Diffusion

Diffusion - Mass transport by atomic motion

Mechanisms

•Gases & Liquids – random (Brownian) motion

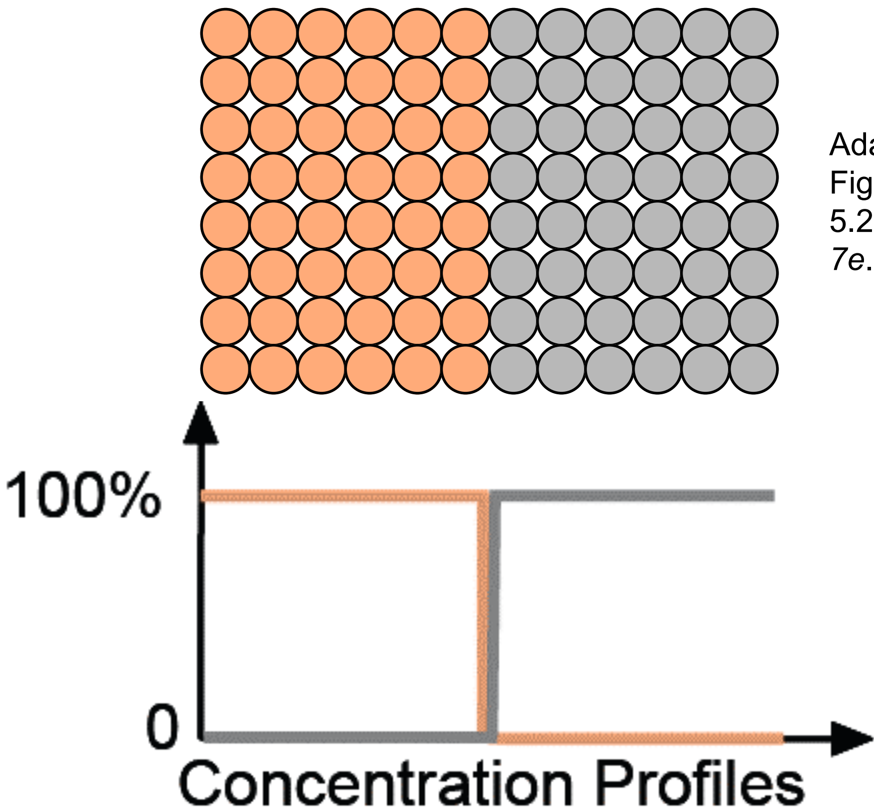
•Solids – vacancy diffusion or interstitial diffusion

Interdiffusion: In an alloy, atoms tend to migrate from regions of high conc. to regions of low conc.

Self-diffusion: In an elemental solid, atoms also migrate.

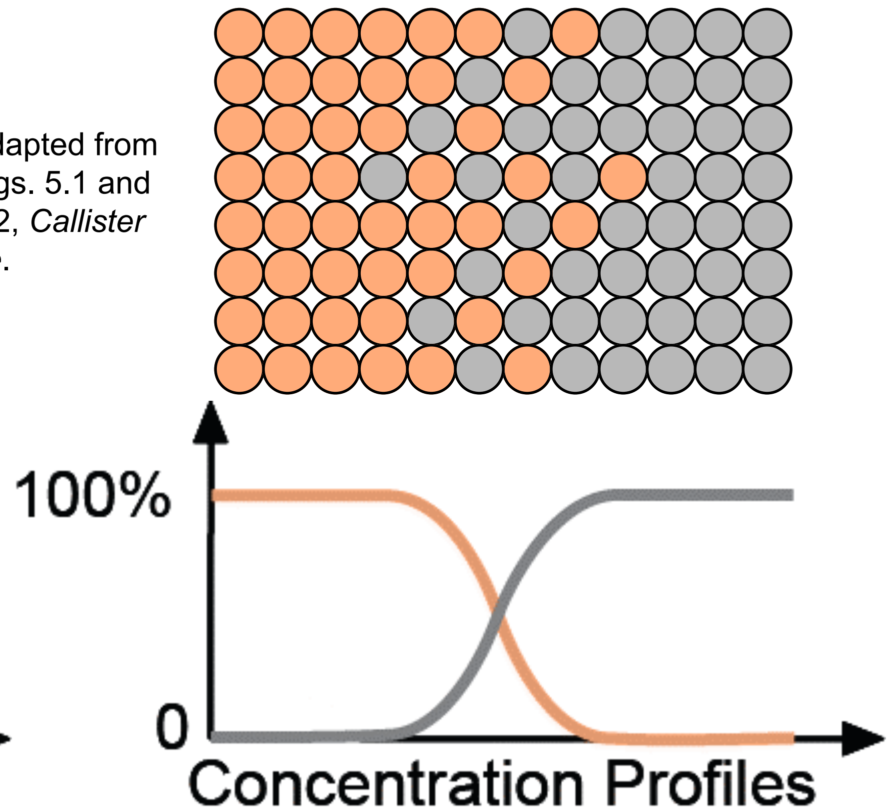
Interdiffusion

Initially



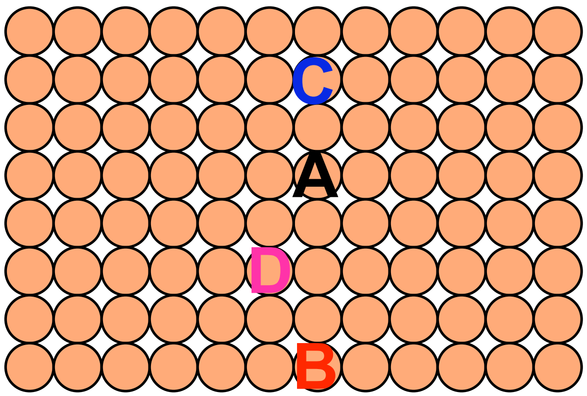
Adapted from Figs. 5.1 and 5.2, *Callister 7e*.

After some time

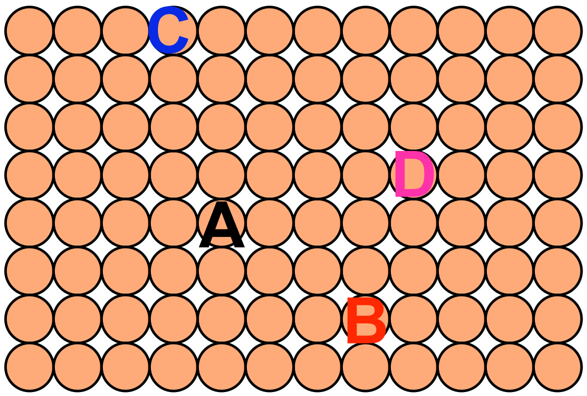


Self-diffusion

Label some atoms



After some time



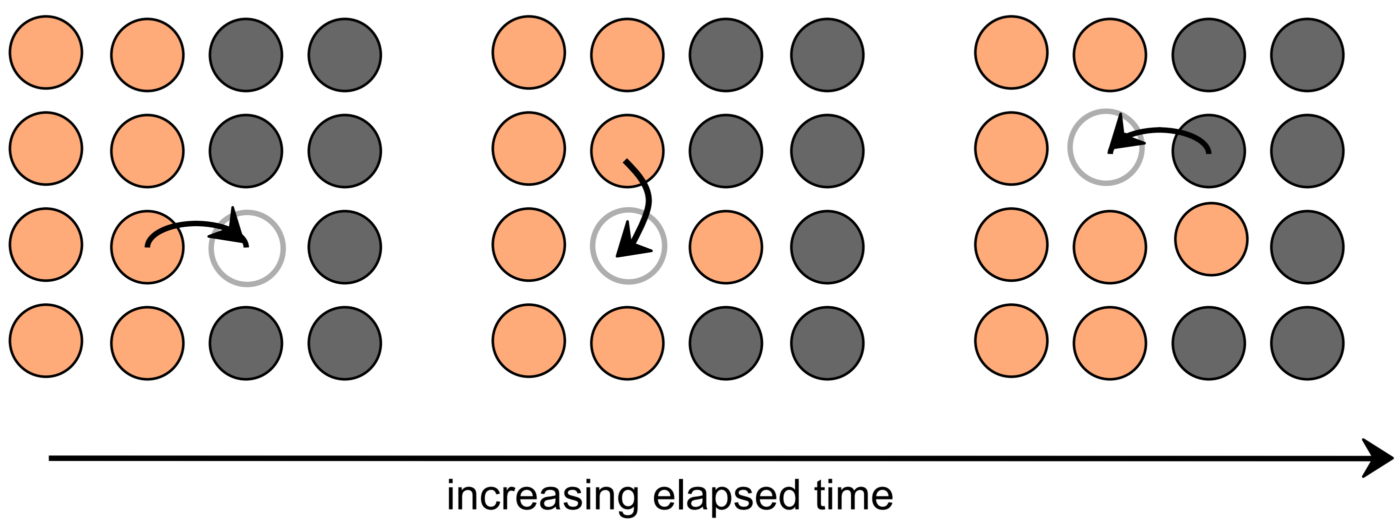
Diffusion mechanisms

Conditions:

