# Basics of Solid Mechanics
# in Nanostructures

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Course Website: **nanoHUB.org**
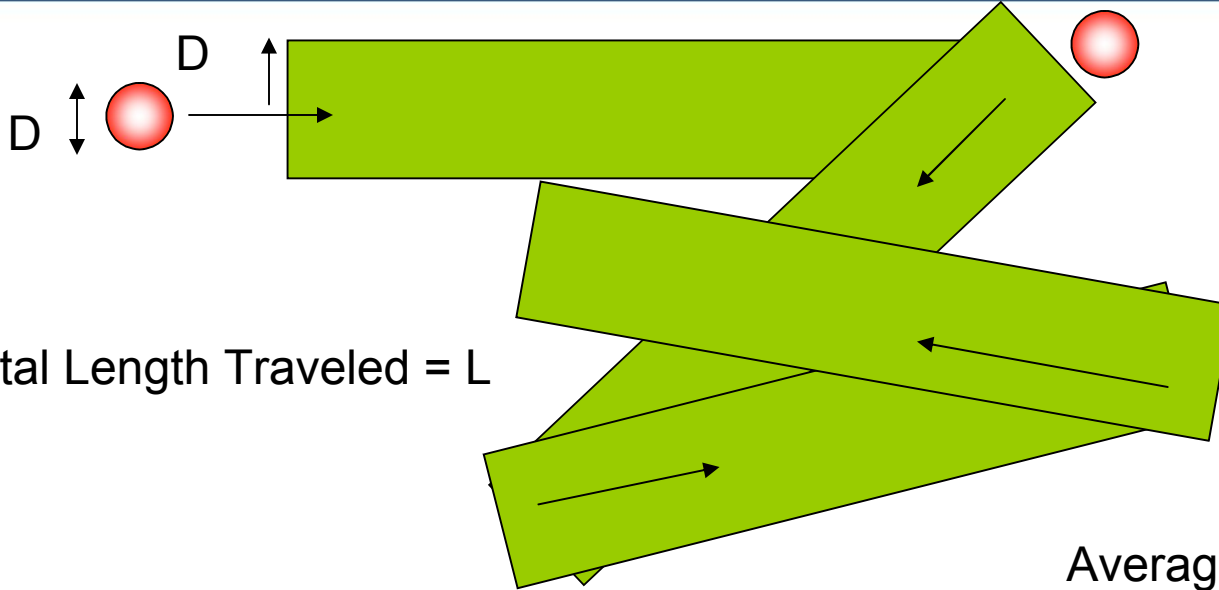**Compass.illinois.edu**

To understand nanoscale transport and energy conversion, we need to know:

— **How much energy/momentum can a particle have?**

— **How many particles have the specified energy E?**

— **How fast do they move?**

— **How do they interact with each other?**

— **How far can they travel?**

D

D

Total Length Traveled = L

Average Distance between Collisions, $\lambda_{mc}$ = L/(#of collisions)

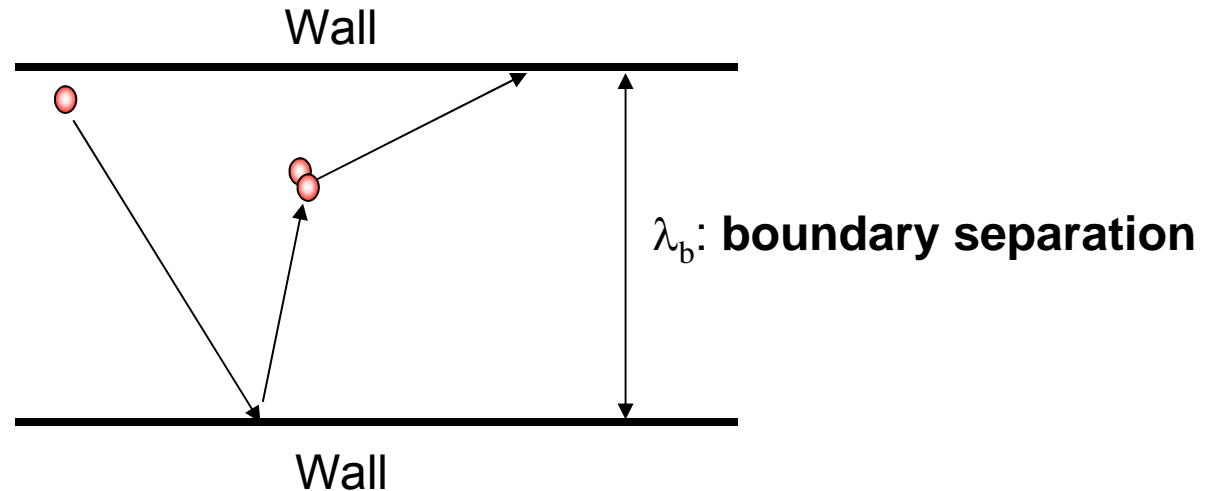E.G. Ideal Gas:
Total Collision Volume
Swept = $\pi D^2 L$

