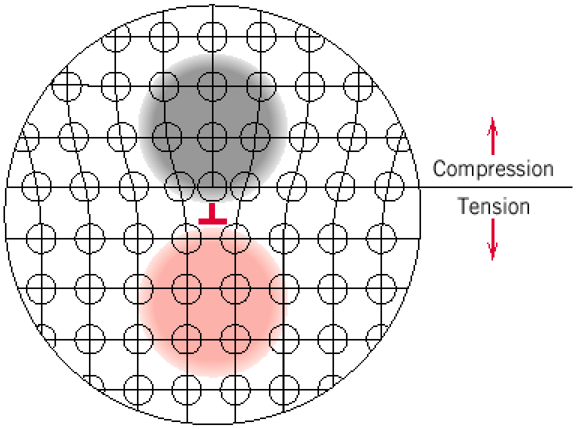
Example of Hall-Petch behavior in $Cu_{70}Zn_{30}$ (brass)

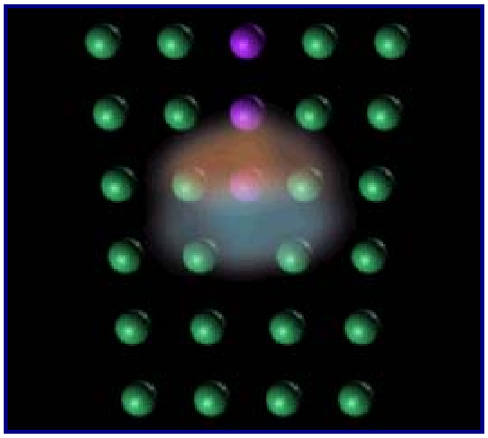
Note how the yield strength varies by over a factor of 4 just due to grain size alone!

(There is evidence that at extremely small grain sizes, i.e., on the order of nanometers (10^{-9} m), dislocation generation is significantly reduced because of the difficulty of operating a Frank-Reed source in such a small volume.)

Dislocation motion is also impaired by strain fields within a crystal.

- Recall that every dislocation has associated with it a strain field:





    - Dislocations of the same sign exert a repulsive force on one another
    - On the average, multiple dislocation interactions are repulsive

- An increase in dislocation density ⇒ increase in number of repulsive strain fields throughout the crystal ⇒ dislocation movement is hindered.

- Whenever dislocation movement is impaired or restricted, a material becomes stronger

    - Implication: **increasing dislocation density increases strength**

Q: How do we increase dislocation density?

A: Plastically deform it.

If we plastically deform a metal (at a temperature much lower than the absolute melting temperature), the process is termed **cold working**.

The amount of cold work (and presumably the dislocation density) is proportional to the percent area reduction:

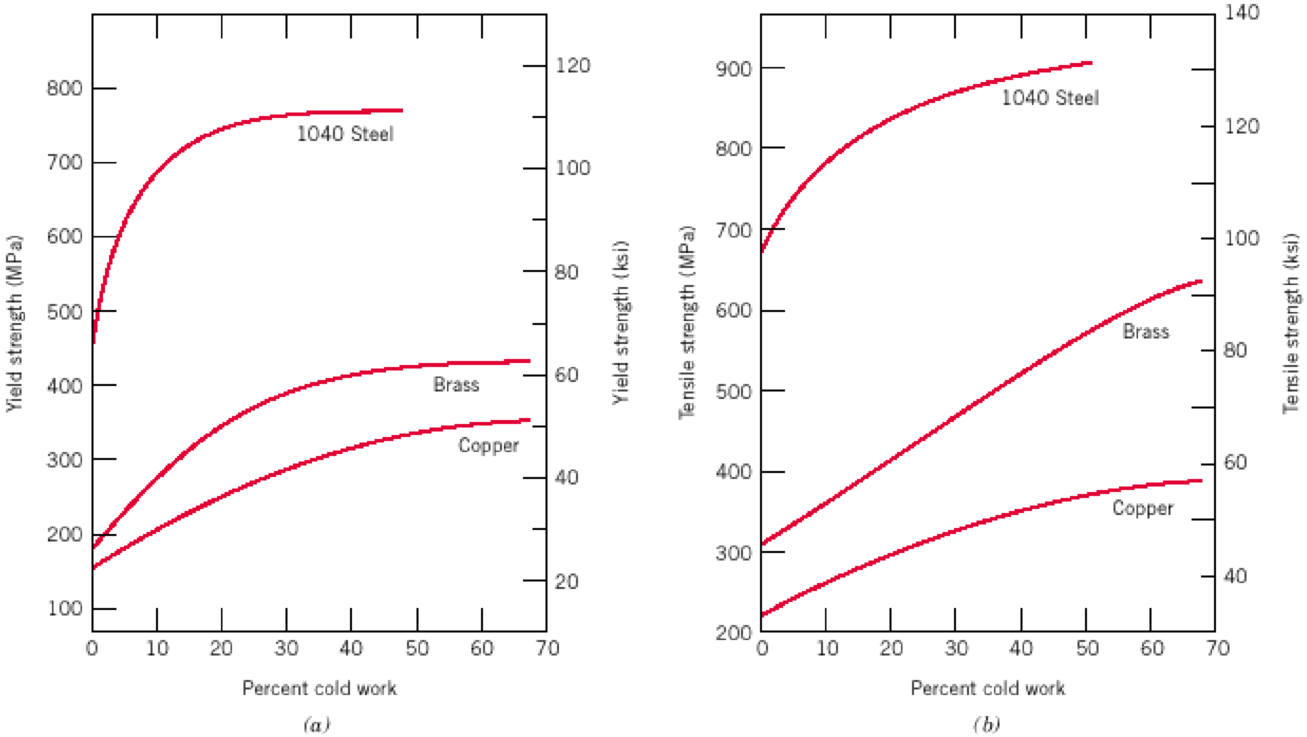
$$\%CW = \left(\frac{A_o - A_d}{A_o} \right) x100\%$$