- There must be an empty site available
- Atoms must have the energy to make the jump

Vacancy Diffusion:

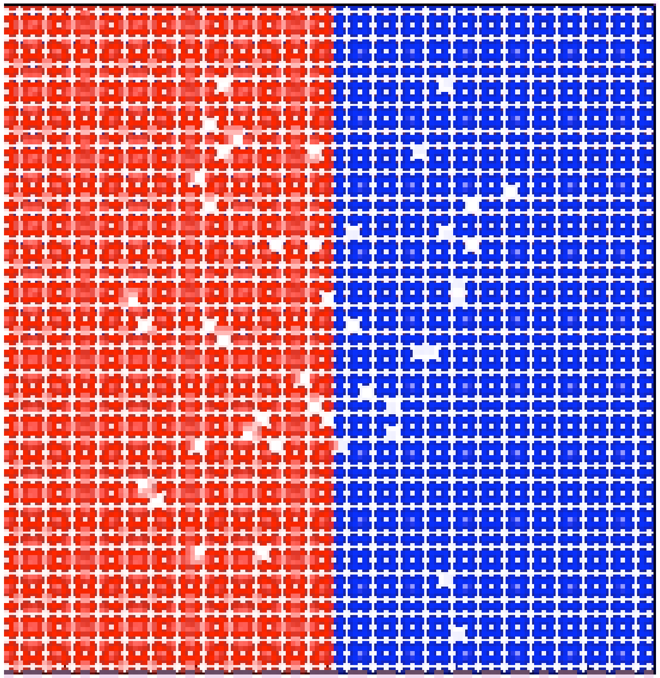
- atoms exchange with vacancies
- applies to substitutional impurities atoms
- rate depends on:
  - --number of vacancies
  - --activation energy to exchange.



Diffusion simulation

• Simulation of interdiffusion across an interface:

• Rate of substitutional diffusion depends on:
  --vacancy concentration
  --frequency of jumping.



(Courtesy P.M. Anderson)

Diffusion flux

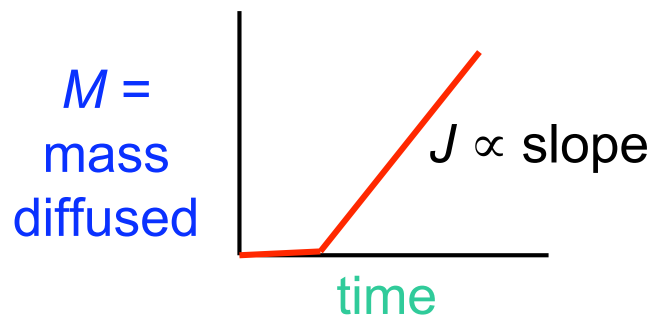
How do we quantify the amount or rate of diffusion?

$$J \equiv \text{Flux} \equiv \frac{\text{moles (or mass) diffusing}}{(\text{surface area})(\text{time})} = \frac{\text{mol}}{\text{cm}^2\text{s}} \text{ or } \frac{\text{kg}}{\text{m}^2\text{s}}$$

Measured empirically

- Make thin film (membrane) of known surface area
- Impose concentration gradient
- Measure how fast atoms or molecules diffuse through the membrane

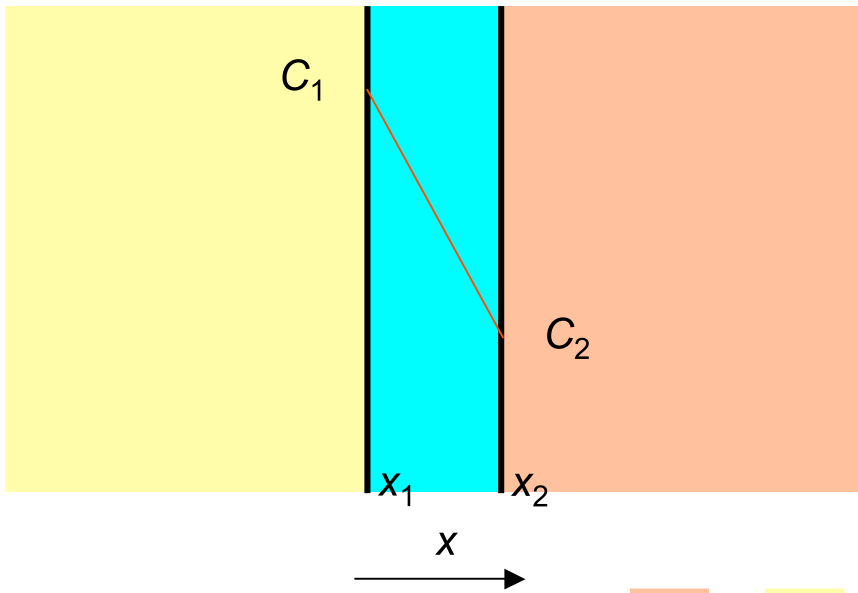
$$J = \frac{M}{At} = \frac{1}{A}\frac{dM}{dt}$$



Steady-state diffusion

Rate of diffusion independent of time

Flux proportional to concentration gradient = $\dfrac{dC}{dx}$



Fick's first law of diffusion

$$\boxed{J = -D\frac{dC}{dx}}$$

$D \equiv$ diffusion coefficient

$$\text{if linear } \frac{dC}{dx} \cong \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1}$$

Diffusion and temperature

- Diffusion coefficient increases with increasing *T*.

$$D = D_o \exp\left(-\frac{Q_d}{R\,T}\right)$$

D = diffusion coefficient [m^2/s]

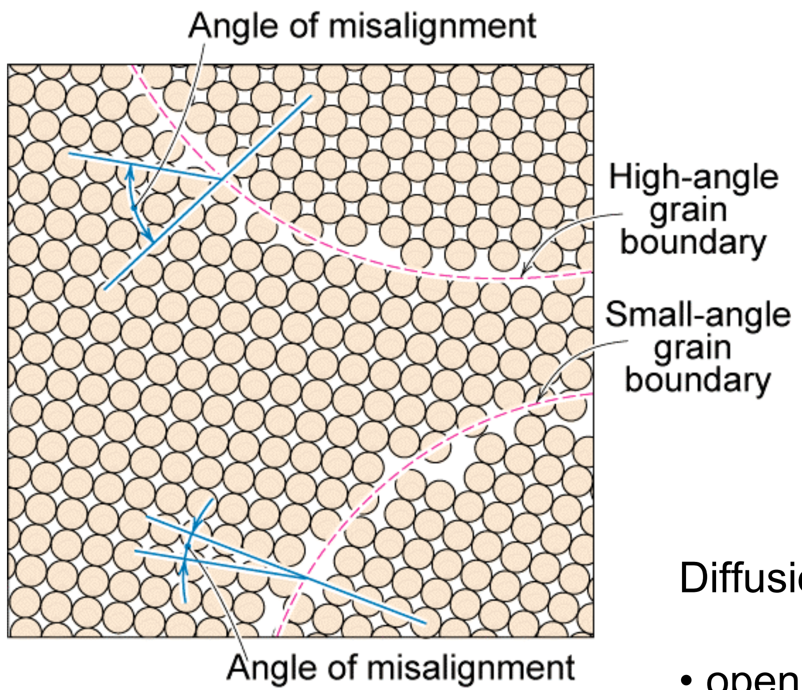
D_o = pre-exponential [m^2/s]

Q_d = activation energy [J/mol or eV/atom]

R = gas constant [8.314 J/mol-K]

T = absolute temperature [K]

Diffusion paths



Diffusion FASTER for...

- open crystal structures
- materials w/secondary bonding
- smaller diffusing atoms
- lower density materials

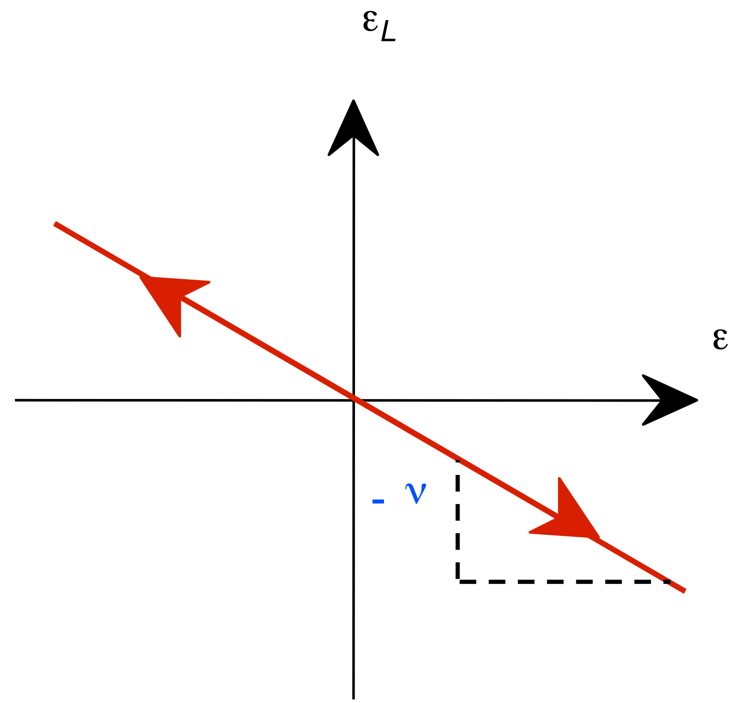
Diffusion SLOWER for...

