Diffusion

Diffusion - Mass transport by atomic motion

Mechanisms

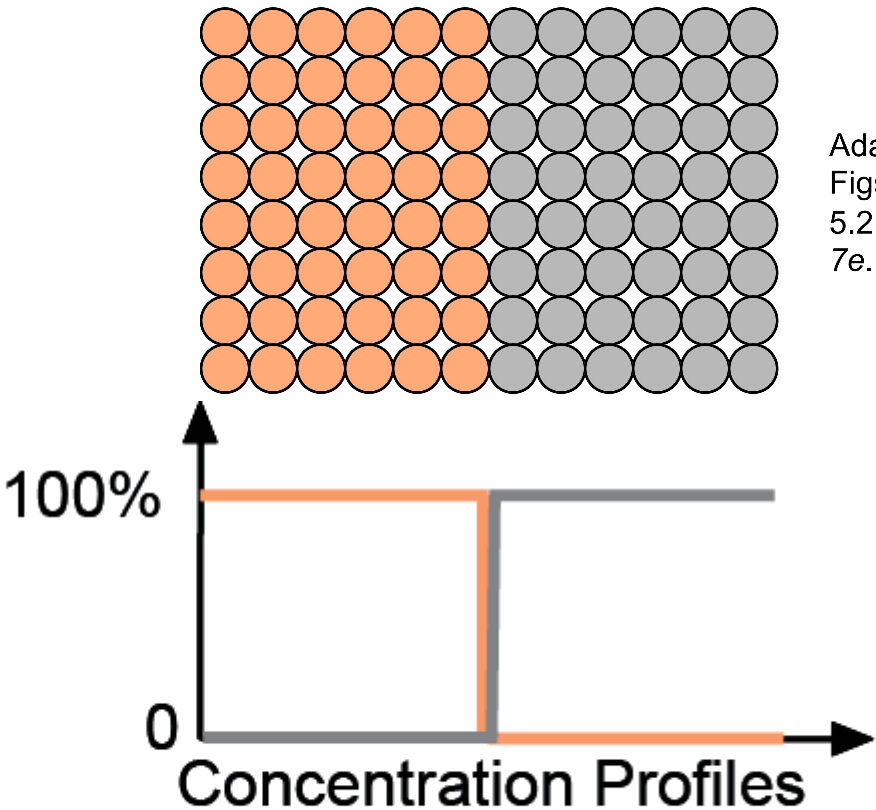
- Gases & Liquids – random (Brownian) motion
- Solids – vacancy diffusion or interstitial diffusion

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.

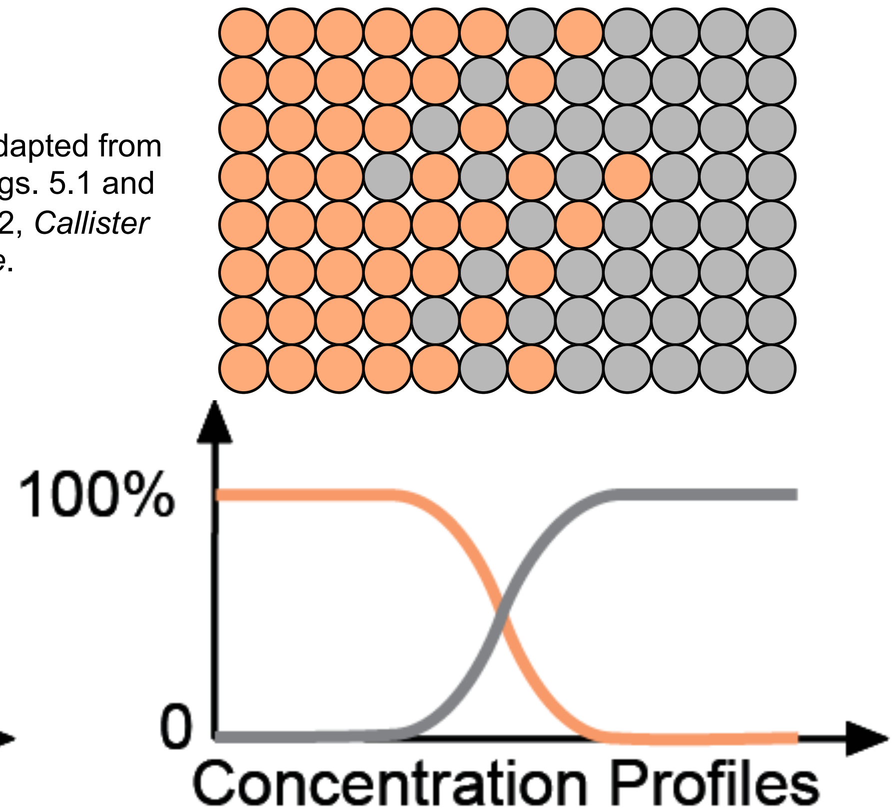
Interdiffusion

Initially



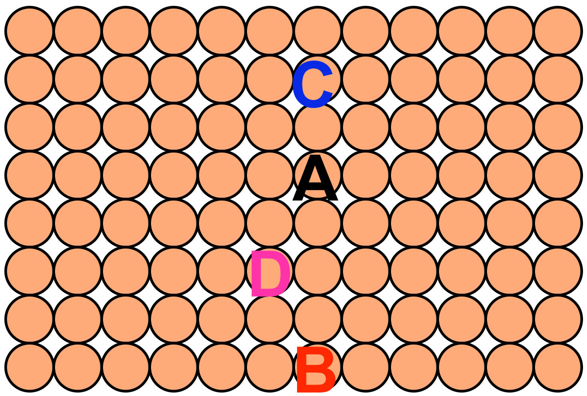
Adapted from Figs. 5.1 and 5.2, *Callister 7e*.

After some time

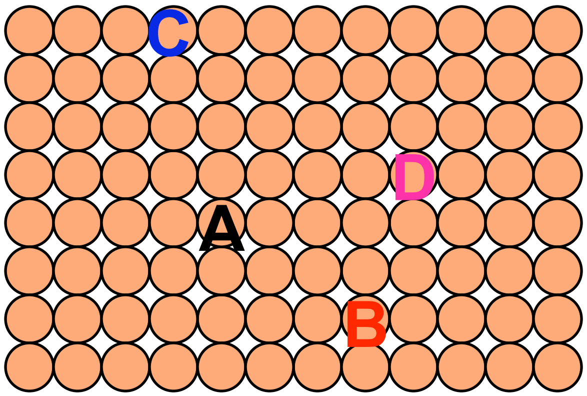


Self-diffusion

Label some atoms



After some time



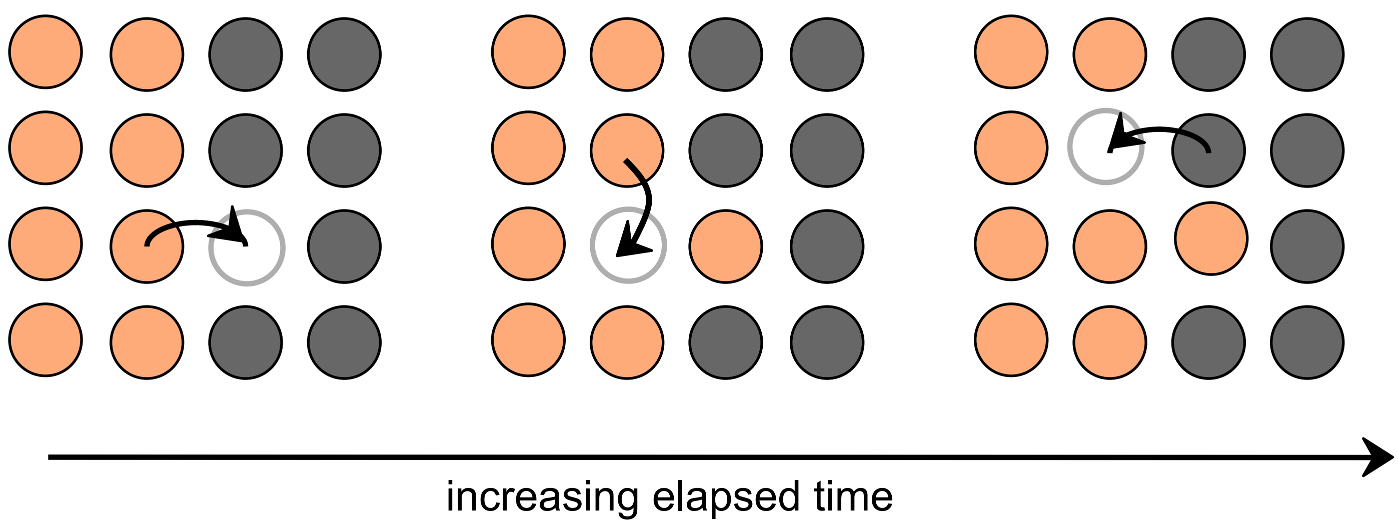
Diffusion mechanisms

Conditions:

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

Vacancy Diffusion:

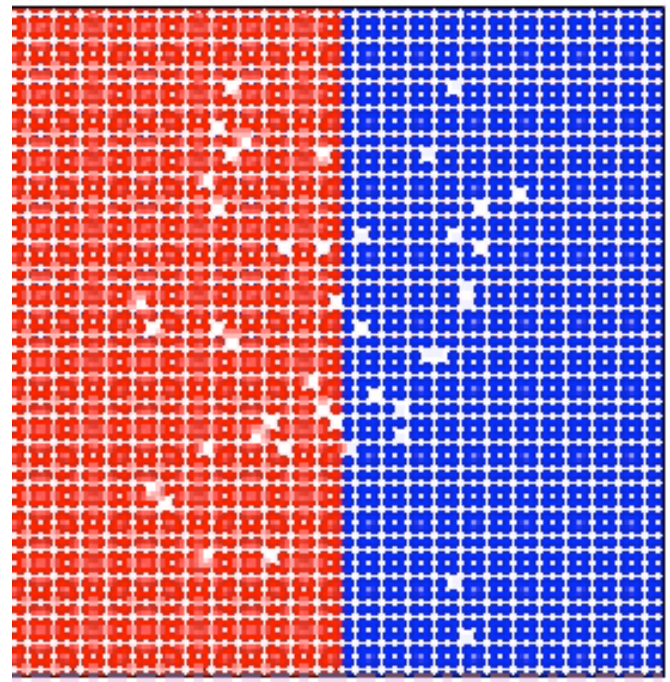
- atoms exchange with vacancies
- applies to substitutional impurities atoms
- rate depends on:
  - --number of vacancies
  - --activation energy to exchange.