where A_o is the initial diameter and A_d the diameter after deformation.

During plastic deformation (in other than ultra-fine grained materials), dislocations are generated by Frank-Reed sources.

- Average separation between dislocations decreases
- Each dislocation experiences an increasing resistance to movement
- We see the material as becoming stronger

Examples:


Yield strength (MPa)
800
700
600
500
400
300
200
100
Yield strength (ksi)
120
100
80
60
40
20
1040 Steel
Brass
Copper
0
10
20
30
40
50
60
70
Percent cold work
(a)
Tensile strength (MPa)
900
800
700
600
500
400
300
200
Tensile strength (ksi)
140
120
100
80
60
40
1040 Steel
Brass
Copper
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50
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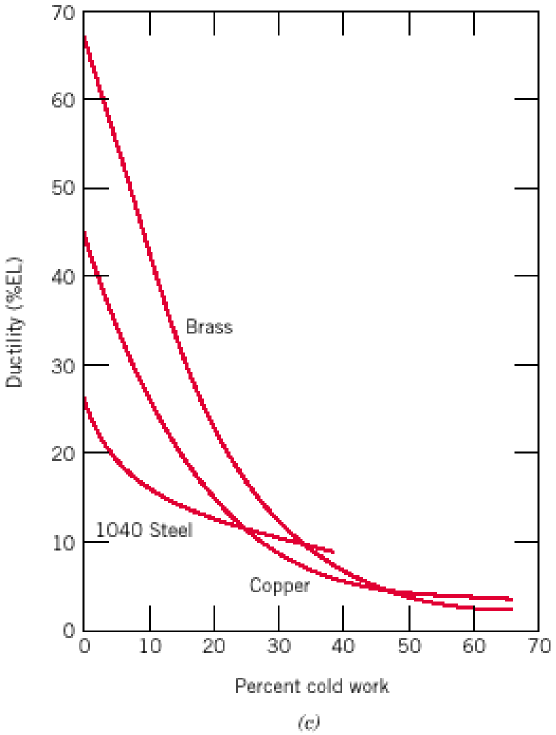
70
Percent cold work
(b)



Examples of yield strength, tensile strength, and ductility (in terms of % elongation) of three metals (1040 steel, brass, and copper) as a function of the amount of cold work (plastic deformation).

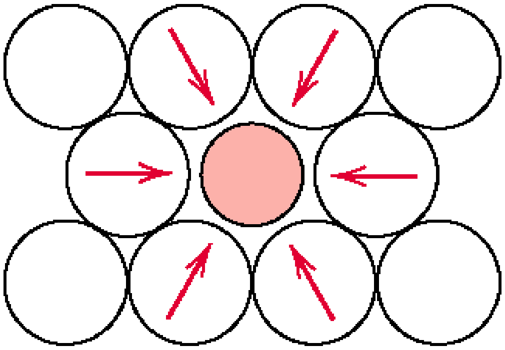
Note that as the strength increases, the ductility decreases.

The effects of strain hardening (or work hardening) may be removed by an appropriate heat treatment

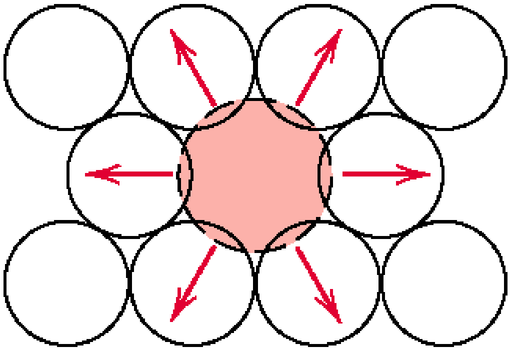
- This process is called **annealing**

If the strain fields associated with dislocations can act to impede their motion and strengthen a material, is there another way to introduce lattice strains?