- close-packed structures
- materials w/covalent bonding
- larger diffusing atoms
- higher density materials

Elastic properties of materials

- **Poisson's ratio, ν:**

$$\nu = -\frac{\varepsilon_L}{\varepsilon}$$



metals: $\nu \sim 0.33$
ceramics: $\nu \sim 0.25$
polymers: $\nu \sim 0.40$

Units:
E: [GPa] or [psi]
ν: dimensionless

–ν > 0.50 density increases

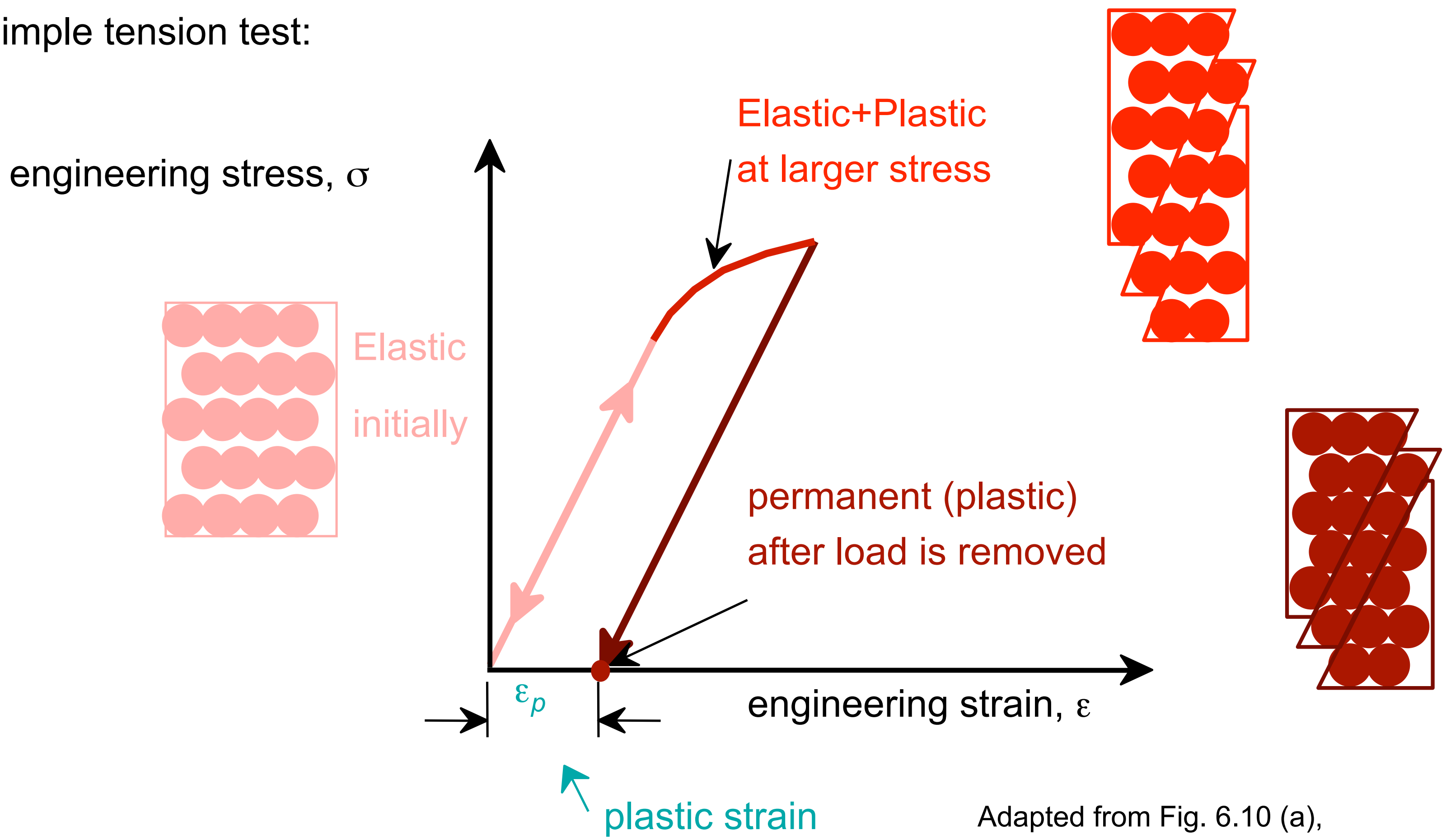
–ν < 0.50 density decreases (voids form)

–For *isotropic* materials

$E = 2G\,(1+\nu)$

Plastic deformation

• Simple tension test:

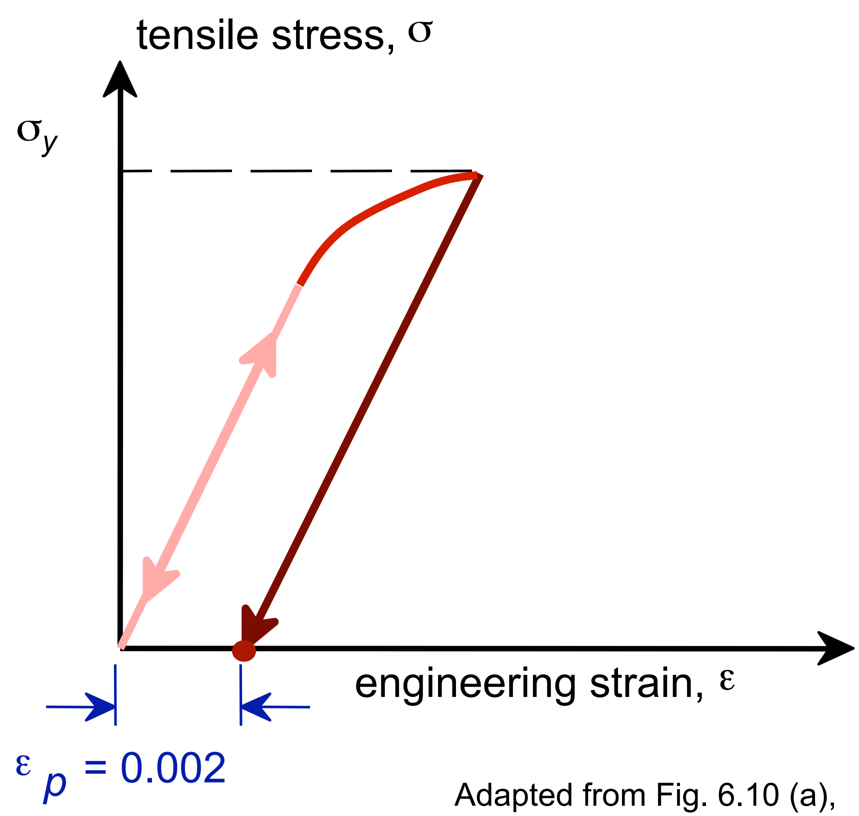


Adapted from Fig. 6.10 (a), *Callister 7e.*

Yield strength, σ_y

- **Stress at which *noticeable* plastic deformation has occurred.**

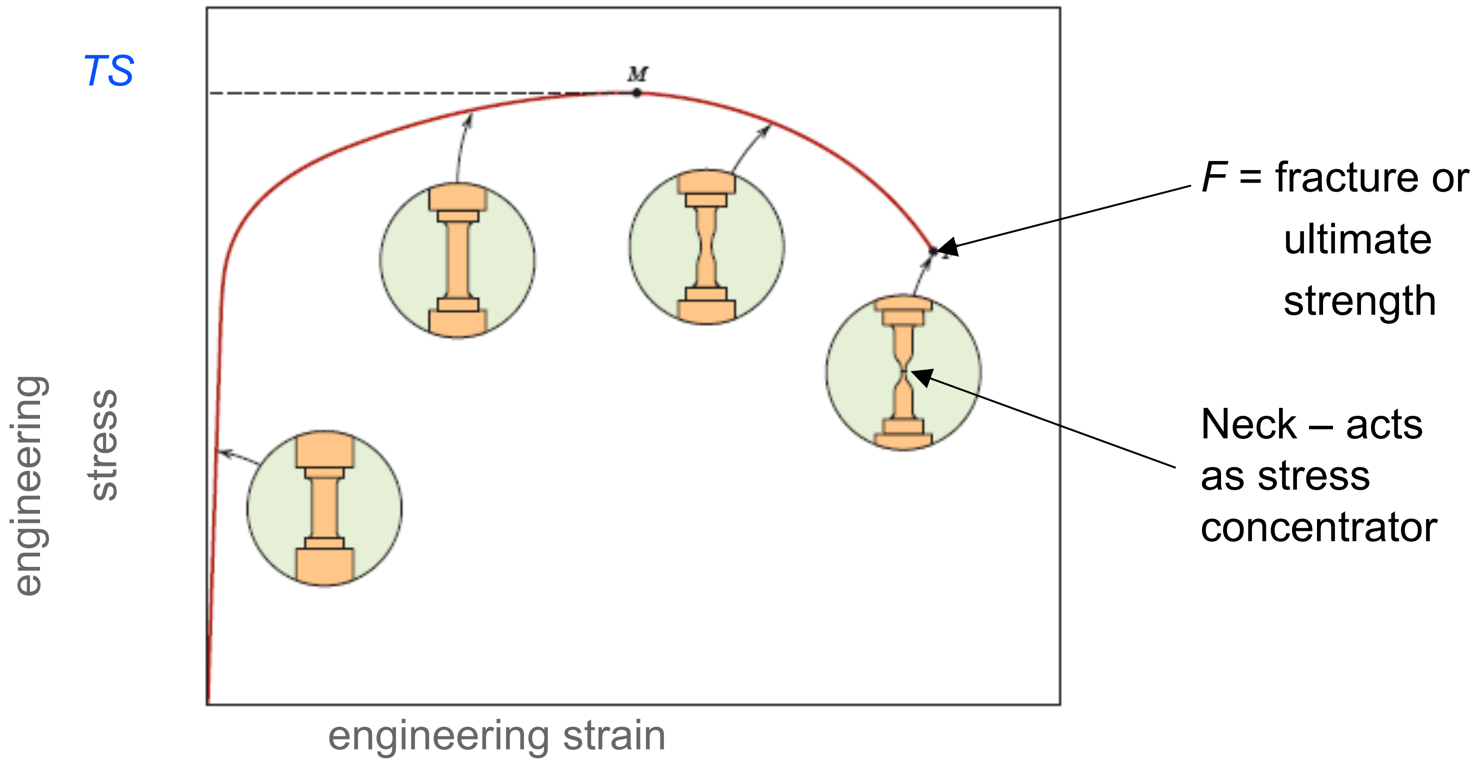
when $\varepsilon_p = 0.002$



Adapted from Fig. 6.10 (a), *Callister 7e.*

Tensile strength, TS

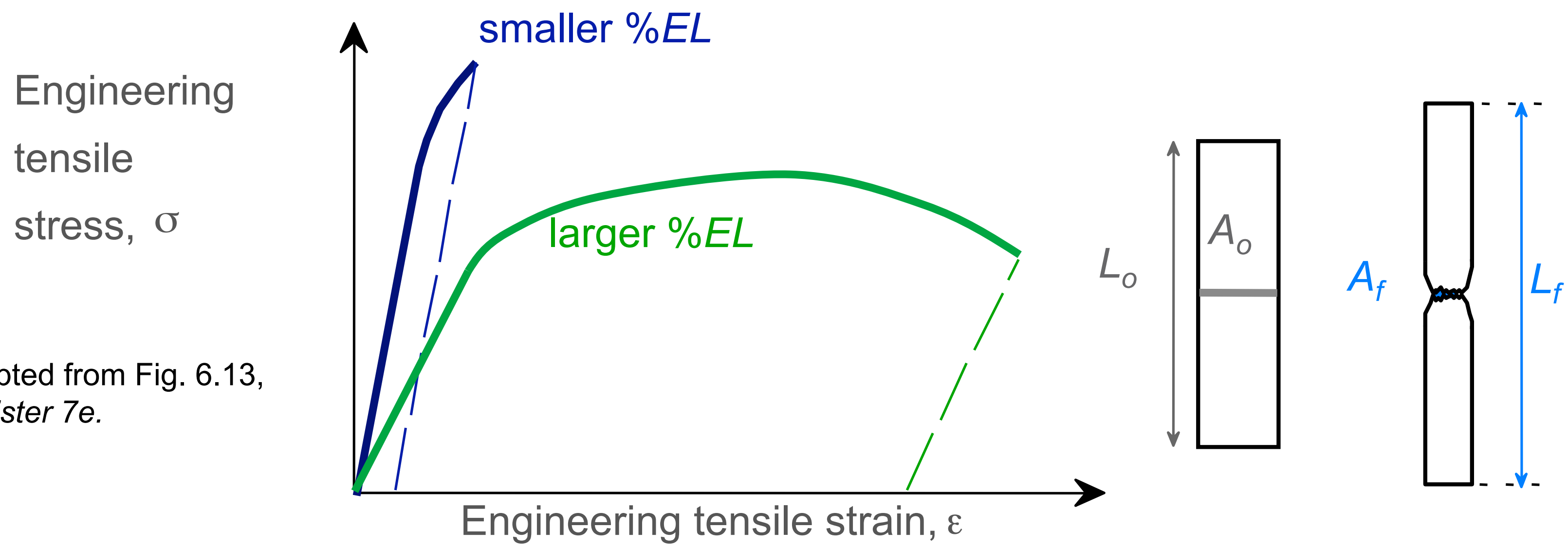
- Maximum stress on engineering stress-strain curve.



- Metals: occurs when noticeable necking starts.
- Polymers: occurs when polymer backbone chains are aligned and about to break.

Ductility

- Plastic tensile strain at failure: $\% EL = \frac{L_f - L_o}{L_o} \times 100$

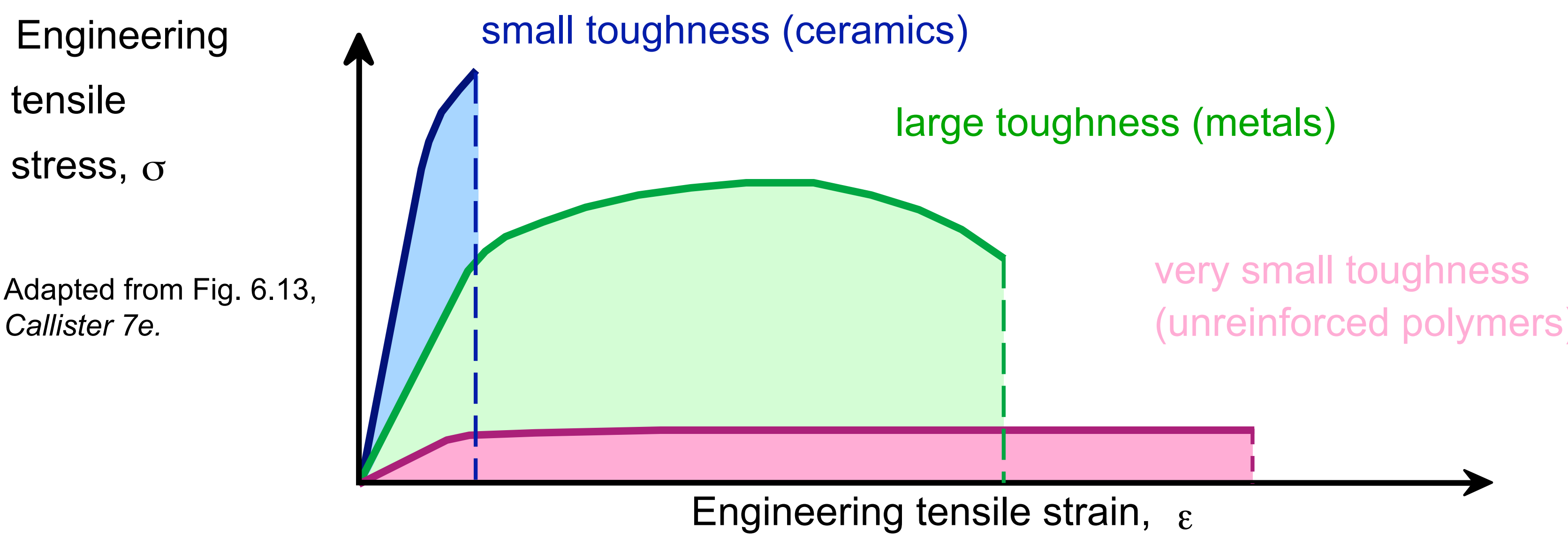


Adapted from Fig. 6.13, *Callister 7e.*

- Another ductility measure: $\% RA = \frac{A_o - A_f}{A_o} \times 100$

Toughness

- Energy to break a unit volume of material
- Approximate by the area under the stress-strain curve.