Number Density of Molecules = n

Total number of molecules encountered in swept collision volume ~ $n\pi D^2 L$

**Mean Free Path**

$$\lambda_{mc} = \frac{L}{n\pi D^2 L} = \frac{1}{n\sigma}$$

$\sigma$: collision cross-sectional area
**~ nm²**

# Effect of Nanoscale confinement

Wall

$\lambda_b$: **boundary separation**

Wall

Effective Mean Free Path:

$$\frac{1}{\lambda} = \frac{1}{\lambda_{mc}} + \frac{1}{\lambda_b}$$

*The smaller dimension governs collision time!*

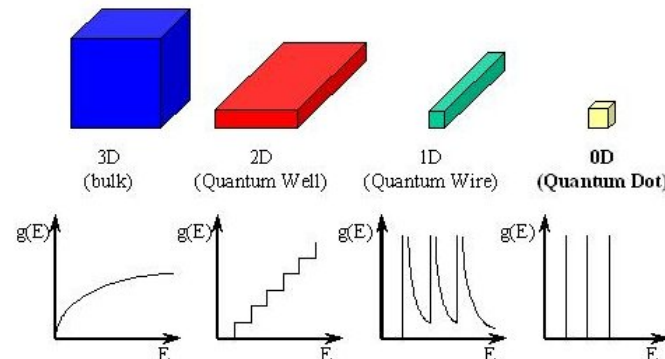# Internal Energy and Specific Heat

- Now we know the energy and momentum of particles/carriers in the material, we can start counting the properties

- E.G. Internal energy

| Boltzmann Distribution | Density of States | Energy of Carrier at Given States |
|---|---|---|

$$p_i = \frac{1}{Z} e^{-E_i/k_B T}$$

3D (bulk)  2D (Quantum Well)  1D (Quantum Wire)  0D (Quantum Dot)

g(E)  g(E)  g(E)  g(E)

E  E  E  E

Translation

Vibration

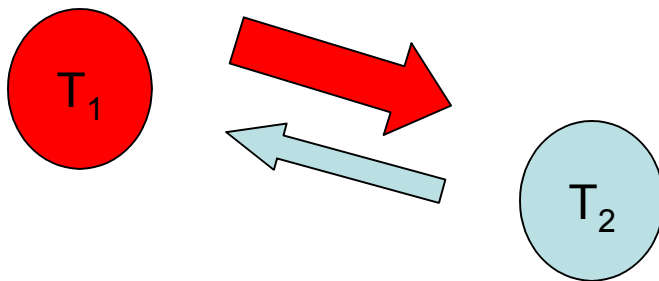Rotation

**Define:** $x = \hbar\omega / k_B T$

$$U(T) = \frac{4\pi N (k_B T)^4}{V(\hbar c)^3} \int_0^{\infty} \frac{x^3}{\exp(x) - 1} dx$$

**The emissive power of Black body radiation:**

$$E(T) = \sigma T^4$$

*Stefan-Boltzmann's Law*

$\sigma = 5.67 \times 10^{-8}$ W/m$^2$ $K^4$ .

$T_1$

$T_2$
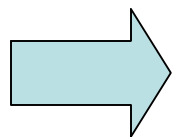
$$q = \sigma \left( T_1^4 - T_2^4 \right)$$
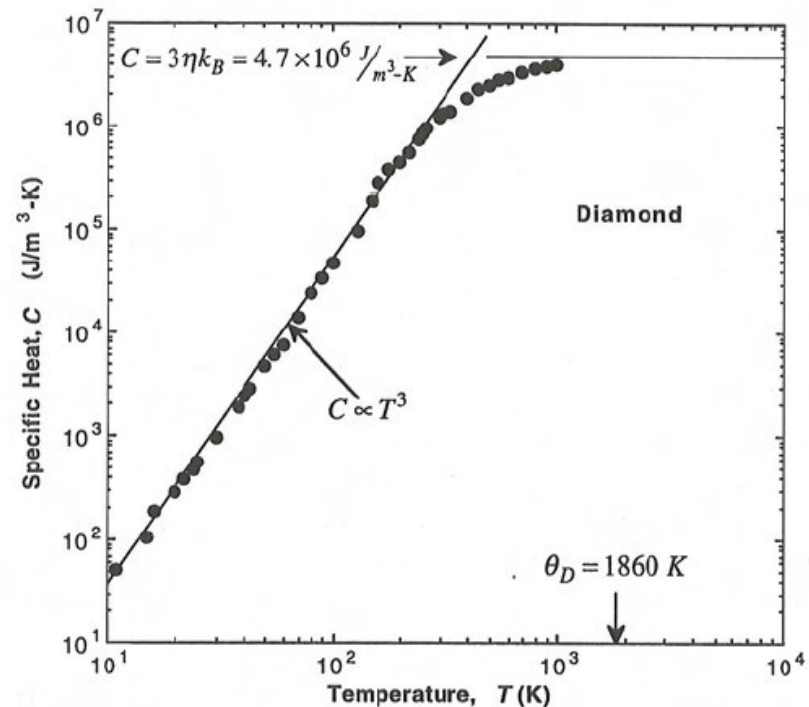
# Specific Heat Capacity