Consider what happens in the case of substitutional alloying:



In the case of a smaller solute atom



and in the caseof a larger solute atom

In both cases, a lattice strain results from the substitution of a different atom onto a given lattice site.

- Tensile in the case of smaller solutes
- Compressive in the case of larger solutes

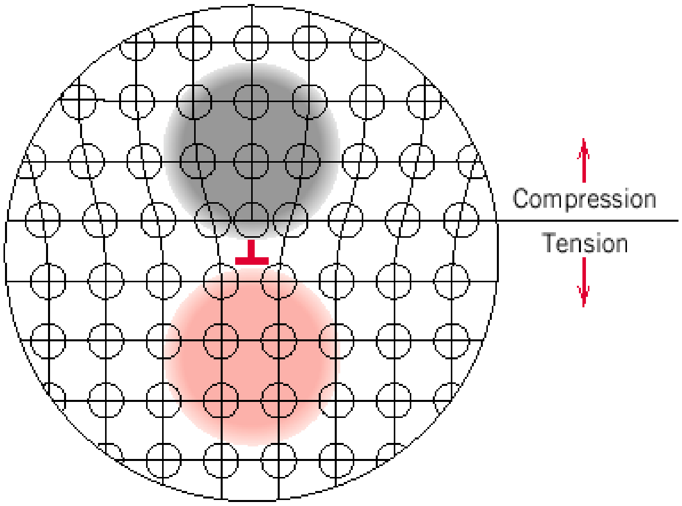
Lattice strain fields resulting from substitutional alloying interact with the dislocation strain fields and impede dislocation movement.

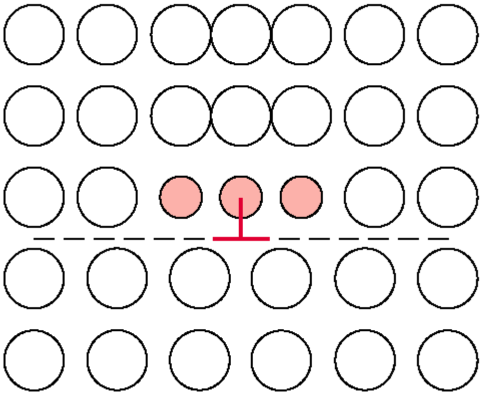
A fundamental principle in solid state physics:

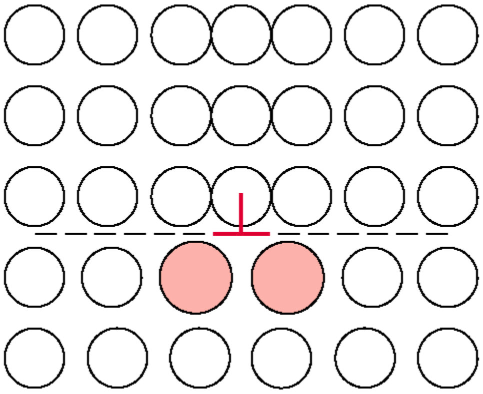
> Materials will respond to stimuli in such a way as to minimize their overall energy.

- There is an energy associated with solute atoms
- There is also an energy associated with dislocations

Diffusion will act to minimize crystalline energy by combining solute atoms and dislocations as shown below:

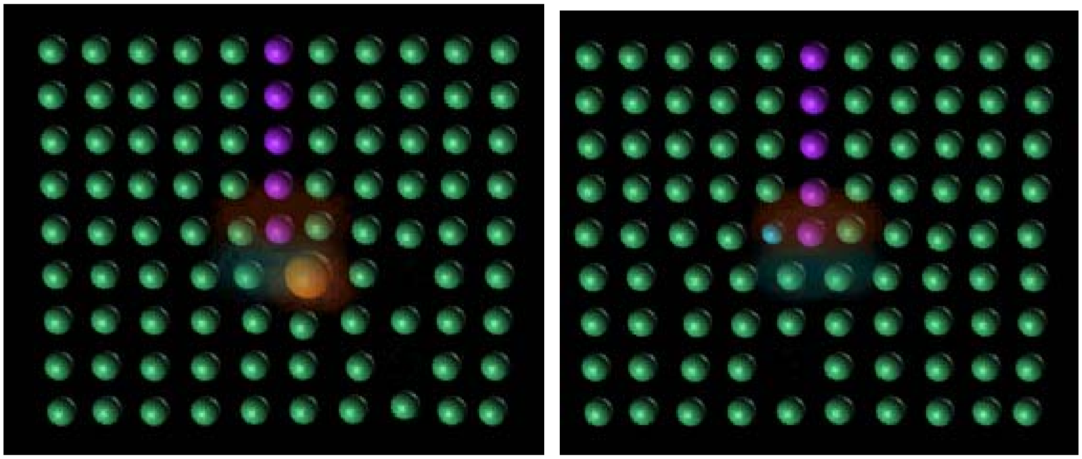






Solute atoms will tend to diffuse to the core of dislocations

- smaller atoms tend to occupy sites within the compressive strain field <u>above</u> the slip plane.
- larger atoms tend to occupy sites within the tensile strain field <u>below</u> the slip plane