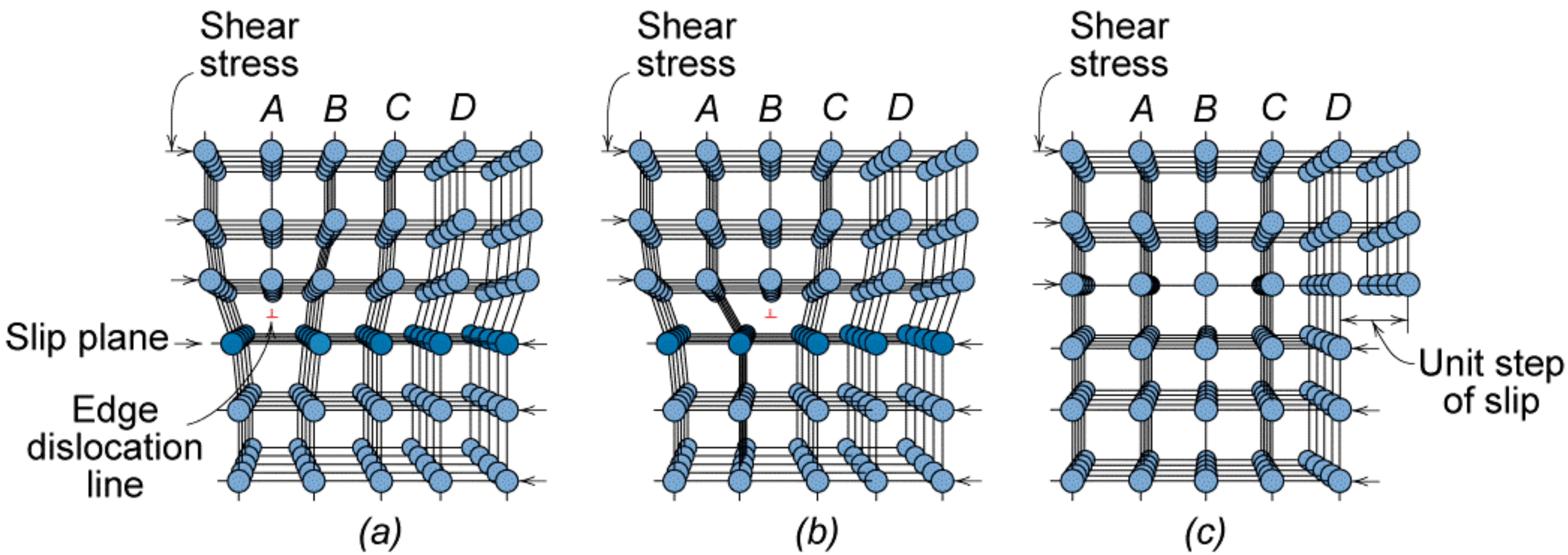


Adapted from Fig. 6.13, *Callister 7e.*

Brittle fracture: elastic energy
Ductile fracture: elastic + plastic energy

Dislocation and plastic deformation

- Cubic & hexagonal metals - plastic deformation by plastic shear or slip where one plane of atoms slides over adjacent plane by defect motion (dislocations).

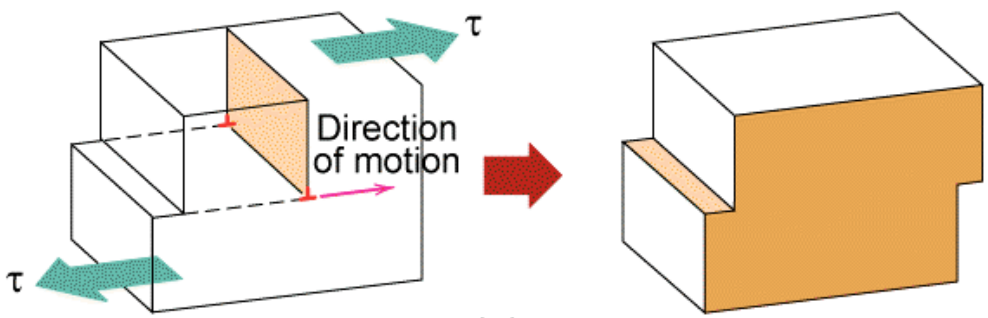


- If dislocations don't move, deformation doesn't occur!

Adapted from Fig. 7.1, *Callister 7e.*

Dislocation motion

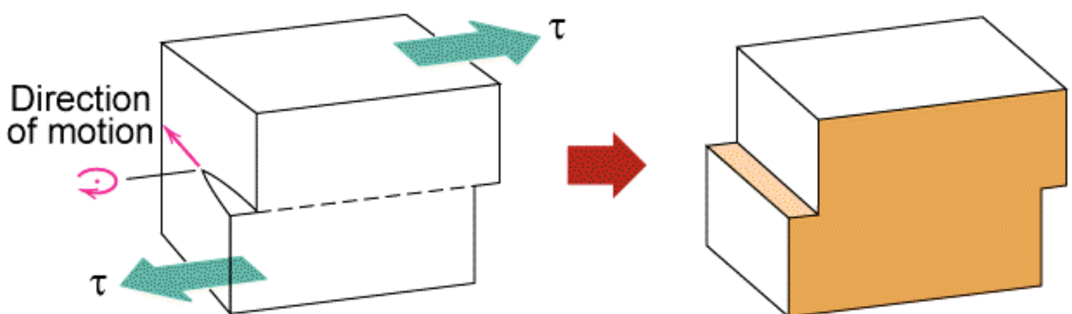
- Dislocation moves along slip plane in slip direction perpendicular to dislocation line
- Edge dislocations move parallel to the applied force, screw dislocations move perpendicular to the applied force



(a)

Edge dislocation

Adapted from Fig. 7.2, *Callister 7e.*

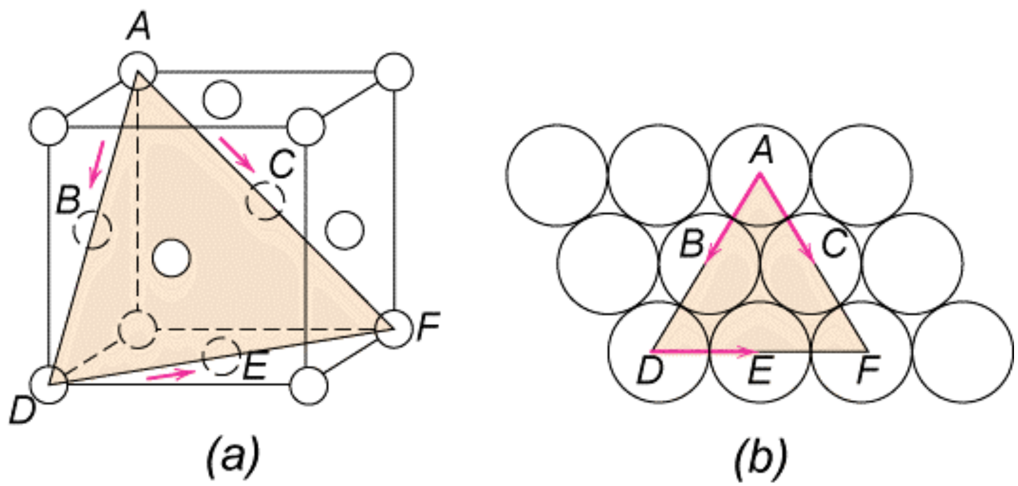


(b)

Screw dislocation

Deformation mechanisms

- Slip System
  - Slip plane - plane allowing easiest slippage
  - Slip direction - direction of movement