- The specific heat capacity is defined by change of internal energy per unit temperature change:

$$C_V = \frac{\partial U}{\partial T}$$

$$U \propto T^4$$

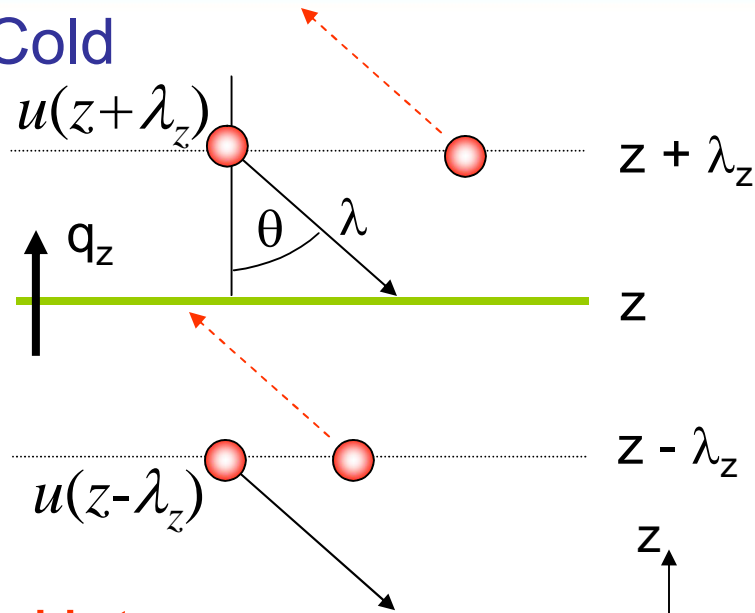$$C_V \propto T^3$$ At low temperature



Specific heat of diamond

(Touloukian and Buyco, 1970).

Cold

$u(z+\lambda_z)$

$z + \lambda_z$

$q_z$

$\theta$ $\lambda$

$z$

$z - \lambda_z$
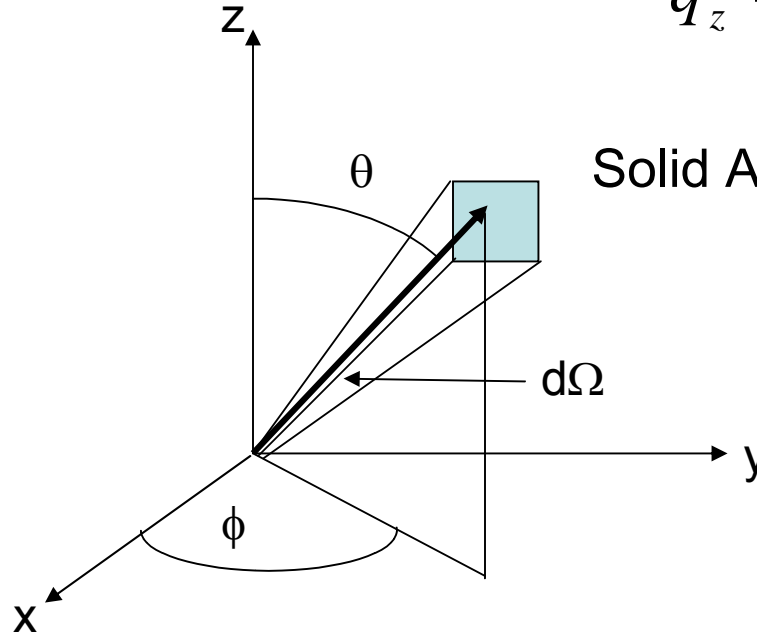
$u(z-\lambda_z)$

Hot

**Net Energy Flux**

$$q_z = \frac{1}{2} v_z \left[ u(z - \lambda_z) - u(z + \lambda_z) \right]$$

through Taylor expansion of $u$

$$q_z = -v_z \lambda_z \frac{du}{dz}$$

$z$

$\theta$

$d\Omega$

$y$

$\phi$

$x$

Solid Angle, $d\Omega = \sin\theta d\theta d\phi$

# Averaging over all the solid angles

$$q_z = -v\lambda \frac{du}{dz} \left[ \frac{\int\limits_{\varphi=0}^{2\pi} \int\limits_{\theta=0}^{\pi/2} \cos^2\theta \sin\theta \, d\theta \, d\varphi}{\int\limits_{\varphi=0}^{2\pi} \int\limits_{\theta=0}^{\pi/2} \sin\theta \, d\theta \, d\varphi} \right] = -v\lambda \frac{du}{dz} \left[ \frac{\int\limits_{\varphi=0}^{2\pi} \int\limits_{\theta=0}^{\pi/2} \cos^2\theta \sin\theta \, d\theta \, d\varphi}{2\pi} \right] = -\frac{1}{3} v\lambda \frac{du}{dz}$$