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

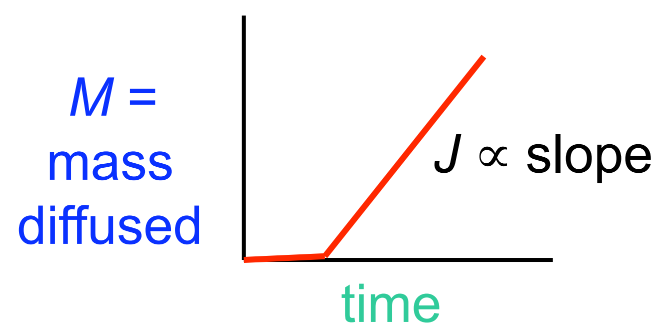
How do we quantify the amount or rate of diffusion?

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

Measured empirically

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

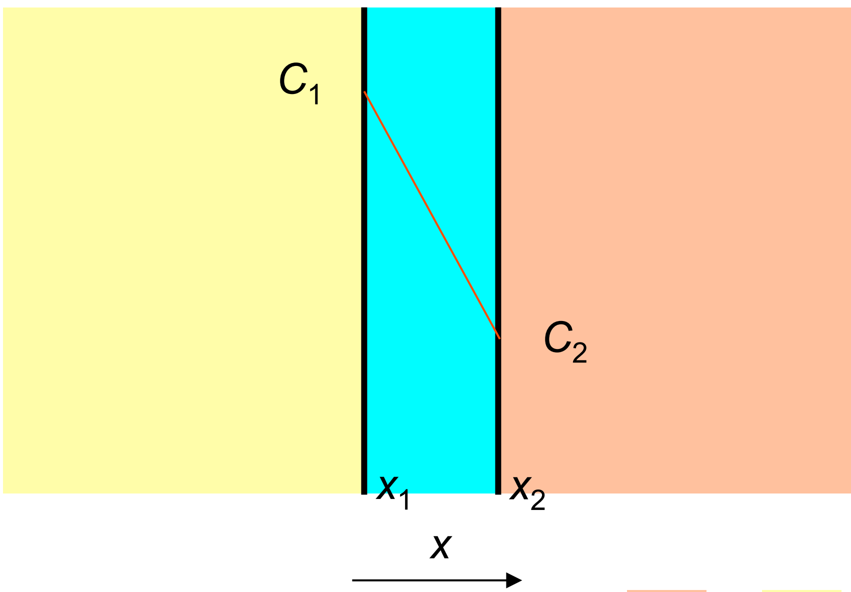
$$J = \frac{M}{At} = \frac{1}{A}\frac{dM}{dt}$$



Steady-state diffusion

Rate of diffusion independent of time

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



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

Fick's first law of diffusion

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

$D \equiv$ diffusion coefficient

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]

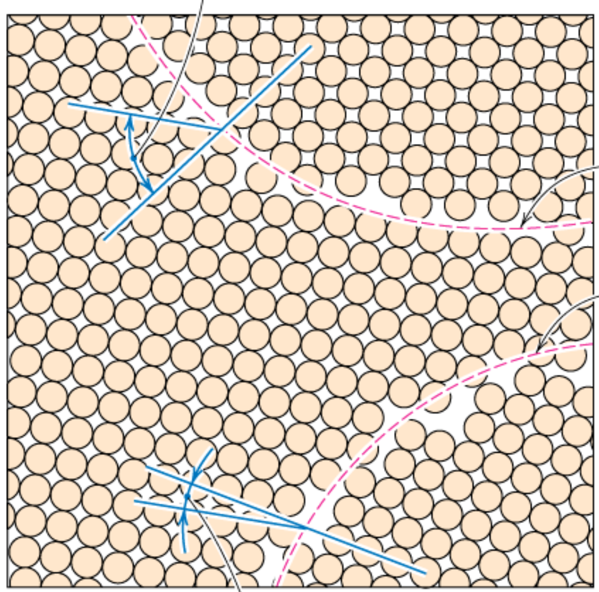
D_o = pre-exponential [m^2/s]

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

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

T = absolute temperature [K]

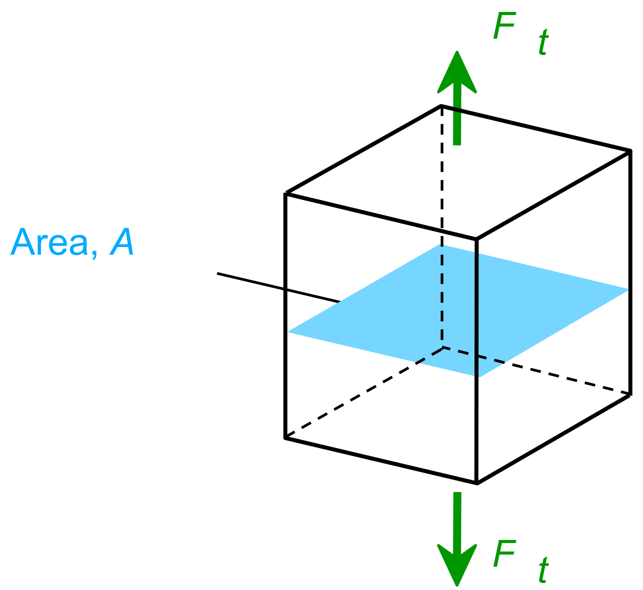
Diffusion paths



Diffusion FASTER for...	Diffusion SLOWER for...
• open crystal structures	• close-packed structures
• materials w/secondary bonding	• materials w/covalent bonding
• smaller diffusing atoms	• larger diffusing atoms
• lower density materials	• higher density materials

Engineering stress

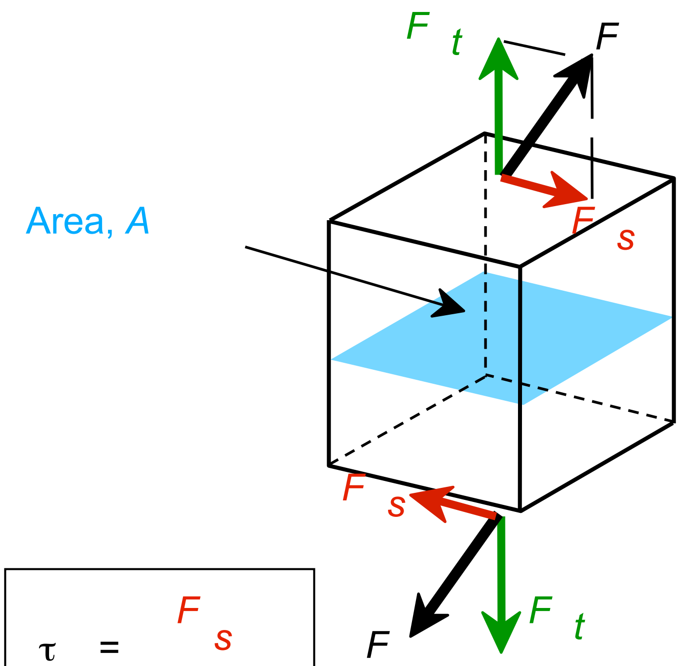
- **Tensile** stress, σ:



$$\sigma = \frac{F_t}{A_o} = \frac{lb_f}{in^2} \text{ or } \frac{N}{m^2}$$

original area before loading

- **Shear** stress, τ:

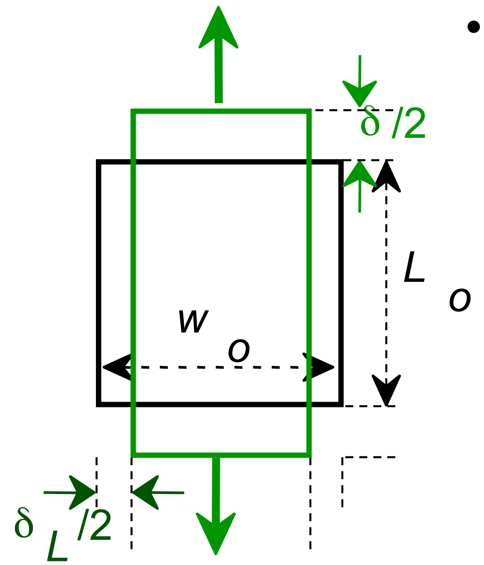


$$\tau = \frac{F_s}{A_o}$$

Engineering strain

- **Tensile strain:**

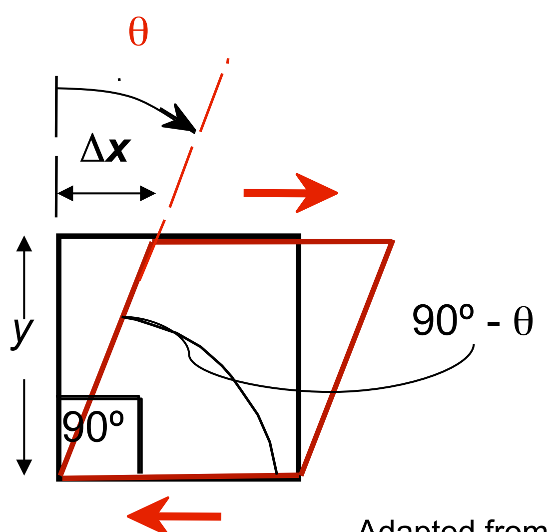
$$\varepsilon = \frac{\delta}{L_o}$$



- **Lateral strain:**

$$\varepsilon_L = \frac{-\delta_L}{w_o}$$

- **Shear strain:**



$$\gamma = \Delta x/y = \tan\theta$$

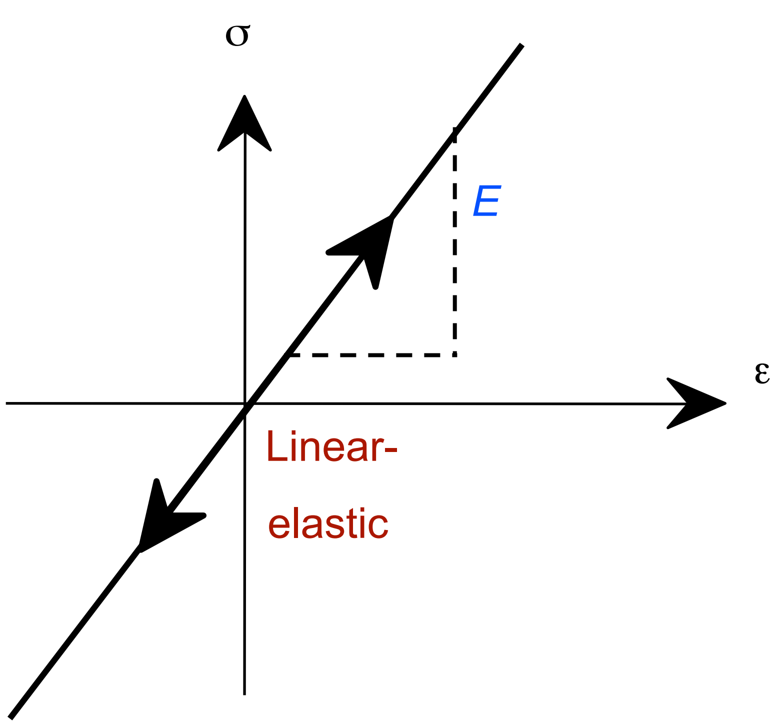
Adapted from Fig. 6.1 (a) and (c), *Callister 7e.*

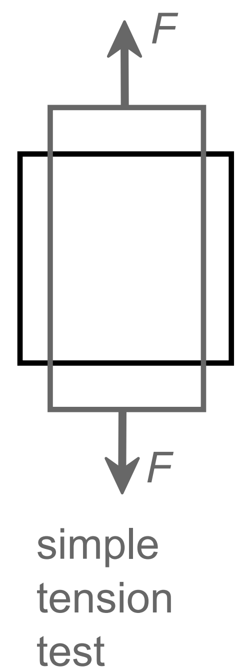
Engineering strain

- **Modulus of Elasticity, *E*:**
  (also known as Young's modulus)

- **Hooke's Law:**

$\sigma = E\,\varepsilon$

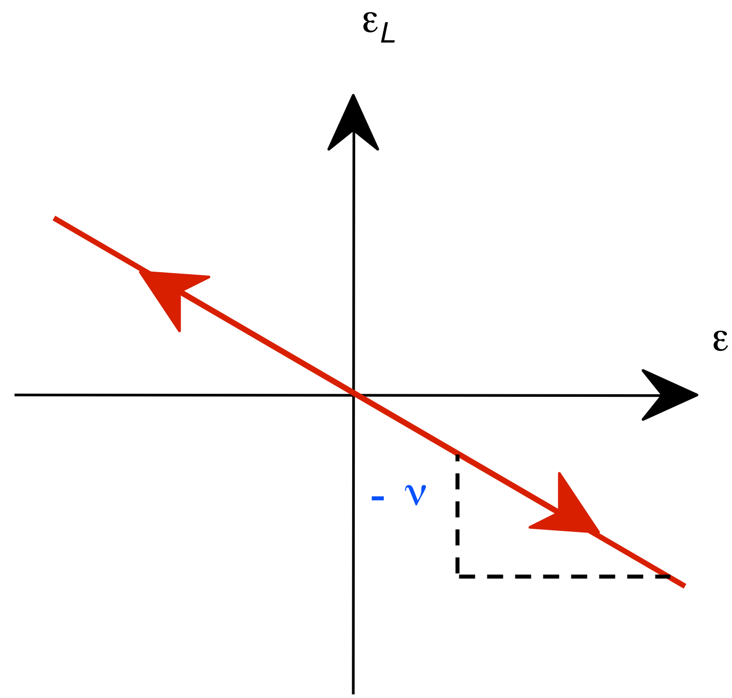




Elastic properties of materials

- **Poisson's ratio, ν:**

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



metals: ν ~ 0.33
ceramics: ν ~ 0.25
polymers: ν ~ 0.40

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

–ν > 0.50 density increases

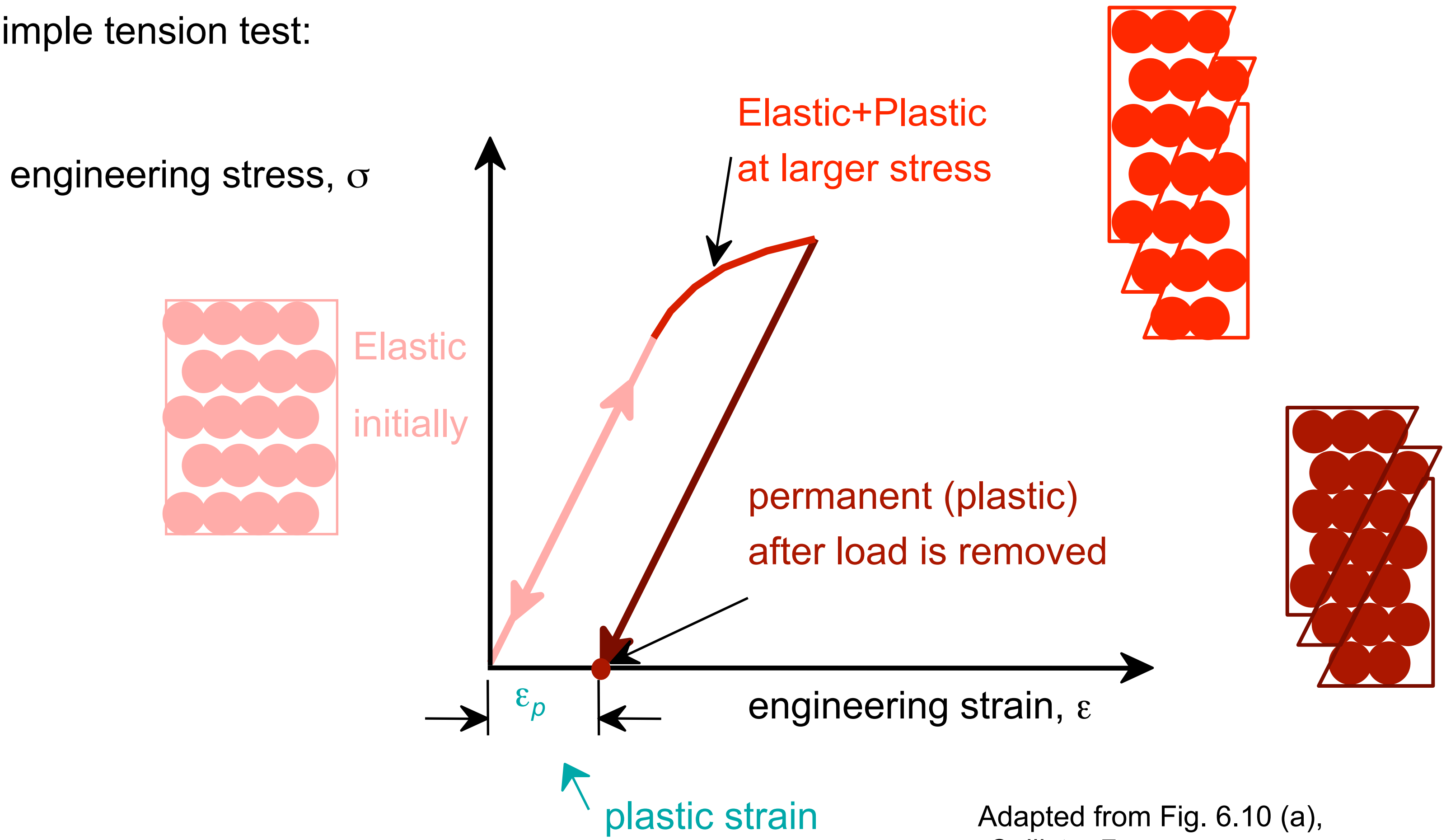
–ν < 0.50 density decreases (voids form)

–For *isotropic* materials

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

Plastic deformation

- Simple tension test:

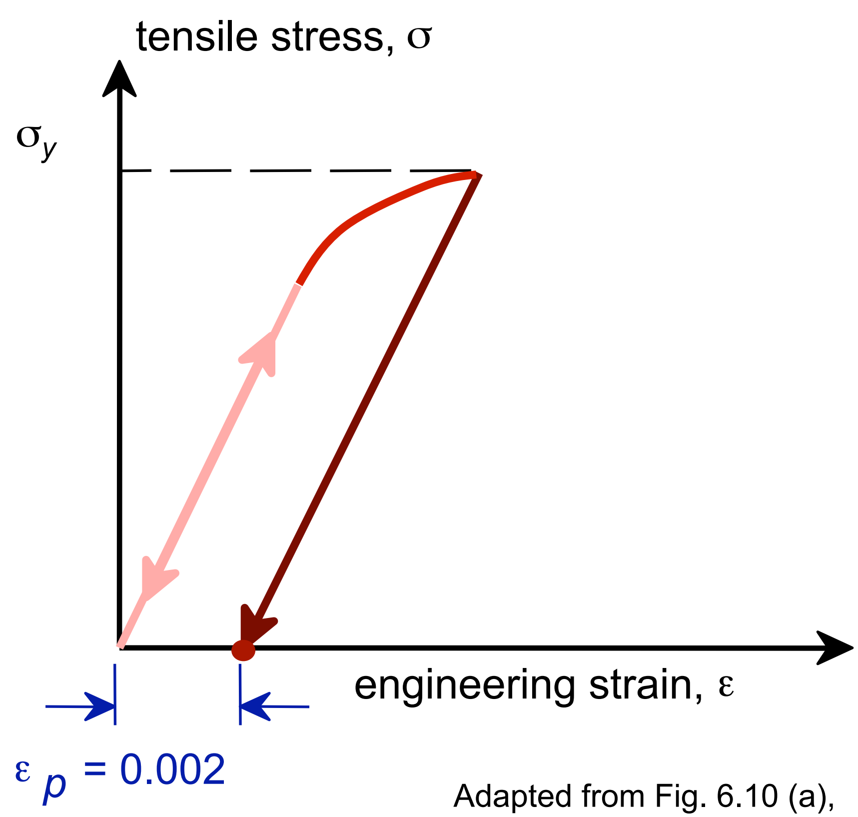


Adapted from Fig. 6.10 (a), *Callister 7e.*

Yield strength, σ_y

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

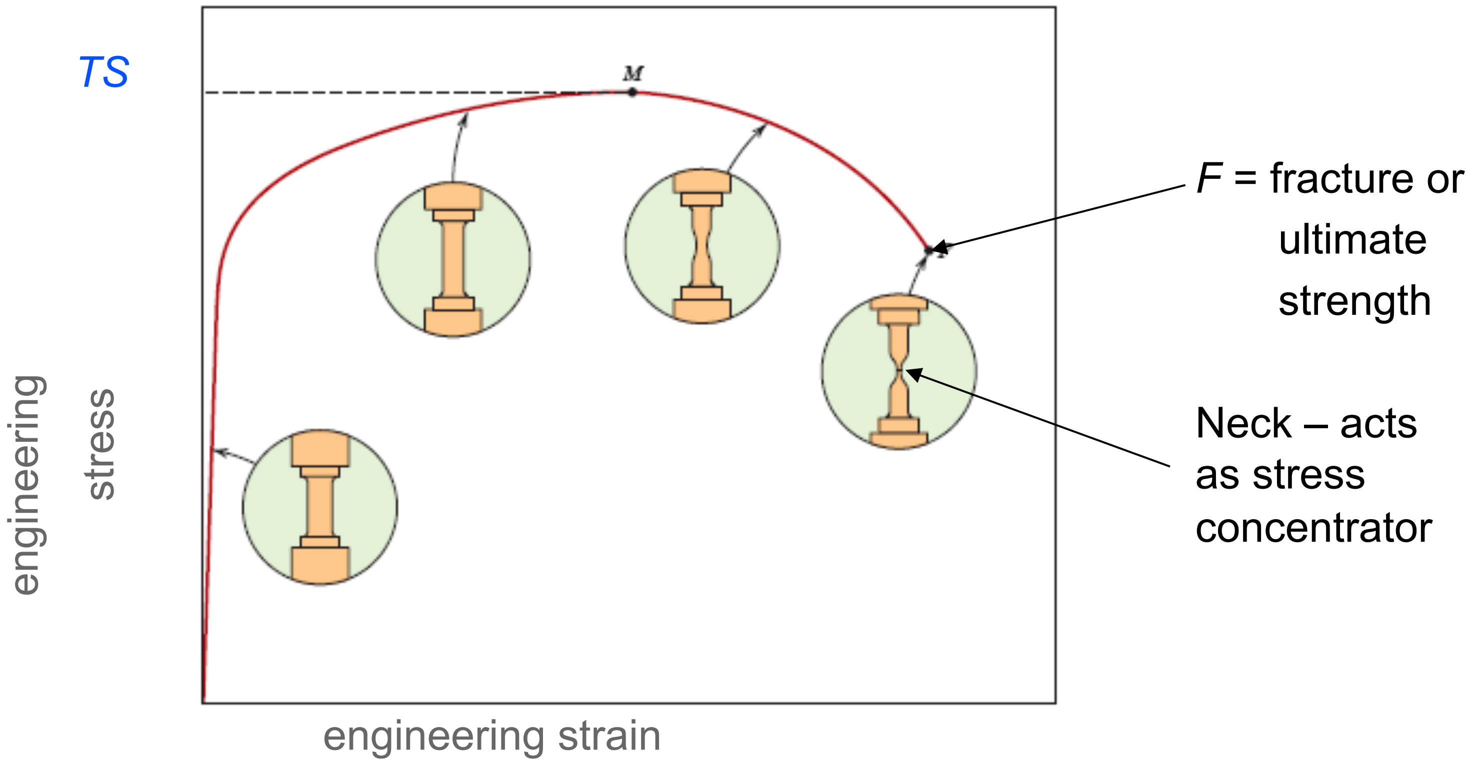
when ε_p = 0.002



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

Tensile strength, TS

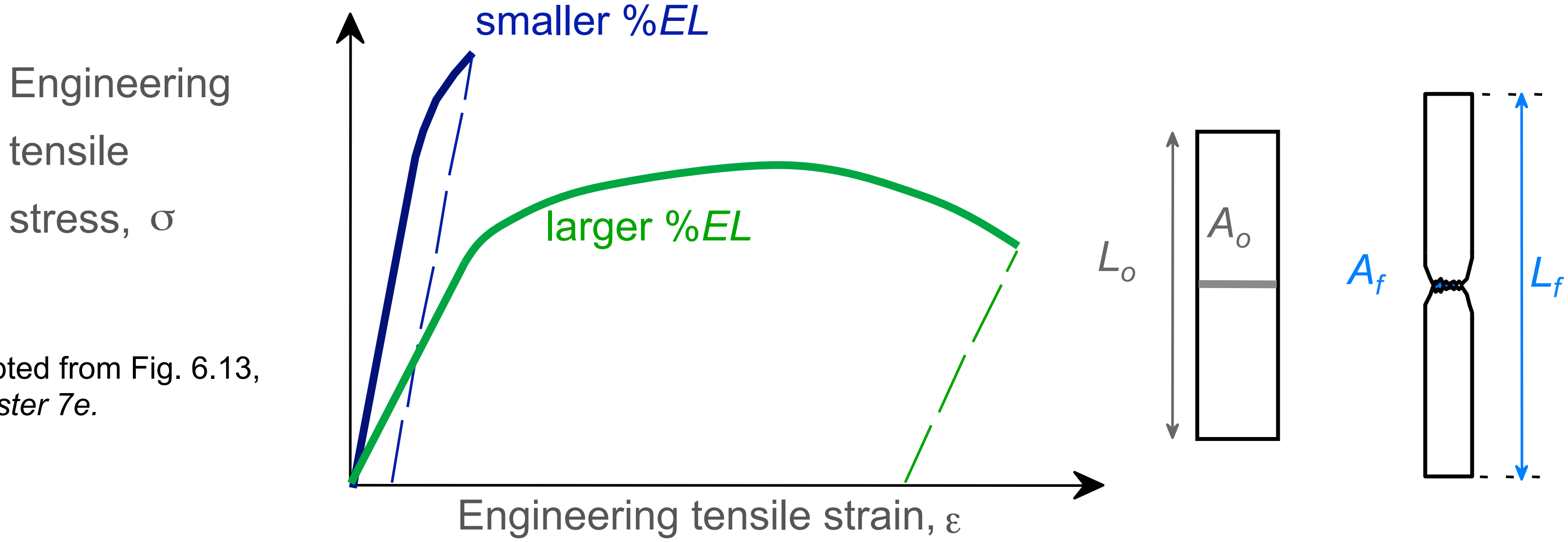
- Maximum stress on engineering stress-strain curve.



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

Ductility

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

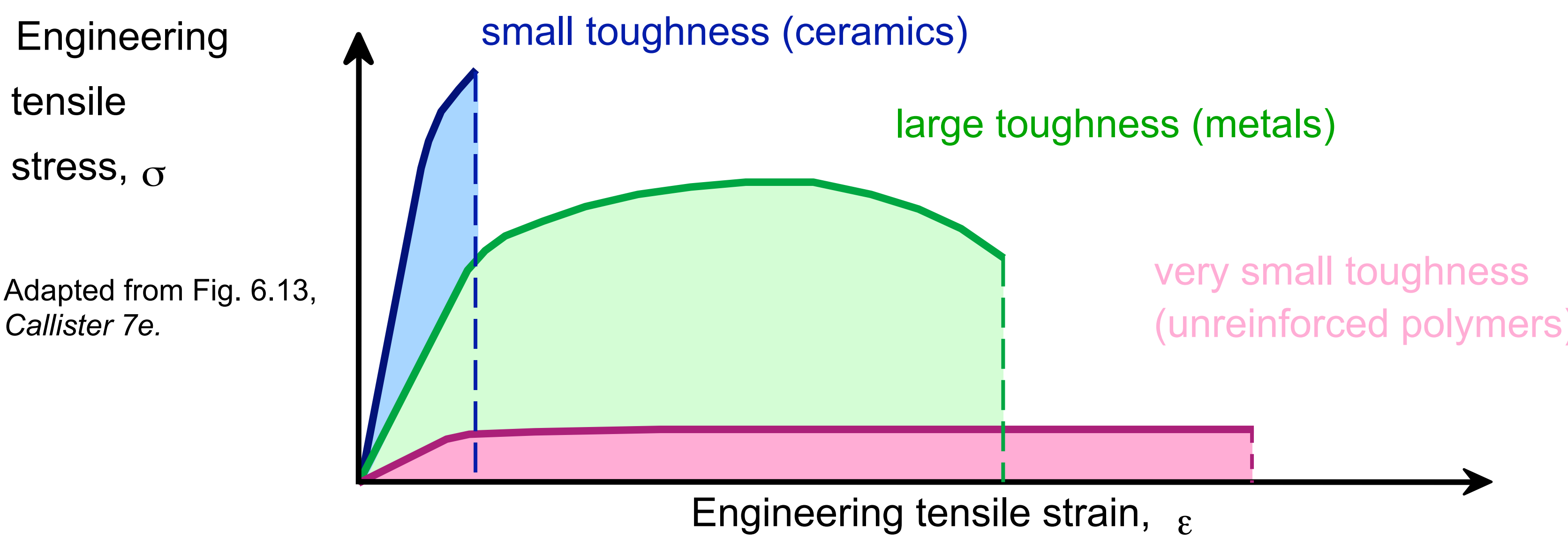


Adapted from Fig. 6.13, *Callister 7e.*

- 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.