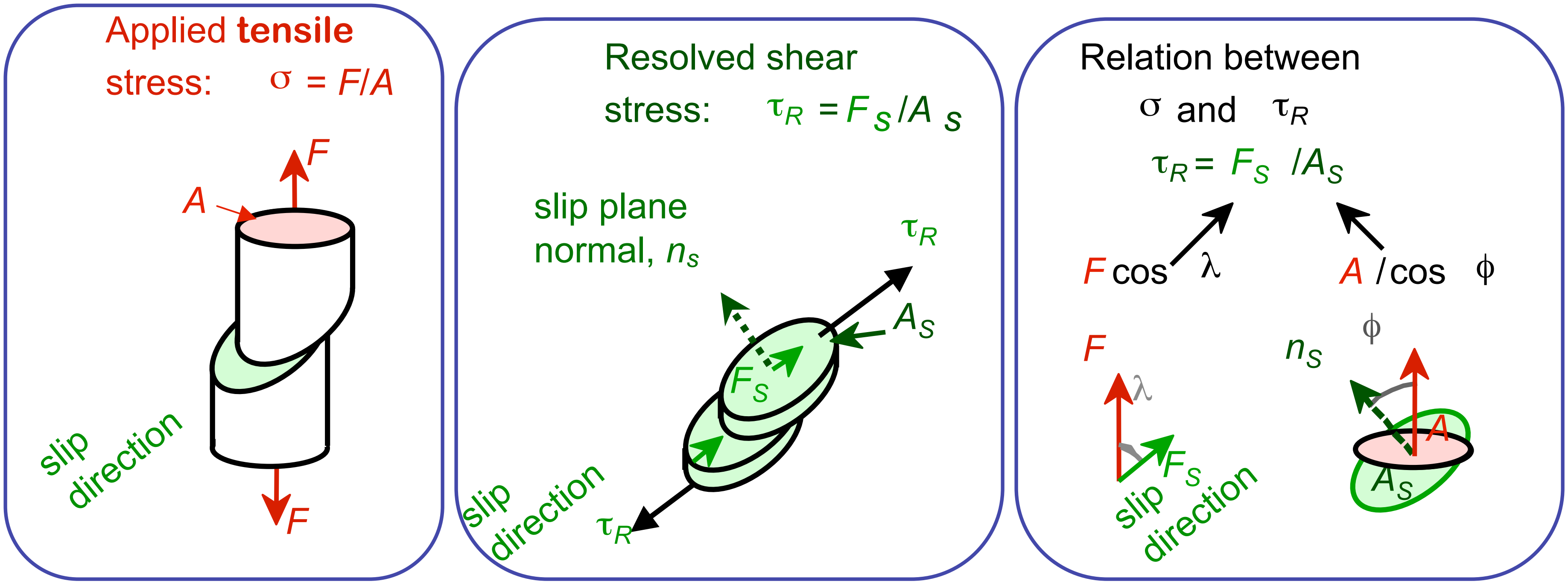


Adapted from Fig. 7.6, *Callister 7e.*

  - FCC Slip occurs on {111} planes (close-packed) in <110> directions (close-packed)
    - => total of 12 slip systems in FCC

Slip in single crystals

- Crystals slip due to a resolved shear stress, τ_R.
- Applied tension can produce such a stress.



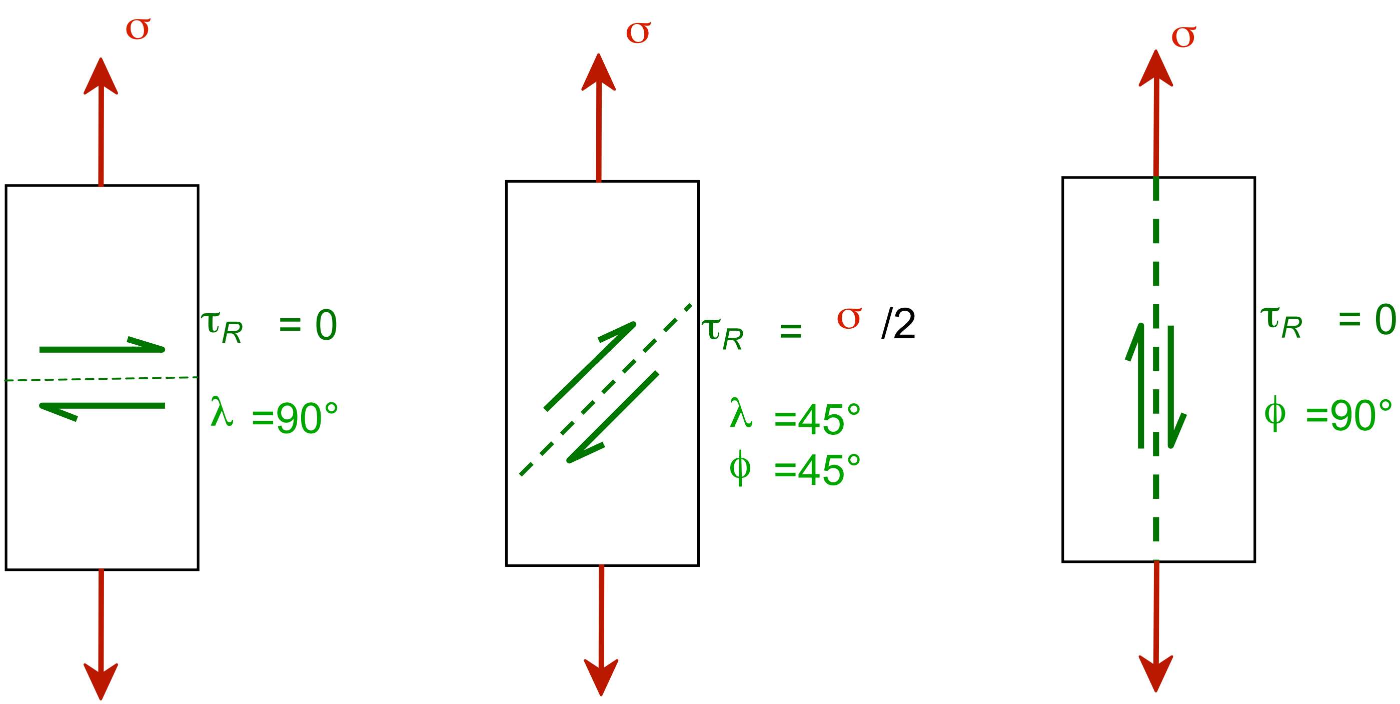
$$\tau_R = \sigma \cos \lambda \cos \phi$$

Critical resolved shear stress

- Condition for dislocation motion: $\tau_R > \tau_{CRSS}$

- Crystal orientation can make it easy or hard to move dislocation

$$\tau_R = \sigma \cos\lambda \cos\phi$$



τ maximum at λ = φ = 45º

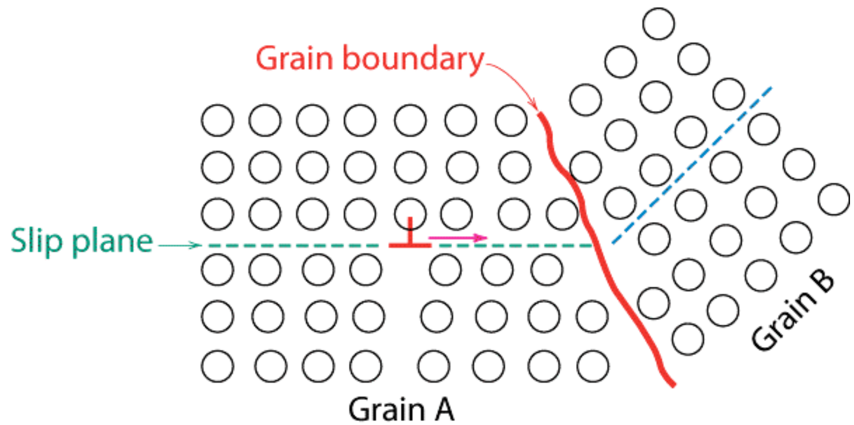
Slip motion in polycrystals

- Stronger - grain boundaries pin deformations
- Slip planes & directions (λ, ϕ) change from one crystal to another.
- τ_R will vary from one crystal to another.
- The crystal with the largest τ_R yields first.
- Other (less favorably oriented) crystals yield later.

Adapted from Fig. 7.10, *Callister 7e.* (Fig. 7.10 is courtesy of C. Brady, National Bureau of Standards [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Strategies for strengthening: grain size reduction

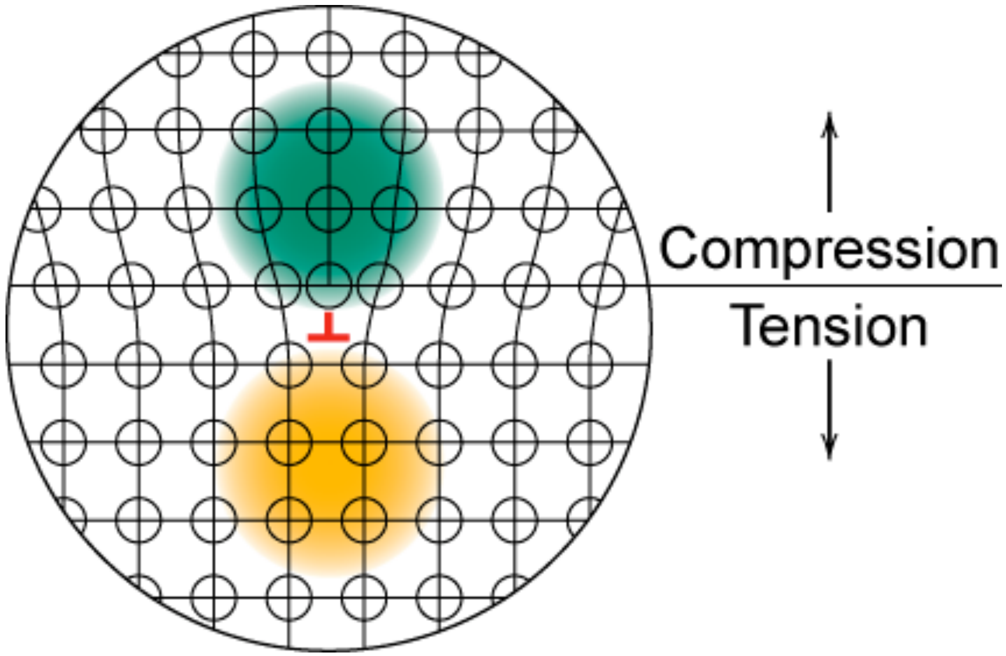
- Grain boundaries are barriers to slip.
- Barrier "strength” increases with increasing angle of misorientation.
- Smaller grain size: more barriers to slip.