Assuming **local thermodynamic equilibrium**: u = u(T)

$$q_z = -\frac{1}{3} v\lambda \frac{du}{dT} \frac{dT}{dz} = -\frac{1}{3} Cv\lambda \frac{dT}{dz}$$
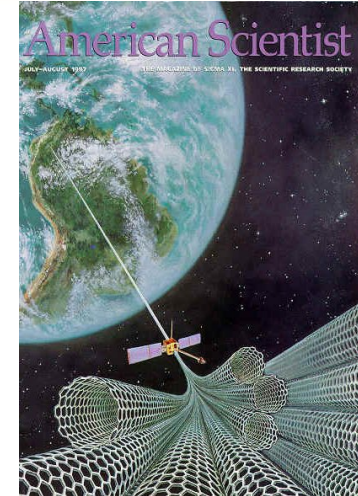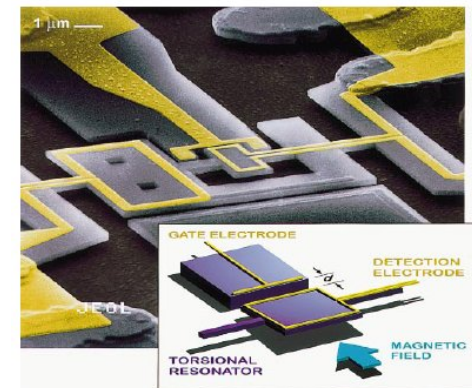
Thermal
Conductivity

$$k = \frac{1}{3} Cv\lambda$$

# Mechanics at Nanoscale

- ## Why?

  - ### Promising material behaviors (reduced defects and faster recovery) (this lecture)

  - ### Coupling and quantum effect on mechanical response

    (E.G. mechanical thermometer)

E.G. artists' view of space elevators using CNTs

Cleland and Roukes, Nature, 1998
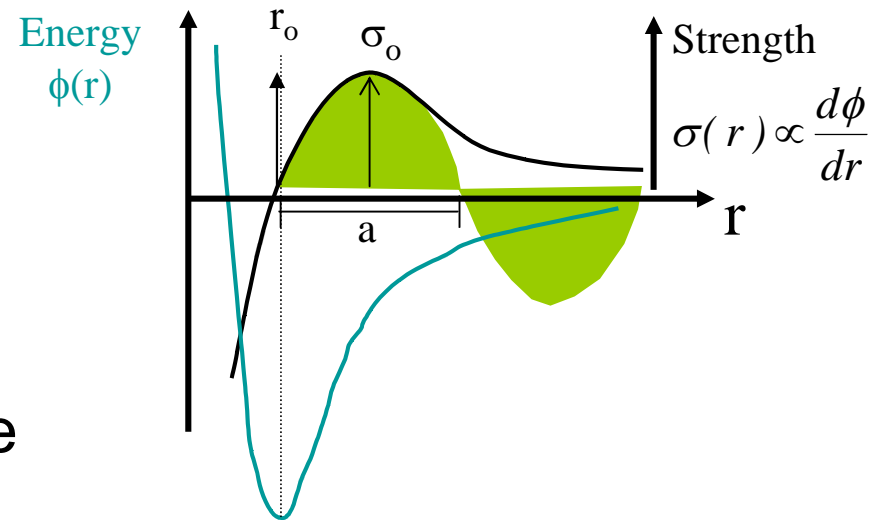
# How Strong Are Crystalline Materials?

- We have learned ...
  - Crystal symmetries, bond potentials and strengths

- Today, we will compute theoretical strength from this background

- Demonstrate why theoretical strength is purely theory
  - Actual strength is 2-3 orders of magnitude lower
  - Defects!!

# Theoretical Cohesive Strength

- Look back at the potential function for two atoms.

- Derivative is related to strength.