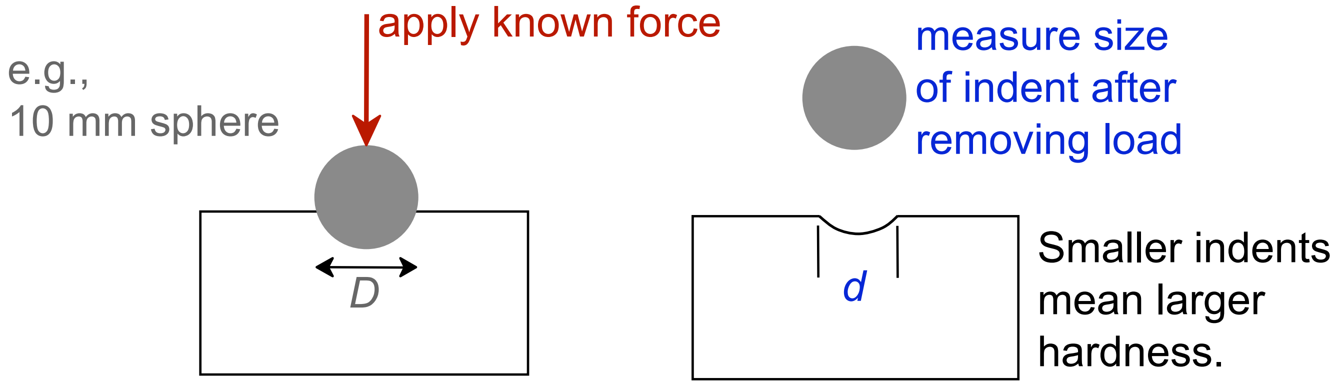


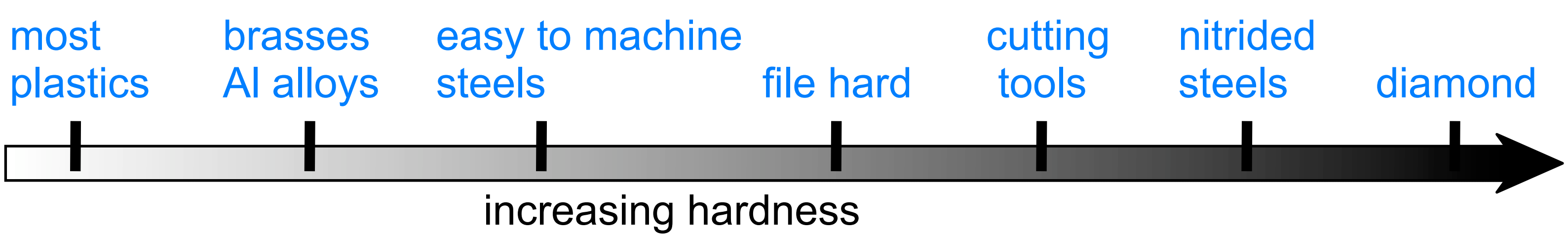
Adapted from Fig. 6.13, *Callister 7e.*

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

Hardness

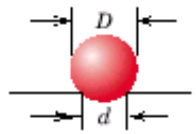
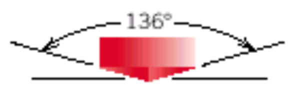
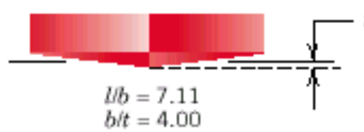
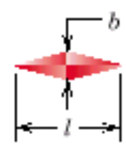
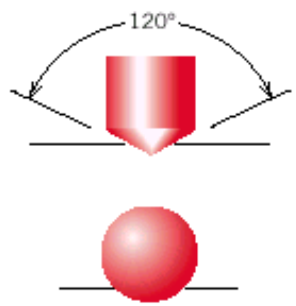
- Resistance to permanently indenting the surface.
- Large hardness means:
  --resistance to plastic deformation or cracking in compression.
  --better wear properties.





Hardness Measurement

Table 6.5 **Hardness Testing Techniques**

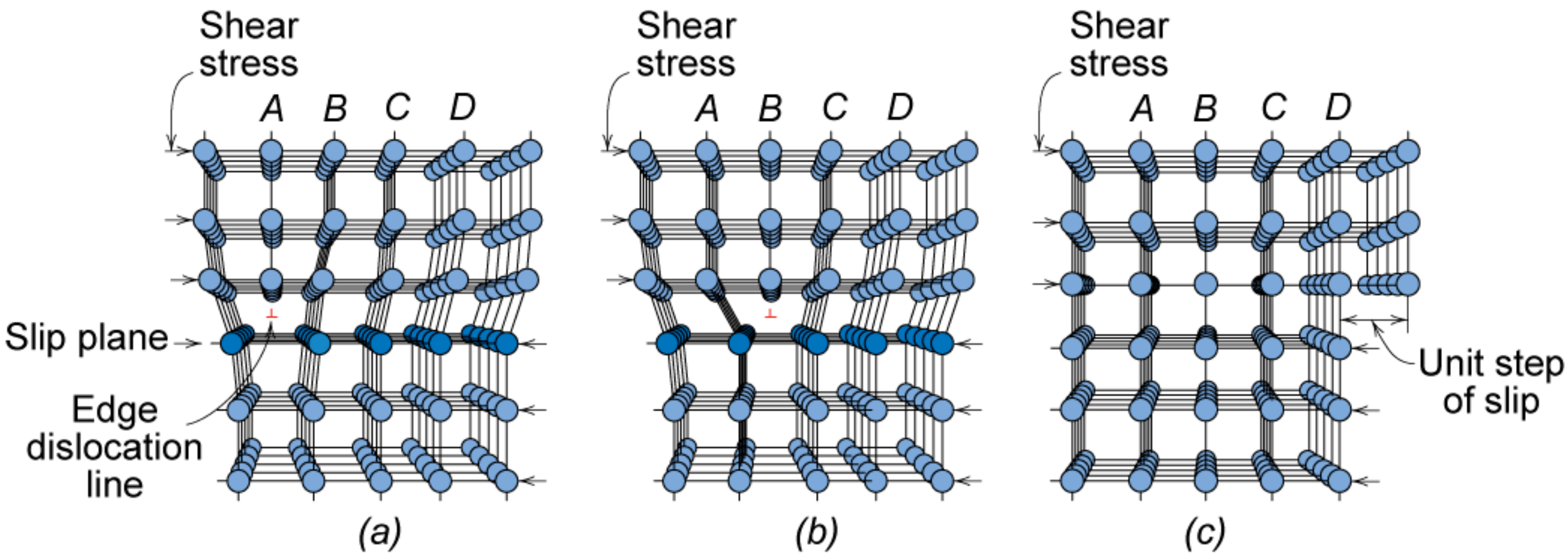
Test	Indenter	Shape of Indentation: Side View	Shape of Indentation: Top View	Load	Formula for Hardness Number[a]
Brinell	10-mm sphere of steel or tungsten carbide			P	$HB = \frac{2P}{\pi D[D - \sqrt{D^2 - d^2}]}$
Vickers microhardness	Diamond pyramid			P	$HV = 1.854P/d_1^2$
Knoop microhardness	Diamond pyramid			P	$HK = 14.2P/l^2$
Rockwell and Superficial Rockwell	{ Diamond cone; $\frac{1}{16}$, $\frac{1}{8}$, $\frac{1}{4}$, $\frac{1}{2}$ in. diameter steel spheres			60 kg 100 kg 150 kg 15 kg 30 kg 45 kg	} Rockwell } Superficial Rockwell

[a] For the hardness formulas given, P (the applied load) is in kg, while D, d, d_1, and l are all in mm.

Source: Adapted from H. W. Hayden, W. G. Moffatt, and J. Wulff, *The Structure and Properties of Materials,* Vol. III, *Mechanical Behavior.* Copyright © 1965 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.

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).