Adapted from Fig. 7.14, *Callister 7e.*
(Fig. 7.14 is from *A Textbook of Materials Technology*, by Van Vlack, Pearson Education, Inc., Upper Saddle River, NJ.)

- Hall-Petch Equation: $\sigma_{yield} = \sigma_o + k_y d^{-1/2}$

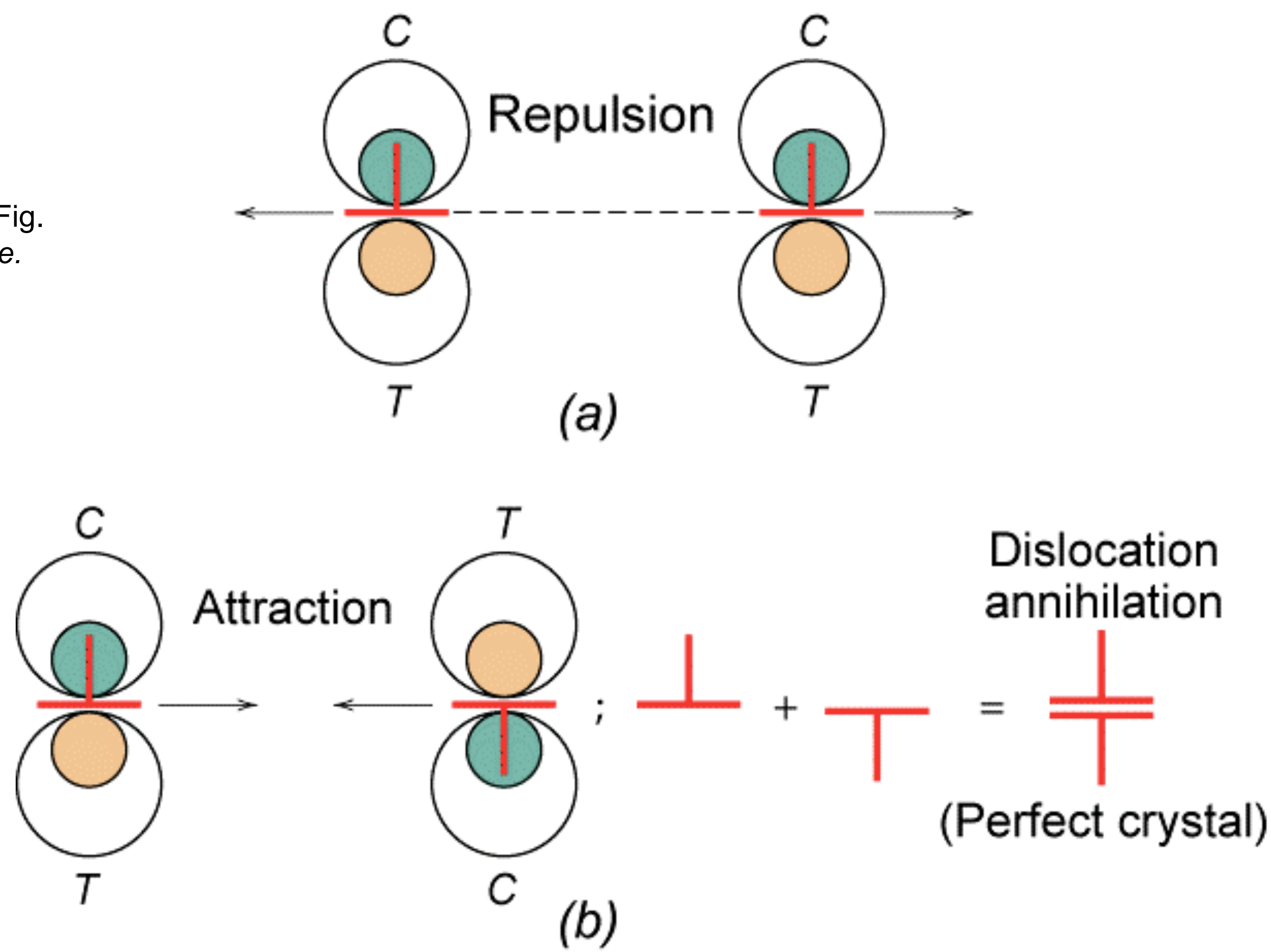
Strategies for strengthening: solid solutions



Adapted from Fig. 7.4, *Callister 7e.*

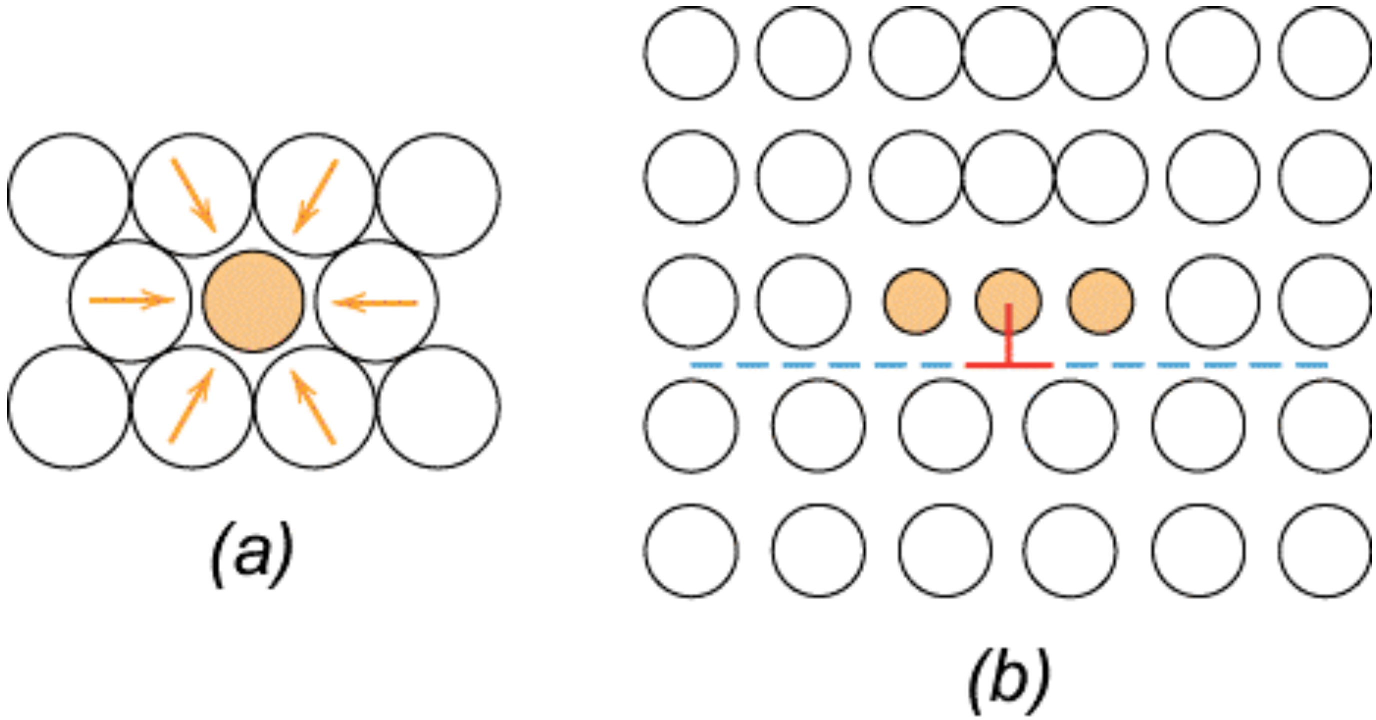
Effects of stress at dislocations

Adapted from Fig. 7.5, *Callister 7e.*



Strengthening by alloying

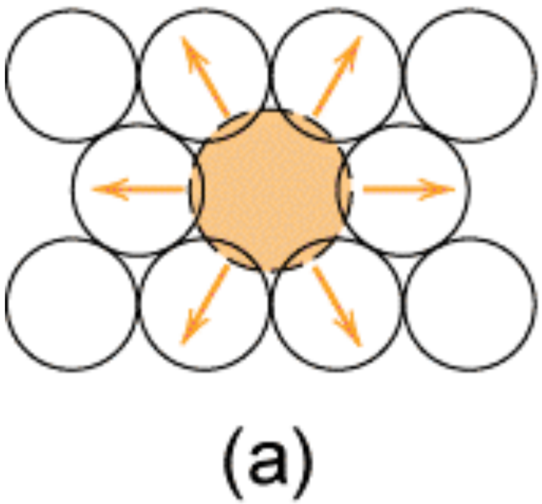
- small impurities tend to concentrate at dislocations
- reduce mobility of dislocation ∴ increase strength