- Approximate strength curve with a sinusoid:

$$\sigma = \sigma_o \, sin \frac{\pi r}{a}$$

– $\sigma_o$ = theoretical cohesive strength

Energy $\phi(r)$

$r_o$ $\sigma_o$

Strength

$\sigma(r) \propto \dfrac{d\phi}{dr}$

$a$

$r$

- For small atomic displacements,

Displacement from equilibrium ($r_o$) is taken as $r$

$$\sigma = \sigma_o \frac{\pi r}{a} \qquad \Rightarrow \frac{d\sigma}{dr} = \frac{\sigma_o \pi}{a}$$

- Elastic modulus: $\qquad E = \frac{stress}{strain} = \frac{\sigma}{r/r_o}$

- Equating: $\qquad \frac{E}{r_o} = \frac{\sigma_o \pi}{a}$

- For most materials, a ~ $r_0$

$$\sigma_o = \frac{E}{\pi}$$

# How Close is Theory?

- Theory states:

$$\sigma_o = \frac{E}{\pi}$$

- Way too high for common materials (100-1000x too high)

- Look at "whiskers"

  – Small, "defect-free" fibers

  – Agreement is a little better.

| Material | $\sigma_f$ GPa | $\sigma_f$ (psi × 10⁶) | E GPa | E (psi × 10⁶) | $E/\sigma_f$ |
|---|---|---|---|---|---|
| Silica fibers | 24.1 | (3.5) | 97.1 | (14.1) | 4 |
| Iron whisker | 13.1 | (1.91) | 295.2 | (42.9) | 23 |
| Silicon whisker | 6.47 | (0.94) | 165.7 | (24.1) | 26 |
| Alumina whisker | 15.2 | (2.21) | 496.2 | (72.2) | 33 |
| Ausformed steel | 3.14 | (0.46) | 200.1 | (29.1) | 64 |
| Piano wire | 2.75 | (0.40) | 200.1 | (29.1) | 73 |

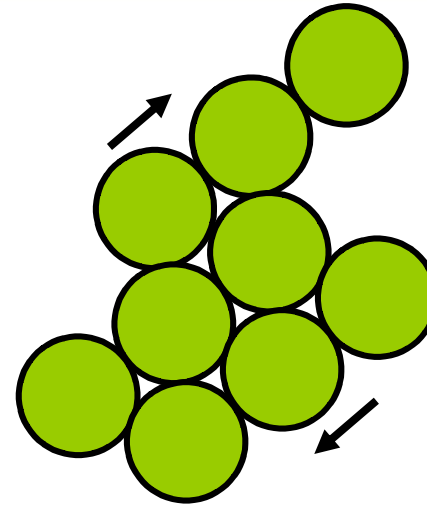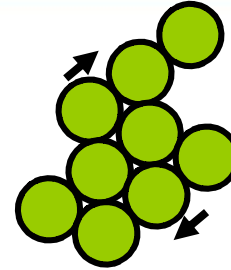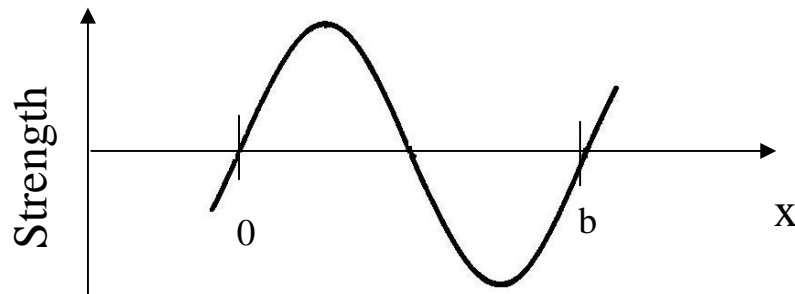**From**: Hertzberg, p.76.
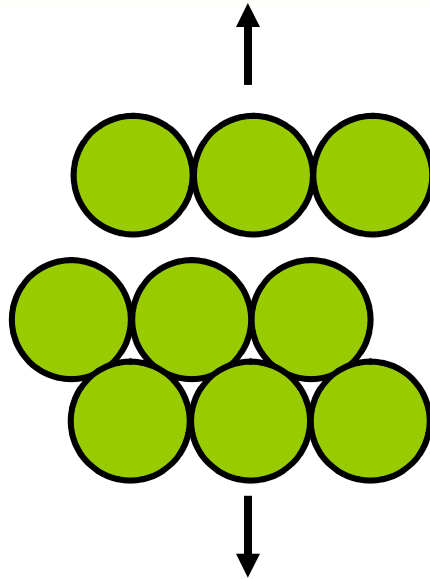
Tensile

Shear

- Previous analysis
  - Energy necessary to tear planes of atoms apart from each other
  - Tensile strength of primary bonds

- What about energy needed to cause slipping in shear?
  - Theoretical yield strength

# Frenkel Analysis



- Approximate as sinusoid, periodic in b,

Shear

$$\tau = \tau_m \, sin \frac{2\pi x}{b}$$

- For small angles,

$$\tau = \tau_m \, sin \frac{2\pi x}{b} \approx \tau_m \frac{2\pi x}{b}$$

- Assume elastic strains,

$$\tau = G\gamma$$

- For small shear strains, where a is the distance between slip planes (a≅b)