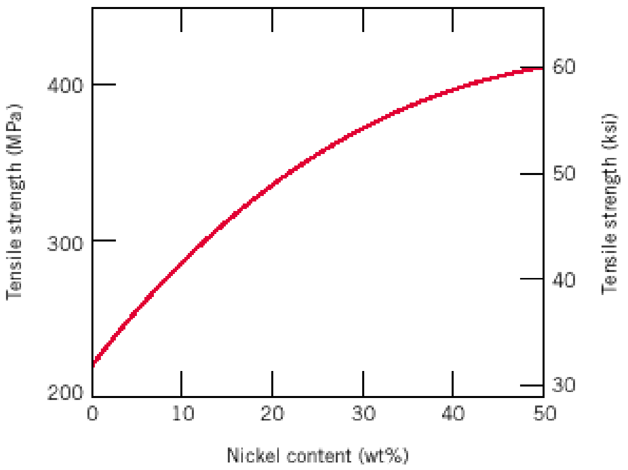
Addition of a larger solute atom (left) or a smaller solute atom (right) partially cancels the dislocation strain field and thereby tends to hold the dislocation in place. The net effect is that the material becomes stronger.

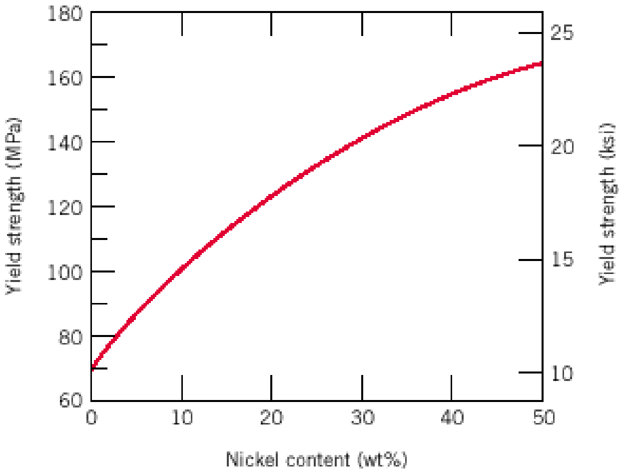
- The net result is that the overall energy of the crystal (i.e., the net strain field) is reduced.

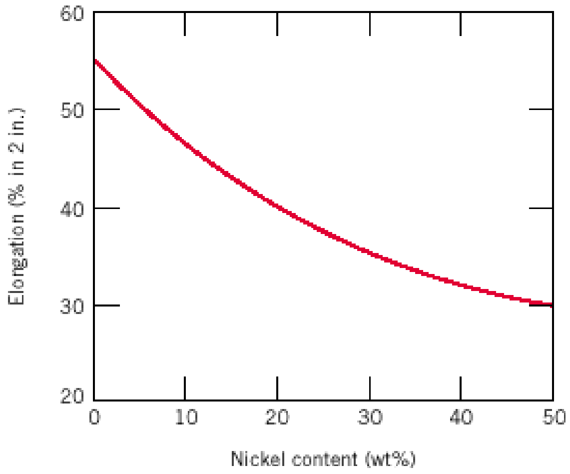
- Since movement of a dislocation would pull it away from the solute atom and increase the overall crystalline energy, this process becomes more difficult (and requires more energy to accomplish)

- Recall the previous in-class tensile test demonstration with ultra-pure Al wire

Examples of the effect of solid solution alloying:







Notice again that as the strength increases, the ductility decreases.

Note also that this argument applied to soluble atoms (insoluble atoms do not have this strengthening effect!)

Thus, our third strengthening mechanism:

Solid solution alloys tend to be stronger than pure metals

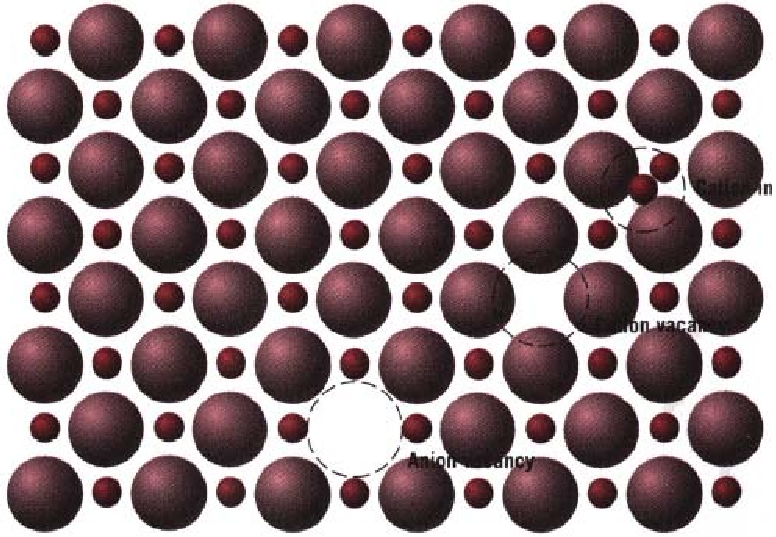
To summarize, the three primary strengthening mechanisms are:

1. **grain size reduction**
2. **work hardening**
3. **solid solution alloying**

A word about ceramics:

Ceramics, as a rule, do not exhibit plastic deformation

- few, if any, active slip systems
- interplanar sliding is not energetically favorable because of the distinct charge distribution of the ions:



- If any plane tries to slip over an adjacent plane, ions of the same charge would be brought closer together (electrostatic repulsion)
- Thus ceramics tend to be intrinsically strong but not very ductile

- **The relevant parameter governing the mechanical behavior of ceramics is not dislocation motion but crack size and crack propagation.**

Finally, the concepts of **Recovery**, **Recrystalliztion**, and **Grain Growth**:

Recovery:

- Plastic deformation ⇒ accumulation of lattice strain
- Elevated temperatures enhance diffusion ⇒ promote mobility of defects
- Higher mobility results in decreased dislocation density ⇒ lower lattice strain

- There is no fixed temperature for recovery. (usually performed slightly above room temperature)
- Recovery does not completely remove all lattice strains
    - Can be useful in dissipating localized high stress regions that could lead to stress-corrosion problems.

Recrystallization:

At sufficiently high temperatures, heavily cold-worked regions produce nuclei of new, stress-free grains.

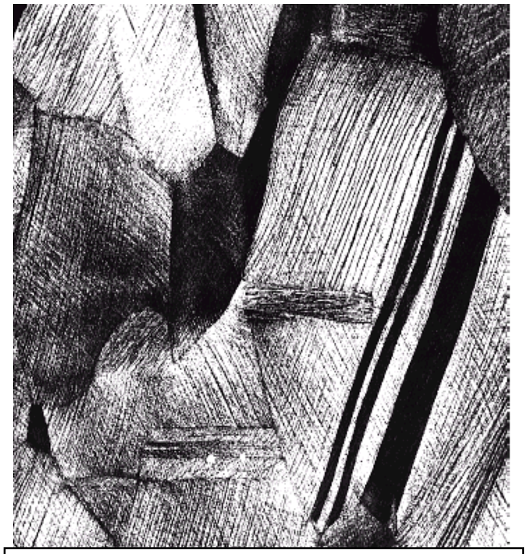
- These nuclei form within regions of highest localized energy such as grain boundaries
    - Grain boundary regions tend to have a high concentration of entangled dislocations
- The nuclei are equiaxed, that is, uniformly-shaped

Why does this happen?

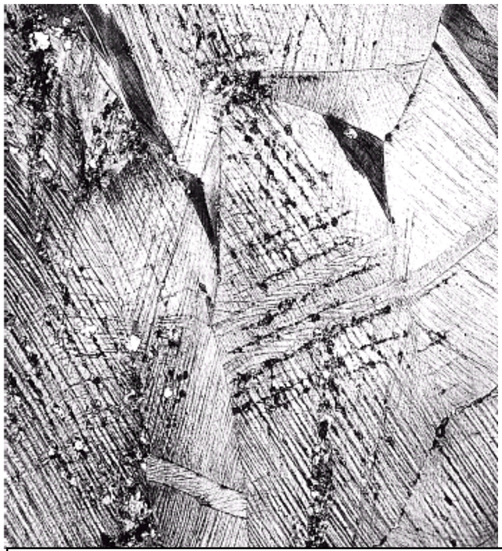
- The driving force for recrystallization is the energy difference between the highly-strained, cold-worked reactants and the strain-free products.
- The crystal "uses" the thermal energy to initiate a "re-arrangement" of atoms to lower the internal strain.
- Mechanical properties of recrystallized metals are restored to their pre-cold worked state (weaker but more ductile).

An example of the effect of recrystallization:

Brass, initially 33% CW:

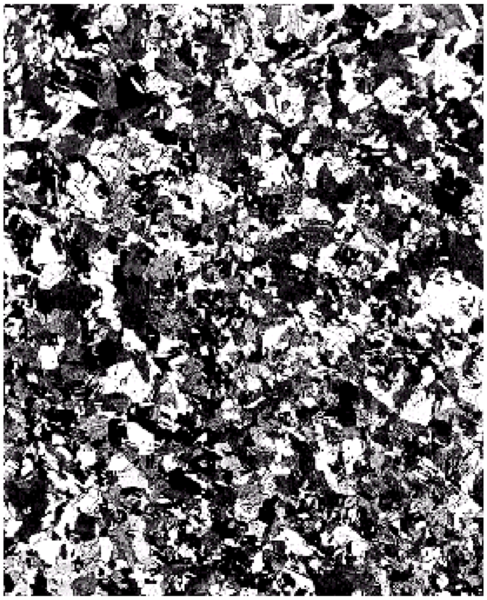


Initial cold-worked microstructure (note the slip lines and twins). These grains contain a considerable amount of potential energy.