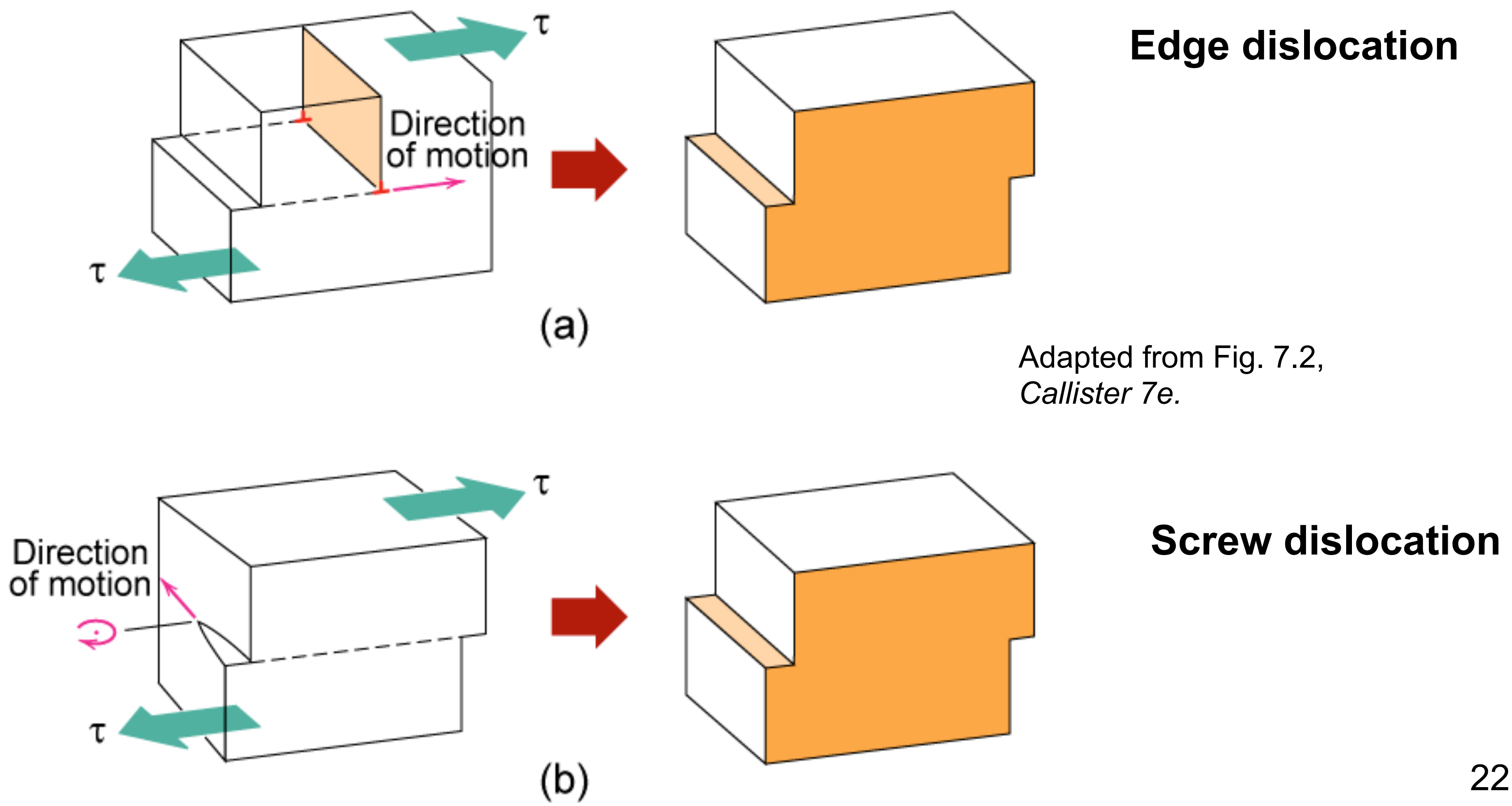


- If dislocations don't move, deformation doesn't occur!

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

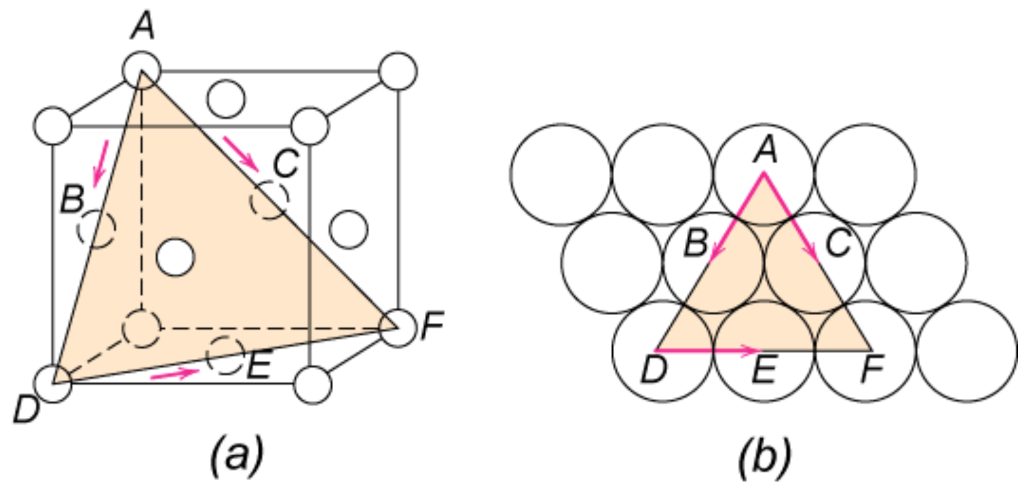


Adapted from Fig. 7.2, *Callister 7e.*

Deformation mechanisms

- Slip System
  - Slip plane - plane allowing easiest slippage

  - Slip direction - direction of movement

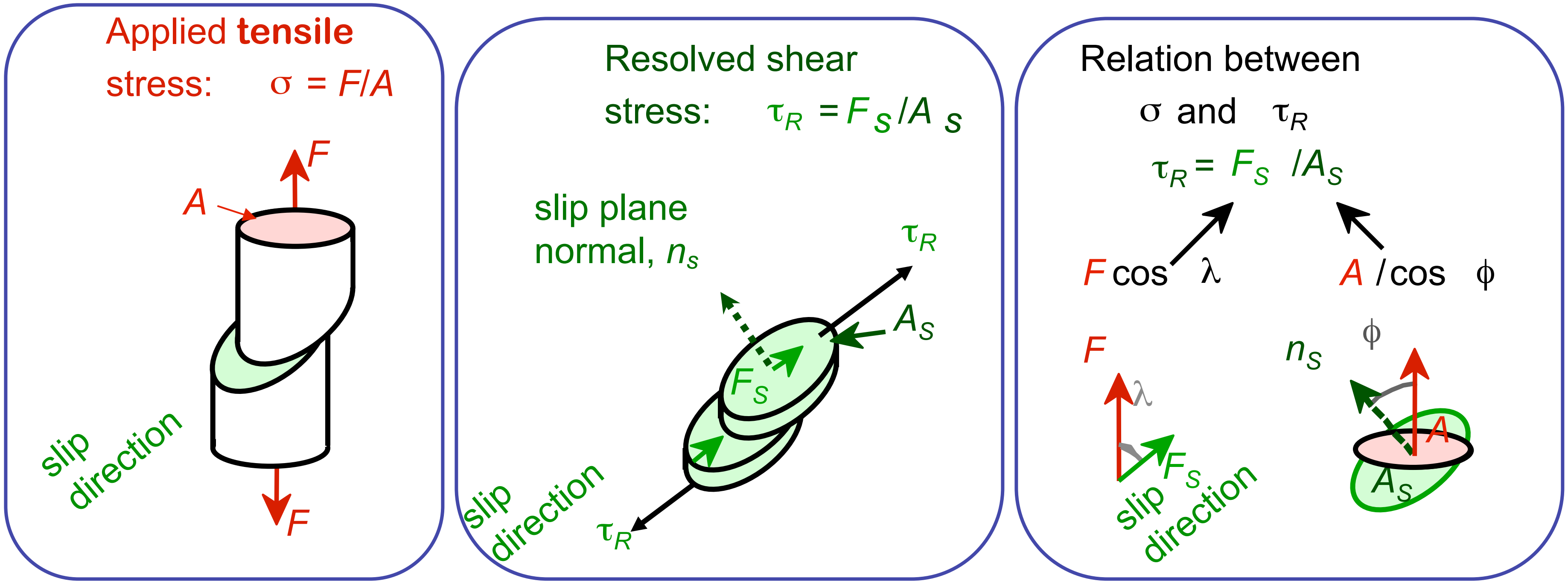


Adapted from Fig. 7.6, *Callister 7e.*

  - 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.