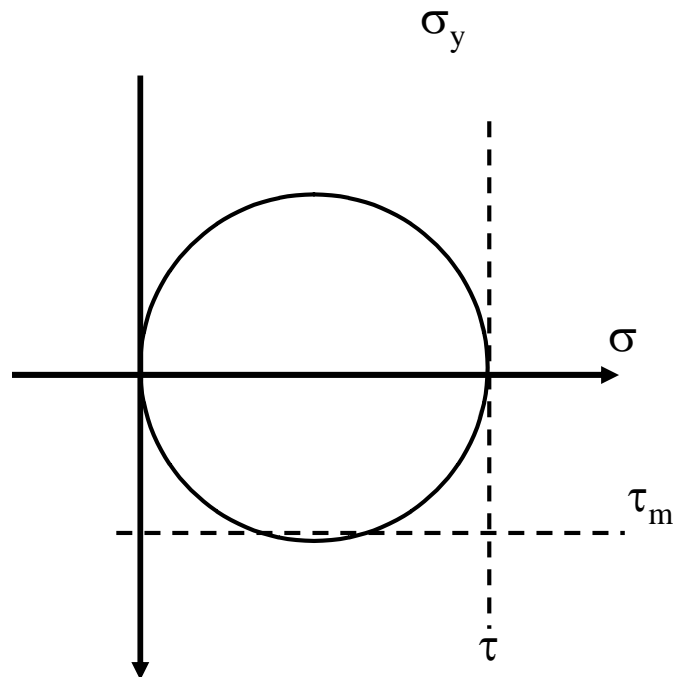$$\gamma \approx \frac{x}{a} \qquad \tau = G\frac{x}{a}$$

- Equating shear stresses

$$G \frac{x}{a} \approx \tau_m \frac{2\pi x}{b}$$

$$\tau_m \approx \frac{Gb}{2\pi a}$$

$$\tau_m \approx \frac{G}{2\pi}$$

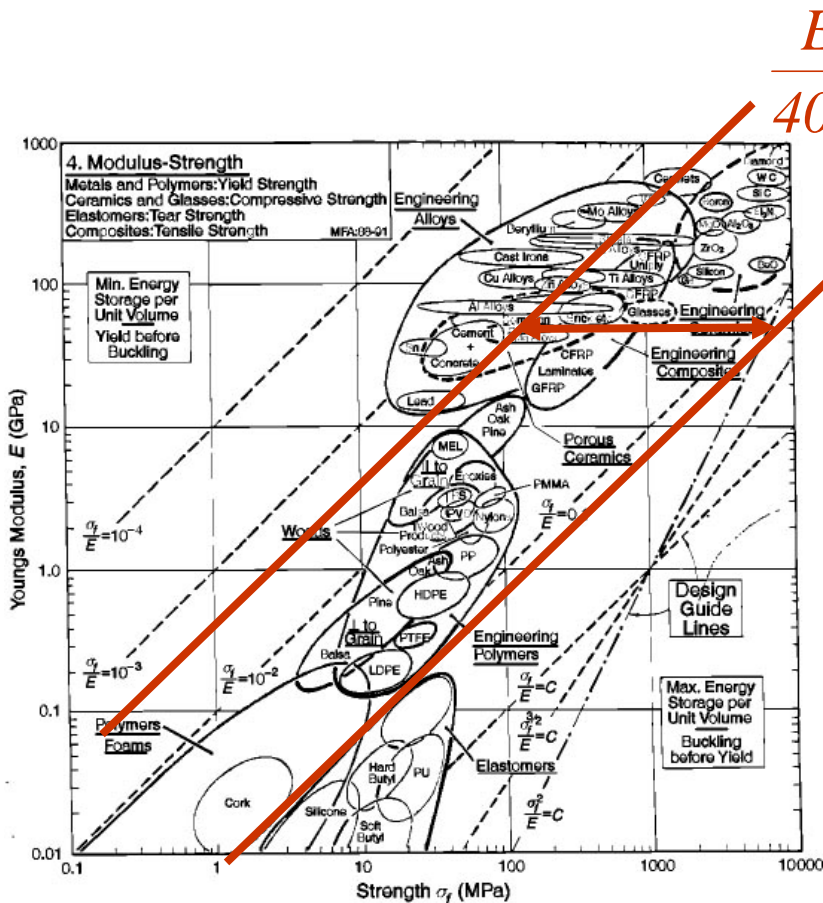- Remember Mohr's circle (uniaxial tension)



$$\sigma_y \approx 2\tau_m$$

$$G = \frac{E}{2(1+v)} \approx \frac{E}{2.6}$$

$$\boxed{\sigma_y \approx \frac{E}{8}}$$

**Still too high!**

$$\frac{E}{400}$$

$$\frac{E}{8}$$

M. F. Ashby, <u>Materials Selection in Mechanical Design</u>, 1999, pg 424

- Experimental strengths ~100x lower than theory
- Some experiments show discrepancy to be ~1000x
- Whiskers and fibers can come close, but not exact.