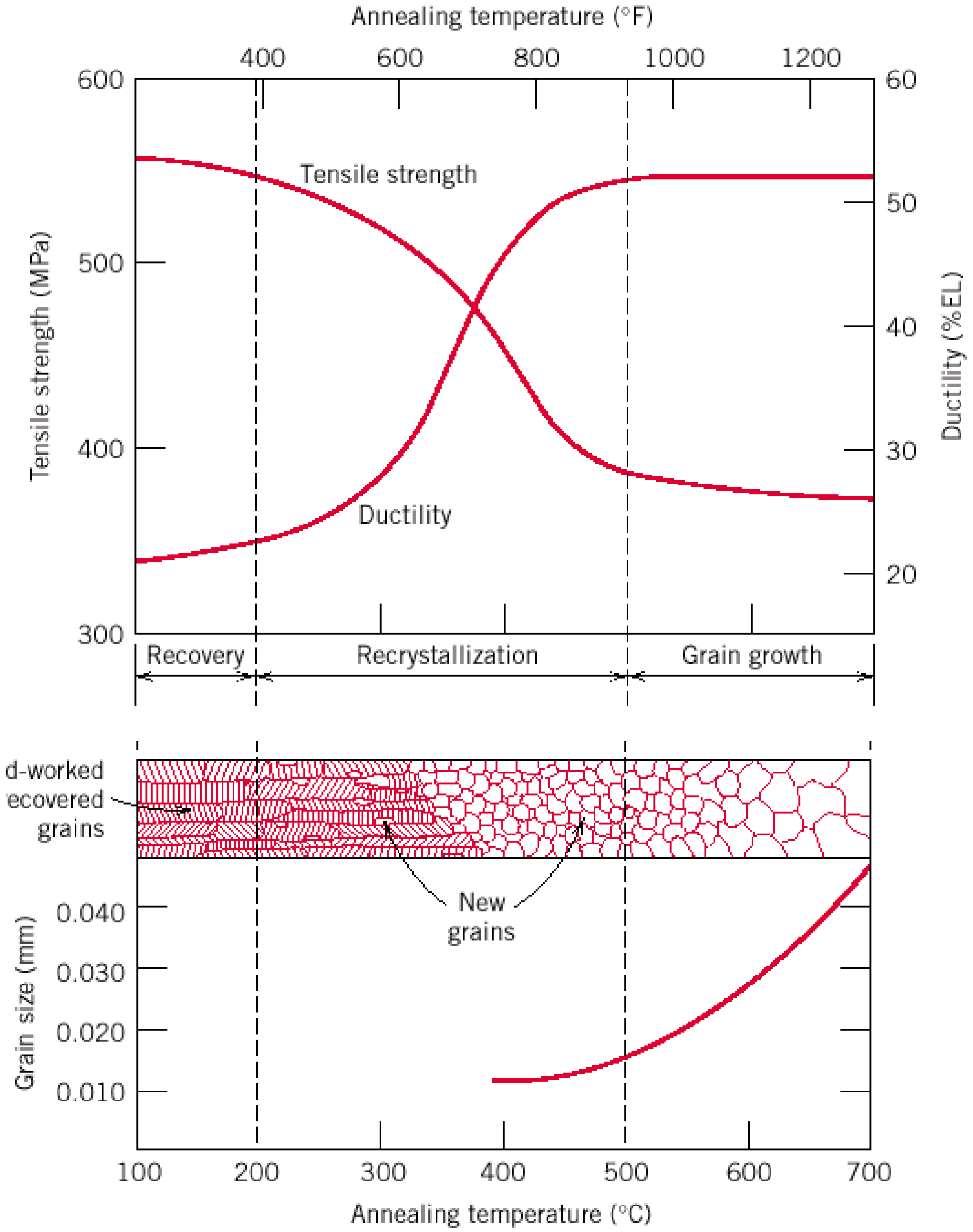
After 3 s at 580°C. Note the presence of miniscule new grains nucleating on slip bands and grain boundaries.

Microstructure after 4 s at 580°C. Notice the large number of new grains that have nucleated



Microstructure after 8 s at 580°C. There has been a complete replacement of cold-worked grains with stress-free grains.