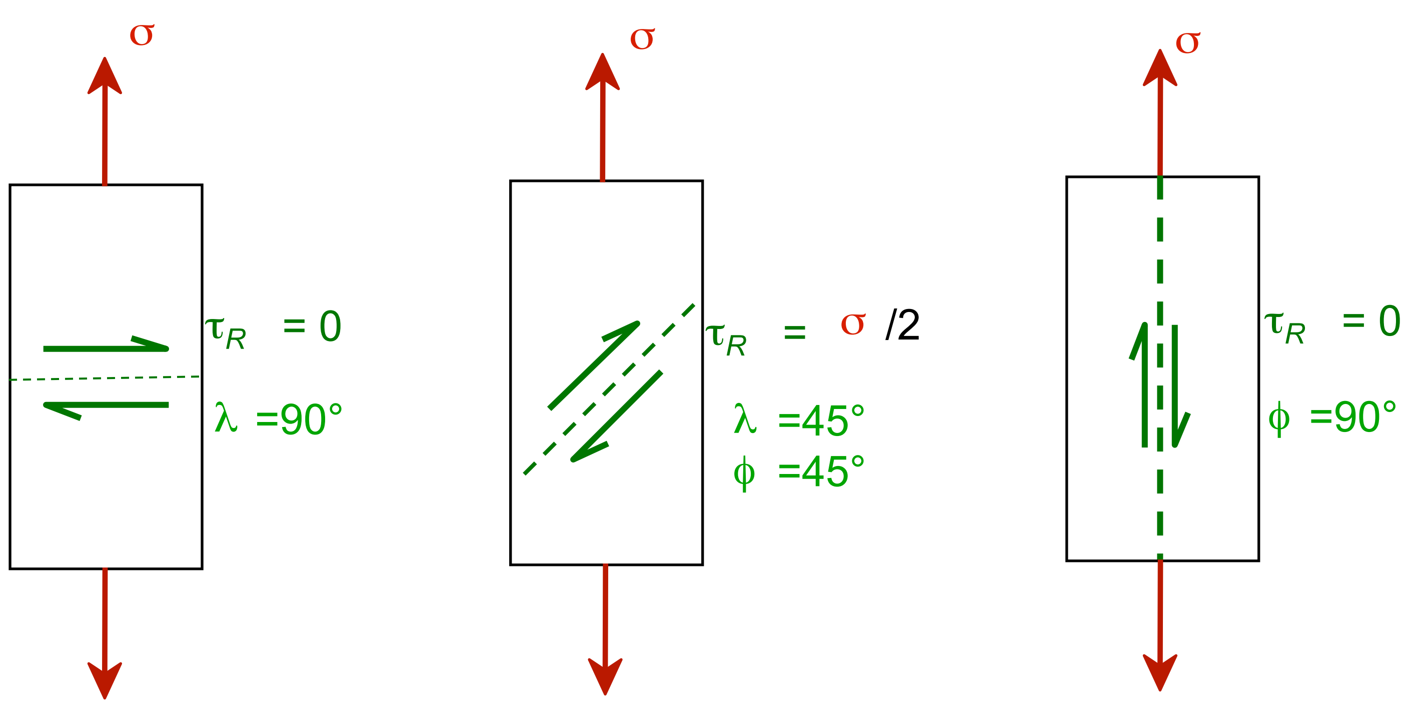


$$\tau_R = \sigma \cos\lambda \cos\phi$$

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 $\lambda = \phi = 45^o$

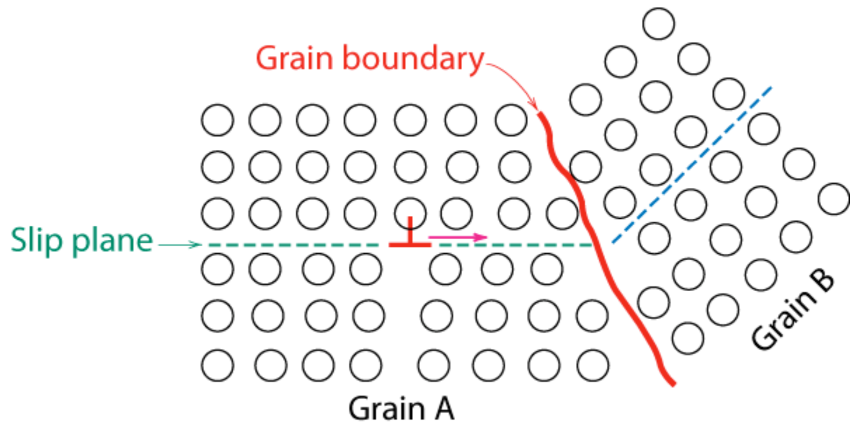
Slip motion in polycrystals

- 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

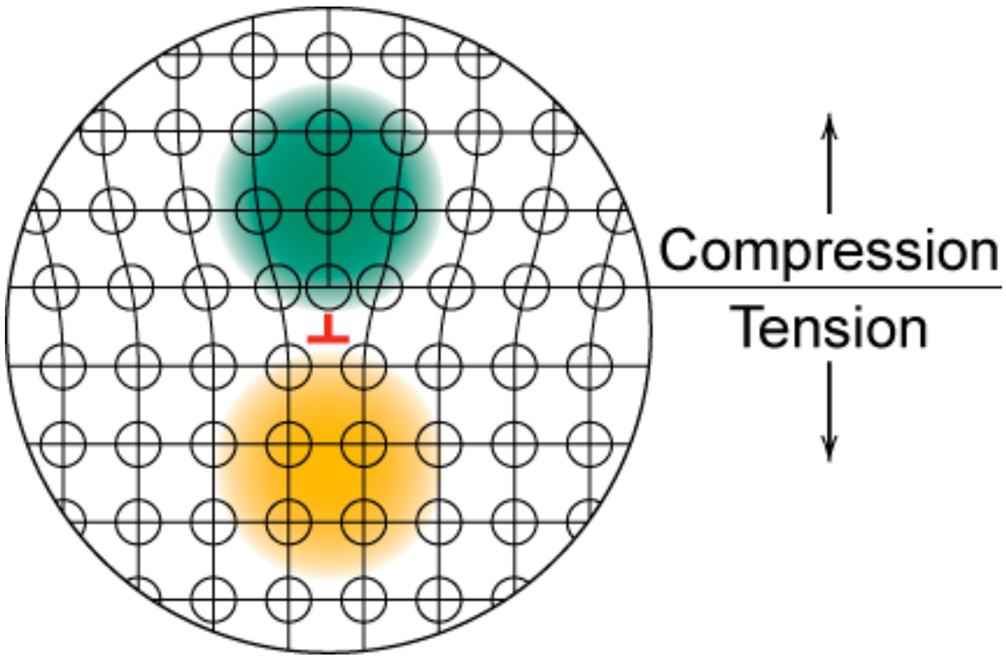
- Grain boundaries are barriers to slip.
- Barrier "strength" increases with increasing angle of misorientation.
- Smaller grain size: more barriers to slip.



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

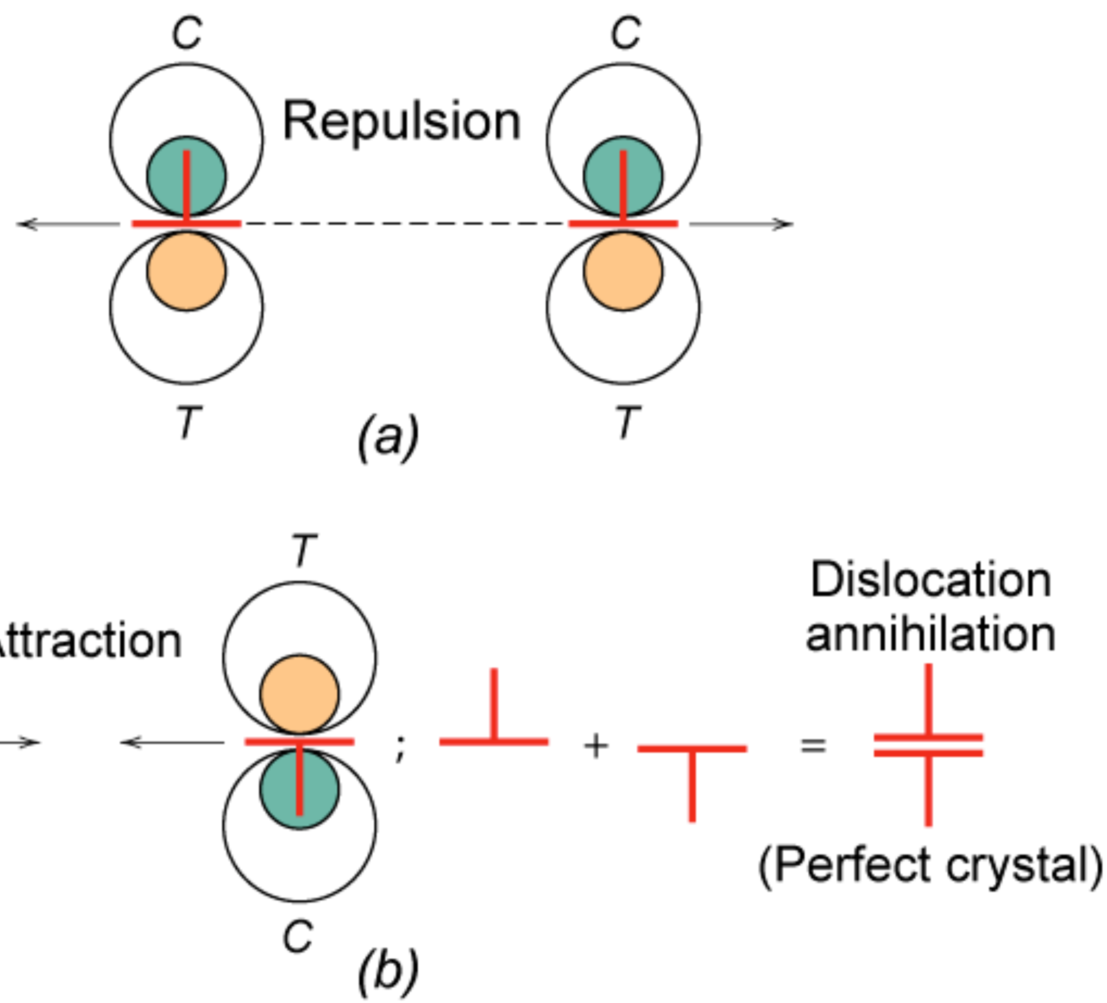
Strategies for strengthening: solid solutions