**TABLE 2.2 Theoretical and Experimental Strengths of Dislocation-Free Crystal (Whiskers)[6]**

| Material | Theoretical Strength $(G/2\pi)$ | | Experimental Strength | | |
|---|---|---|---|---|---|
| | GPa | $10^6$ psi | GPa | $10^6$ psi | Error |
| Copper | 19.1 | 2.77 | 3.0 | 0.44 | ~6 |
| Nickel | 33.4 | 4.84 | 3.9 | 0.57 | ~8.5 |
| Iron | 31.8 | 4.61 | 13 | 1.89 | ~2.5 |
| $B_4C$ | 71.6 | 10.4 | 6.7 | 0.98 | ~10.5 |
| SiC | 132.1 | 19.2 | 11 | 1.60 | ~12 |
| $Al_2O_3$ | 65.3 | 9.47 | 19 | 2.76 | ~3.5 |
| C | 156.0 | 22.6 | 21 | 3.05 | ~7 |

- Need an explanation for lower strength $\Rightarrow$ *defects*!

# Defects in Solids

- To this point we have assumed perfect order in crystals
  - Defects always exist in real materials
  - Sometimes we add "defects" - alloying

- Classifications of defects
  - Usually referring to geometry or dimension of defect
  - **Point** : 1-2 atomic positions ($10^{-10}$ m)- e.g. vacancies, interstitials
  - **Line**: 1-Dimensional ($10^{-9}$ to $10^{-5}$ m)- e.g. dislocations
  - **Interfacial**: 2-Dimensional ($10^{-8}$ – $10^{-2}$ m) - e.g. grain boundaries
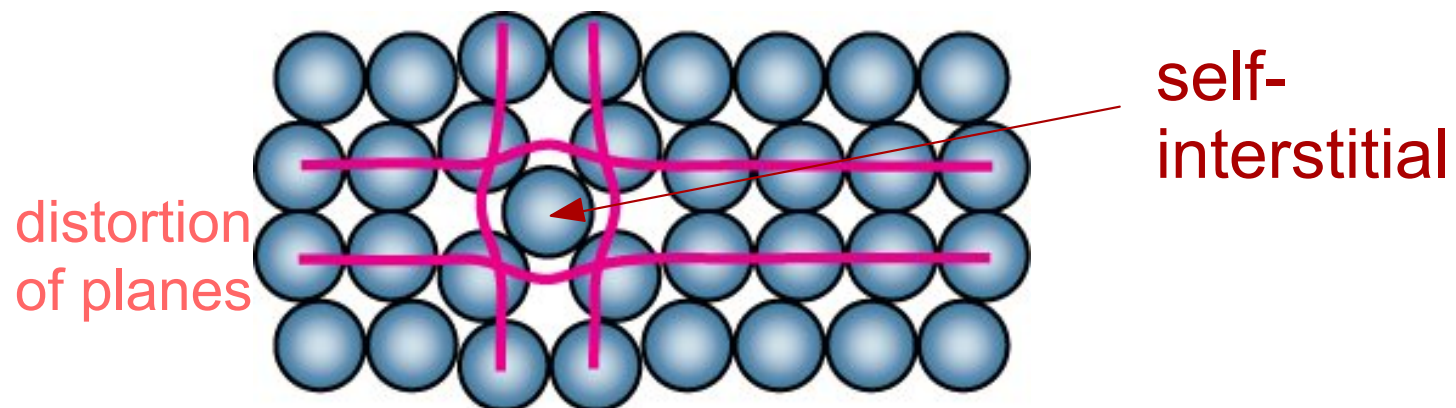  - **Volume**: 3-Dimensional ($10^{-4}$ – $10^{-2}$ m) - e.g. pores, cracks