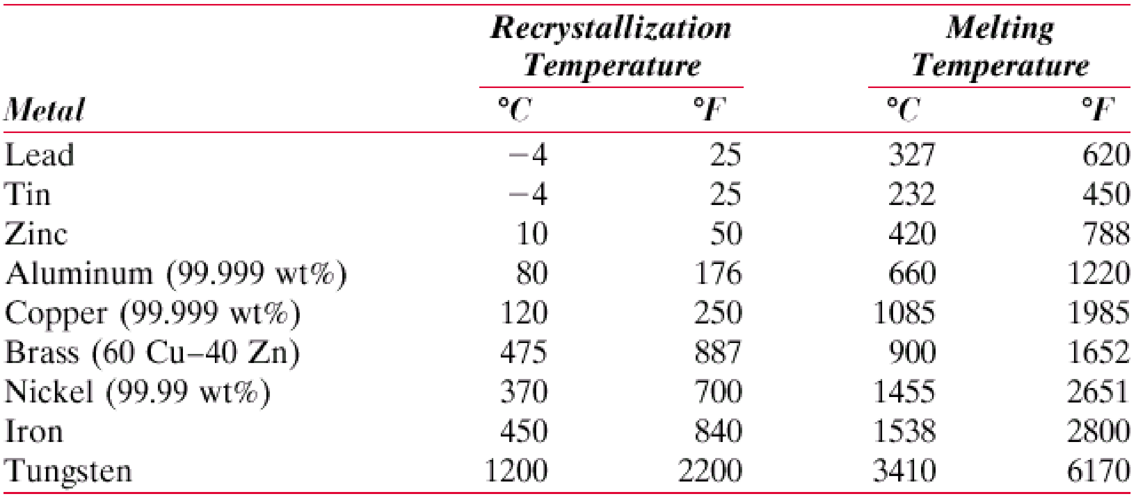
- Recrystallization depends on both time and temperature. Consider the effects of temperature on tensile strength, ductility, and grain size, as shown below:



- Metals are classified by their **recrystallization temperature**
  - (temperature at which recrystallization just reaches completion in 1 hour)
  - $T_{recryst}$(brass) = 450°C

- Rule-of-thumb: recrystallization temperature generally ranges from 33% to 50% of the absolute melting temperature.

The following table lists recrystallization temperatures of various elements and alloys:



	Recrystallization Temperature		*Melting Temperature*	
Metal	*°C*	*°F*	*°C*	*°F*
Lead	−4	25	327	620
Tin	−4	25	232	450
Zinc	10	50	420	788
Aluminum (99.999 wt%)	80	176	660	1220
Copper (99.999 wt%)	120	250	1085	1985
Brass (60 Cu–40 Zn)	475	887	900	1652
Nickel (99.99 wt%)	370	700	1455	2651
Iron	450	840	1538	2800
Tungsten	1200	2200	3410	6170

Note that the recrystallization temperature for Pb, Sn, and Zn is below room temperature. This means that these metals will not work-harden at room temperature.

- These materials continuously recrystallize during work hardening

Finally, **Grain Growth**:

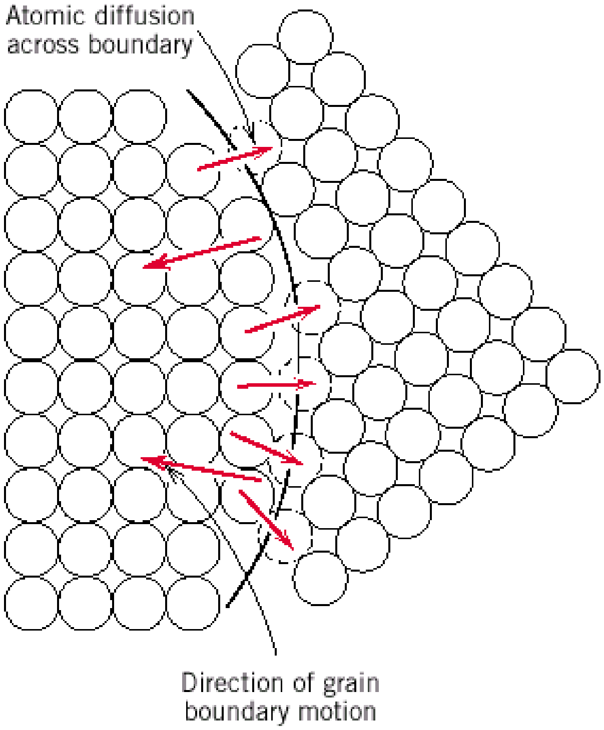
After recrystallization is complete, the material consists of small, stress-free grains.

While the grains themselves may be stress-free, the material now contains a large grain boundary volume.

- Remember that atoms in grain boundaries are in a higher energy configuration than corresponding atoms in the bulk.
- A large volume fraction of grain boundaries contributes to the potential energy of the material.
- There exists a thermodynamic driving force to reduce <u>this excess grain boundary energy</u>
- This process is called grain growth

Grain growth is a diffusional process (which means that it has an explicit temperature dependence)

Grain growth proceeds by the diffusion of atoms across grain boundaries:



Notice how the diffusive flux is in the opposite direction to the grain boundary motion.