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

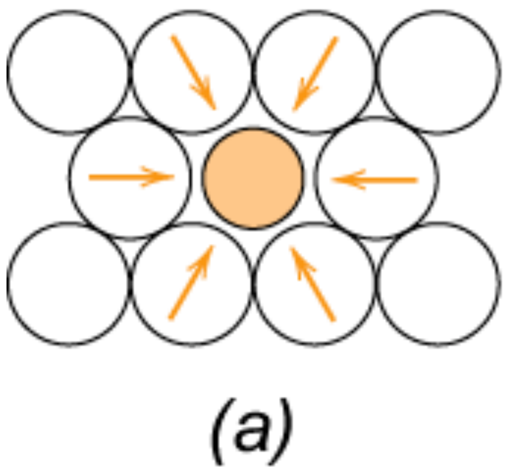
Effects of stress at dislocations

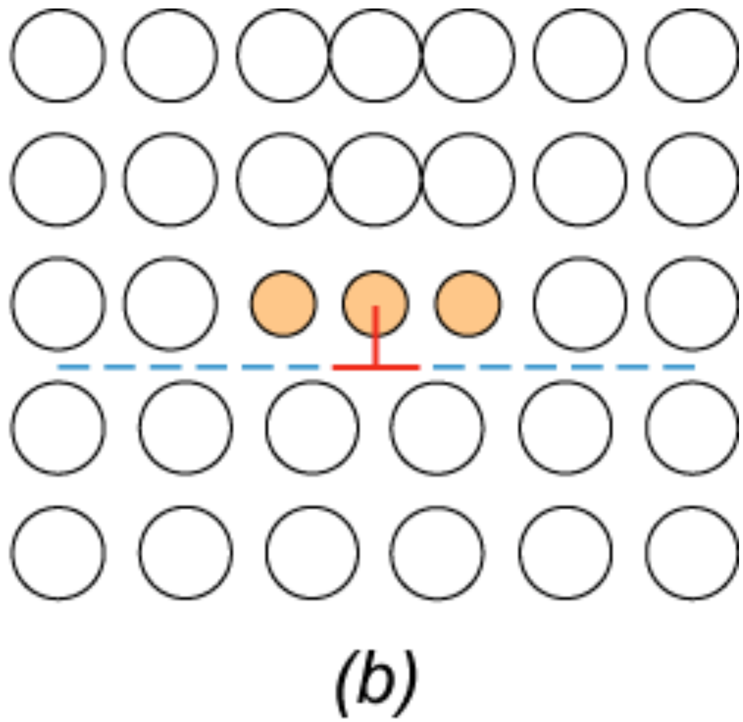
Adapted from Fig. 7.5, *Callister 7e.*



Strengthening by alloying

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

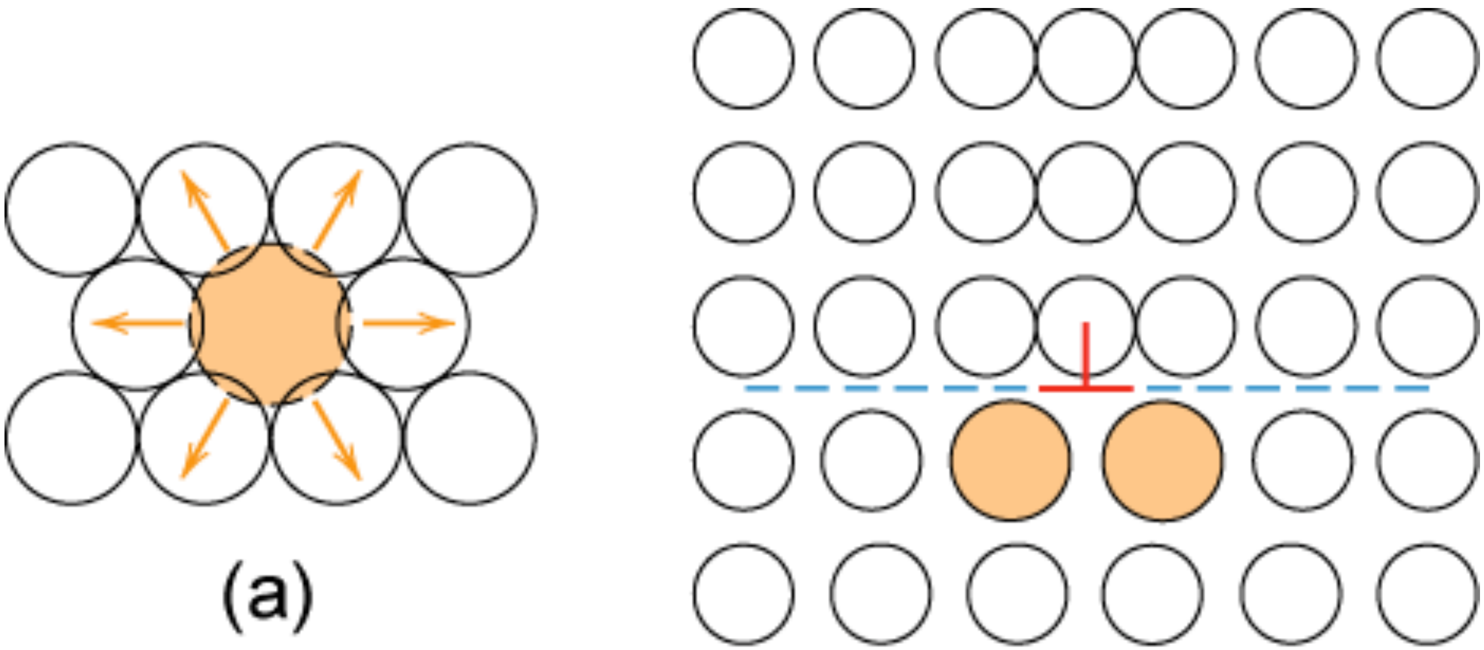




Adapted from Fig. 7.17, *Callister 7e.*

Strengthening by alloying

- large impurities concentrate at dislocations on low density side

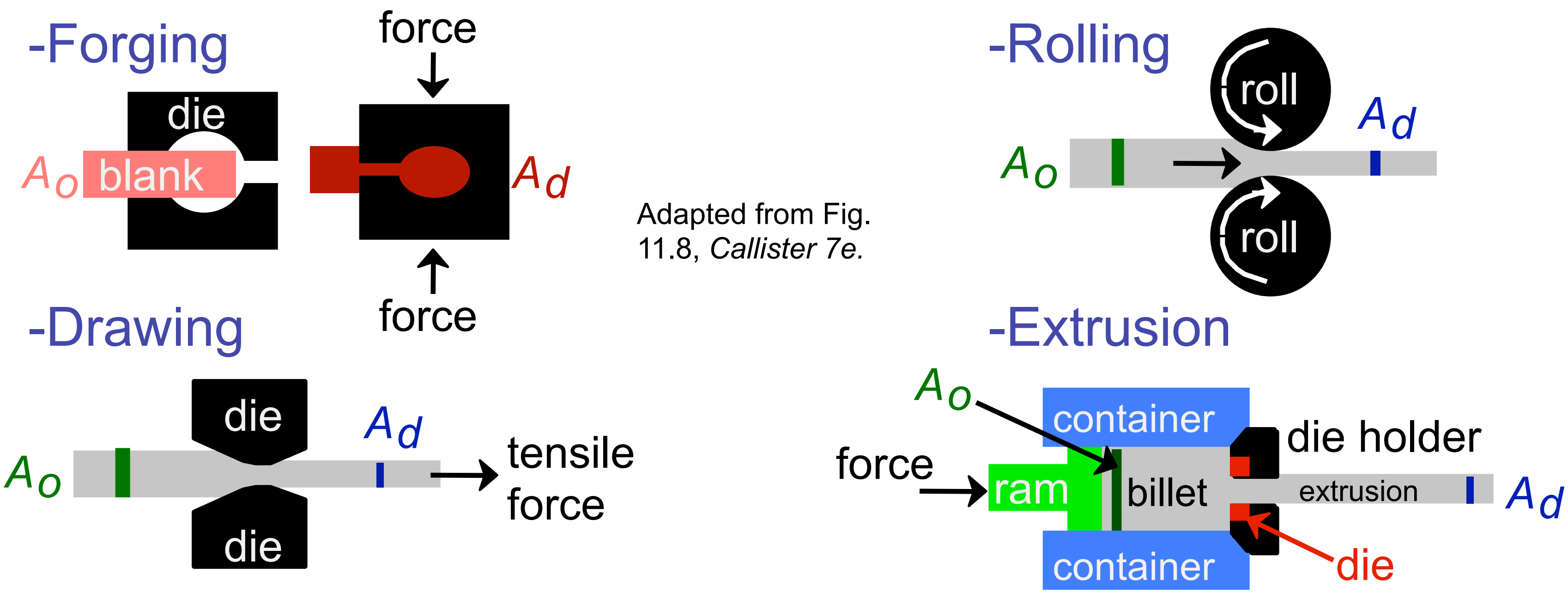


(a) (b)

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

Strategies for strengthening: Cold work (%CW)

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



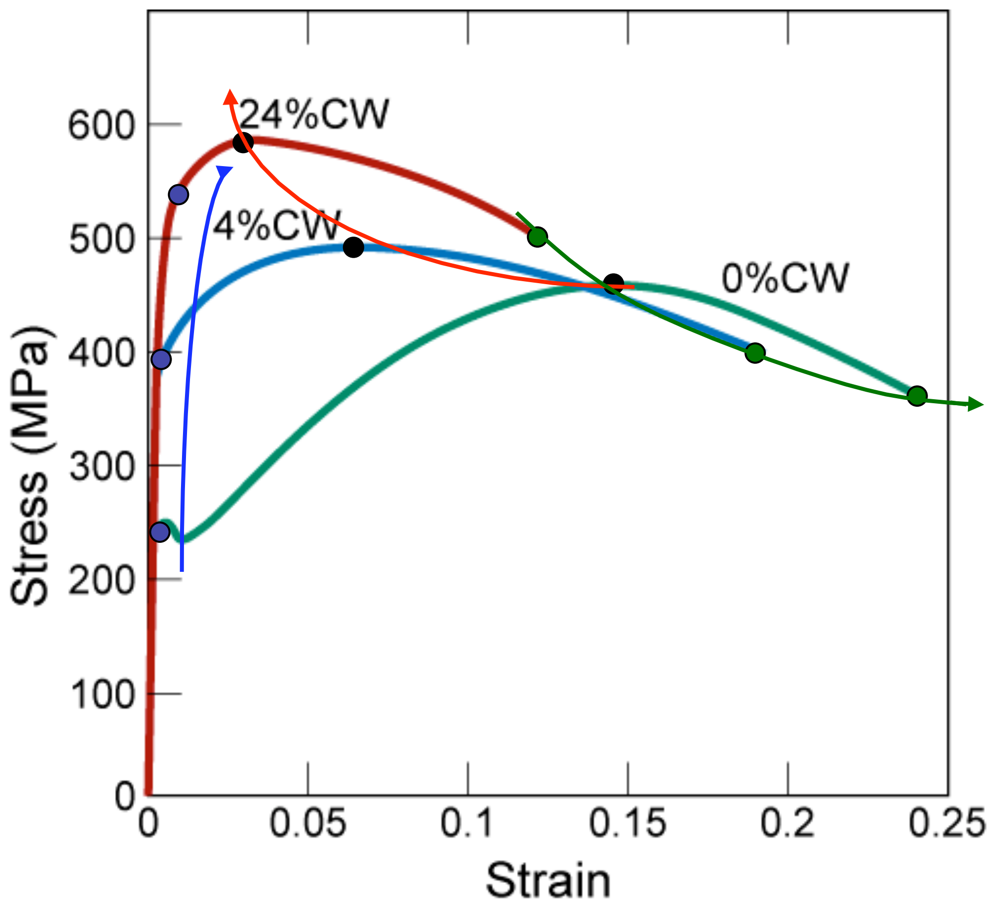
Adapted from Fig. 11.8, *Callister 7e.*

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

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.*