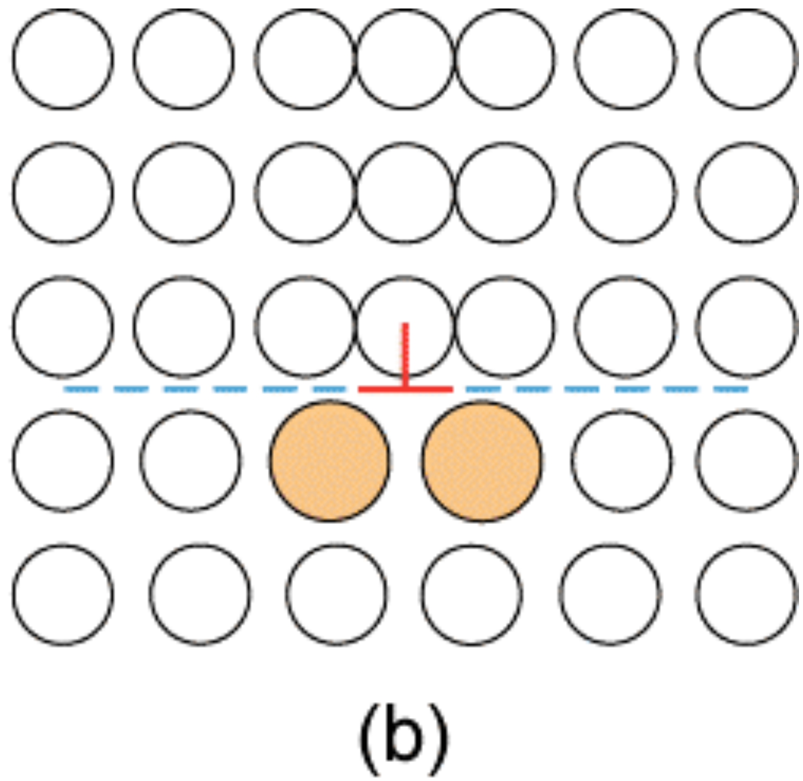


Adapted from Fig. 7.17, *Callister 7e.*

Strengthening by alloying

- large impurities concentrate at dislocations on low density side

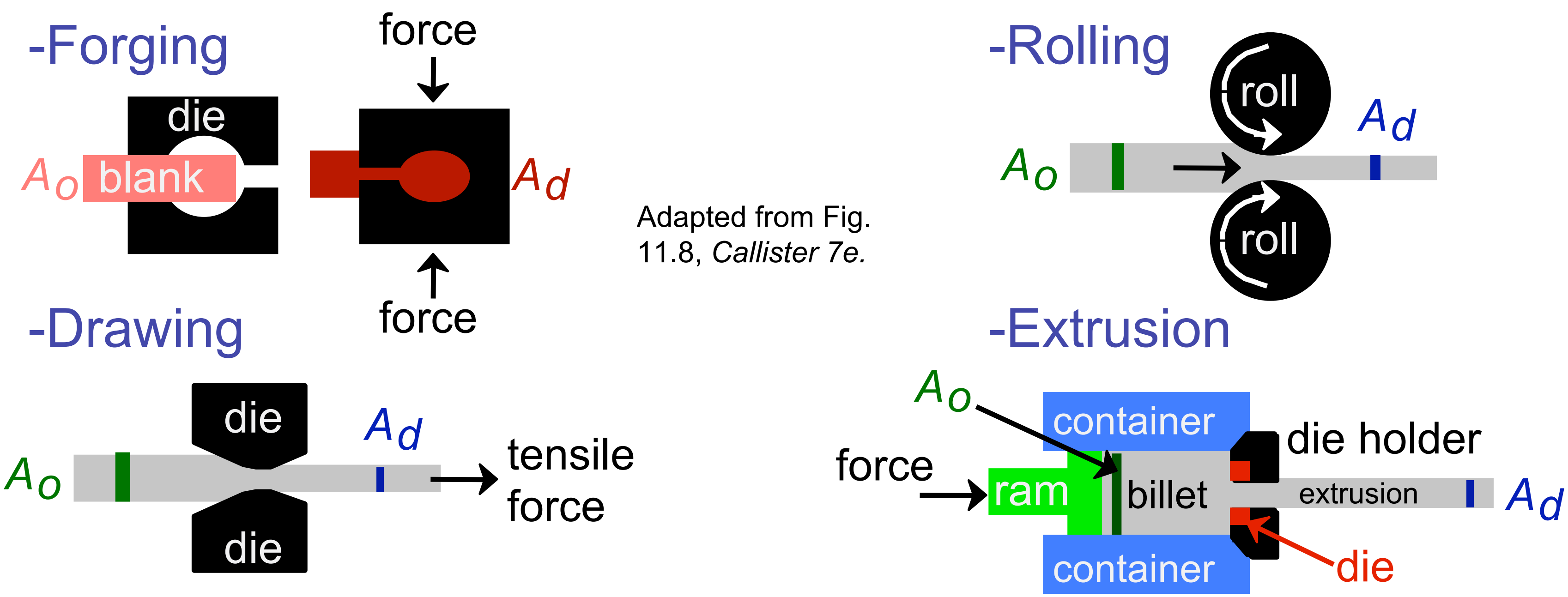




Adapted from Fig. 7.18, *Callister 7e.*

Strategies for strengthening: Cold work (%CW)

- Room temperature deformation.
- Common forming operations change the cross sectional area:



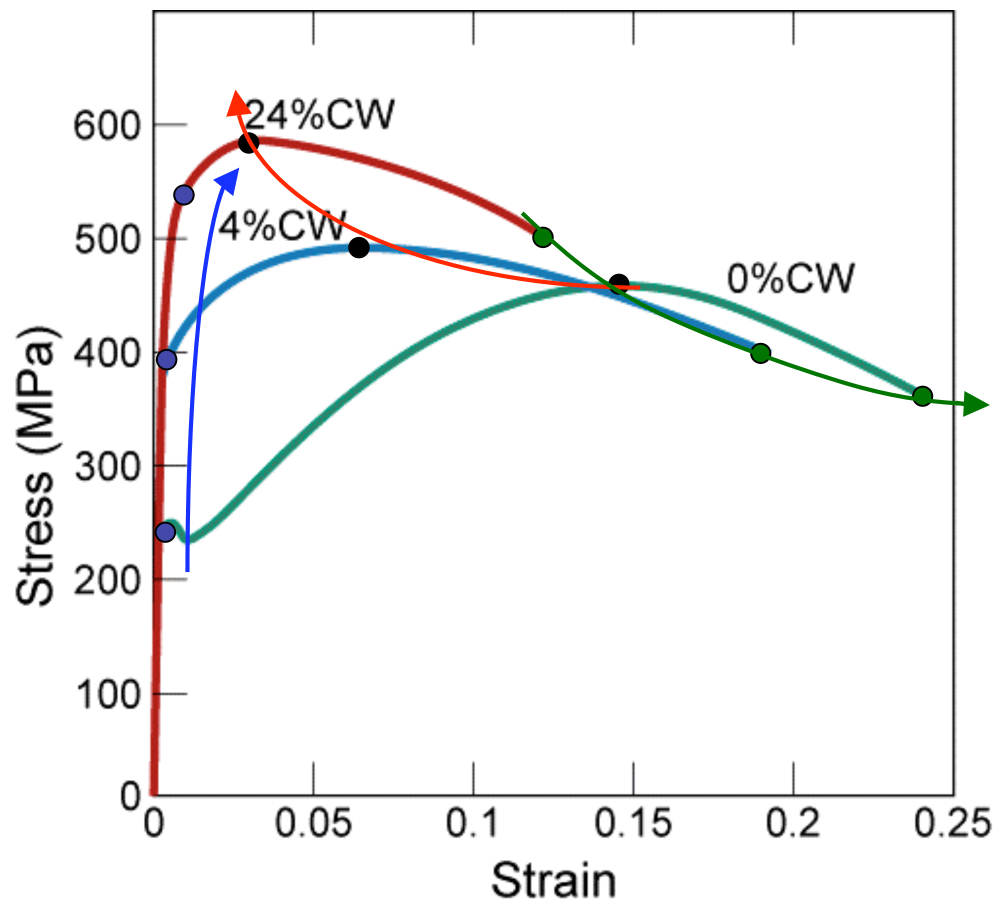
Adapted from Fig. 11.8, *Callister 7e.*

$$\%CW = \frac{A_o - A_d}{A_o} \times 100$$

Impact of cold work

As cold work is increased

- Yield strength (σ_y) increases.
- Tensile strength (*TS*) increases.
- Ductility (%*EL* or %*AR*) decreases.



Adapted from Fig. 7.20, *Callister 7e.*