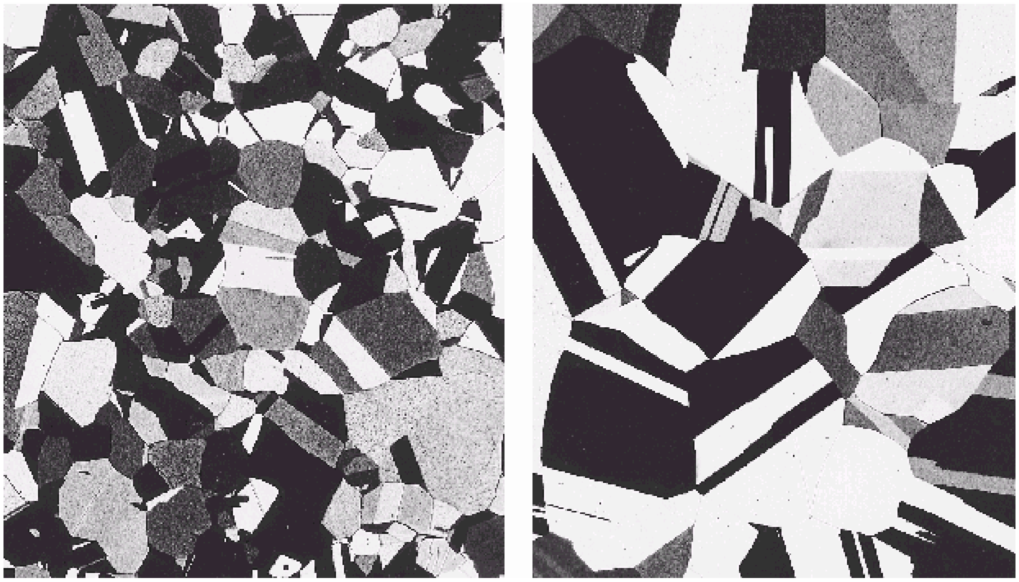
Large grains grow at the expense of small grains

- This is another consequence of thermodynamics

The direction of grain growth is always towards the center of curvature

One can control the grain size (and thus the mechanical properties) by an appropriate heat treatment (a combination of time, temperature, and atmosphere)

Let's revisit the brass specimen that previously experienced recovery and recrystallization. Suppose we continue to hold the material at elevated temperature:

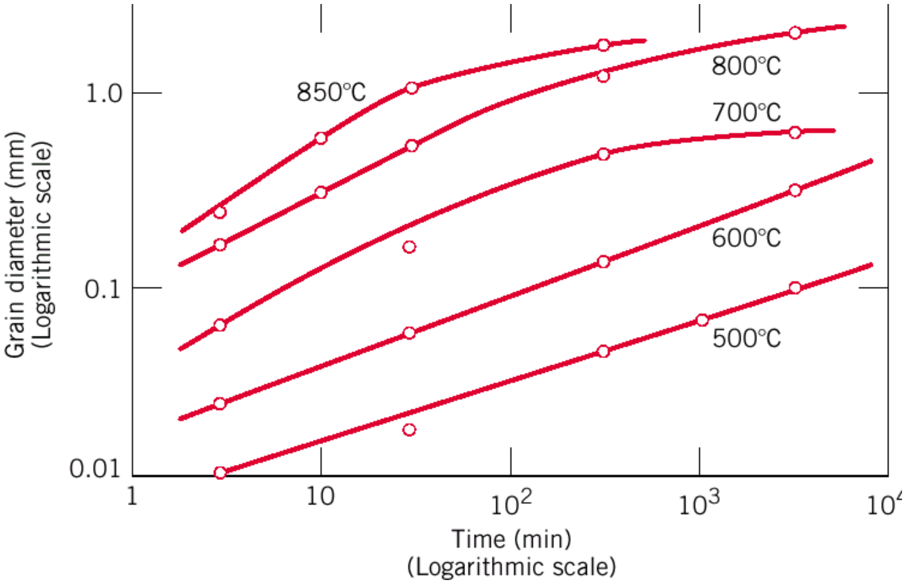


The micrograph on the left show the microstructure after 15 min. at 580°C. The micrograph on the right shows the microstructure after 10 min. at 700°C. Compare the grain size with that immediately after recrystallization.

The rate of grain growth depends on temperature through the relation

$$d^n - d_o^n = Kt$$

where d_o is the initial grain size at time $t = 0$, d^n is the grain size after time t, and K is a constant. For many materials, $n \geq 2$.


850°C
800°C
700°C
600°C
500°C
1.0
0.1
0.01
1
10
10^2
10^3
10^4
Grain diameter (mm)
(Logarithmic scale)
Time (min)
(Logarithmic scale)