# Point Defects

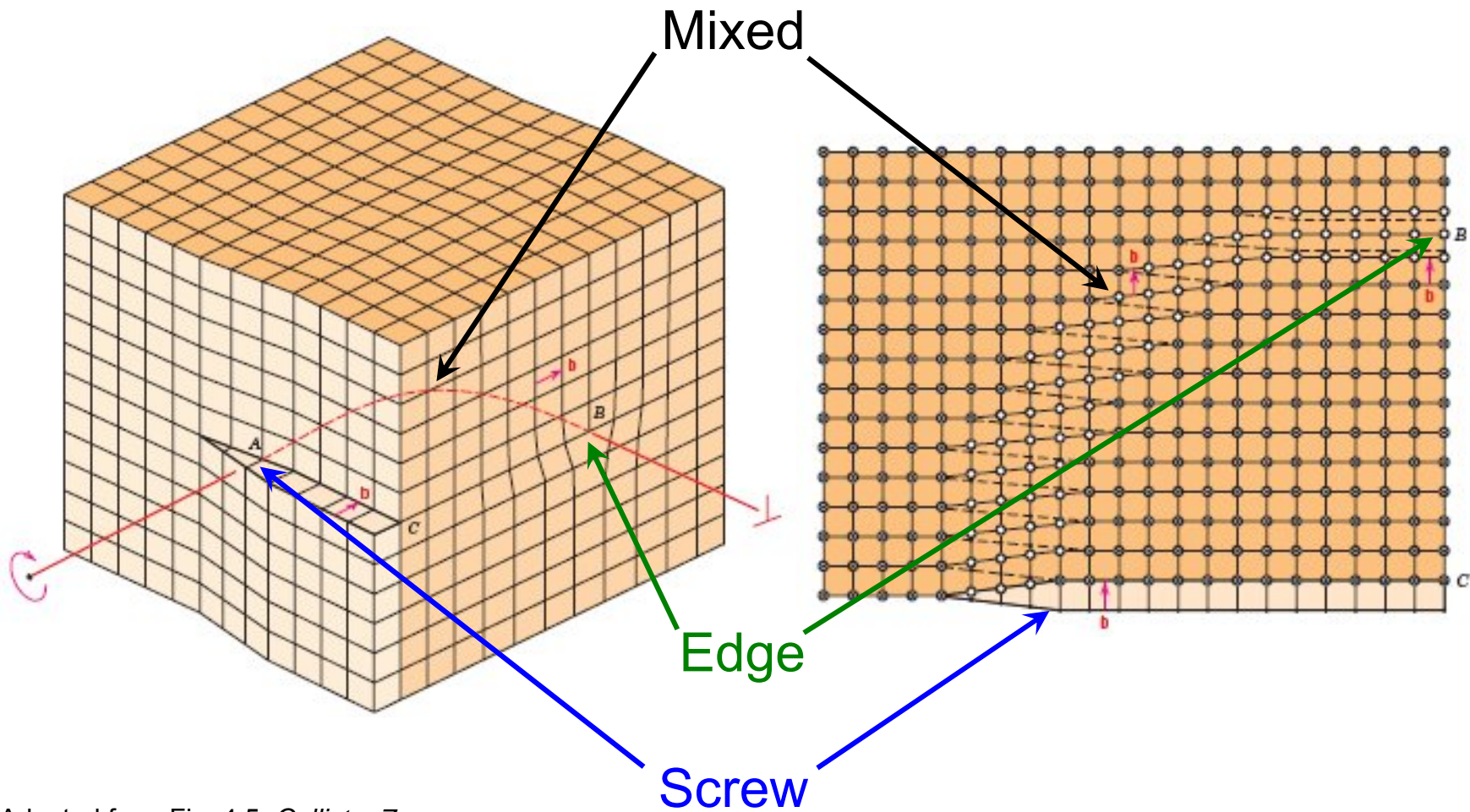- **Vacancies:**
  -vacant atomic sites in a structure.



distortion of planes

Vacancy
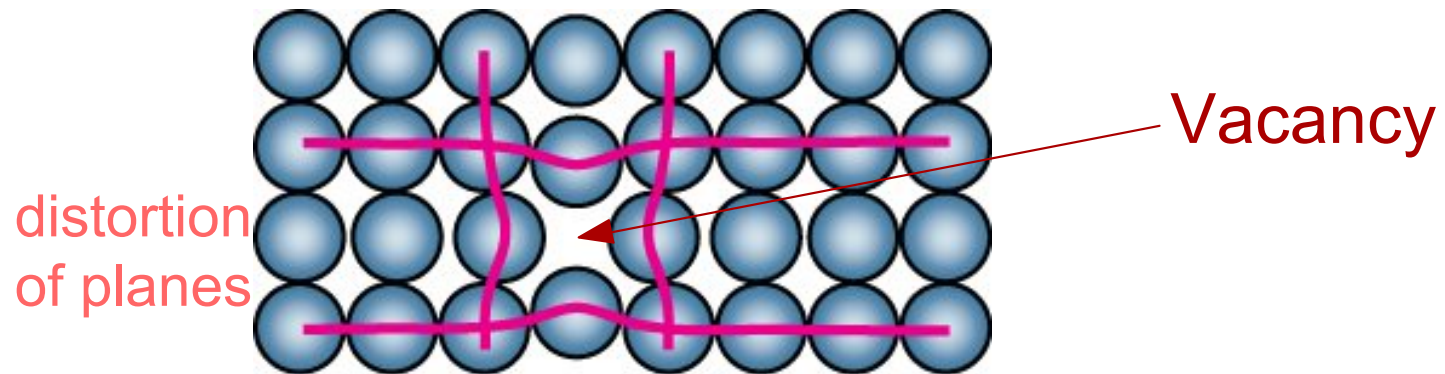
- **Self-Interstitials:**
  -"extra" atoms positioned between atomic sites.



distortion of planes

self-interstitial

Mixed

Edge

Screw

Adapted from Fig. 4.5, *Callister 7e.*
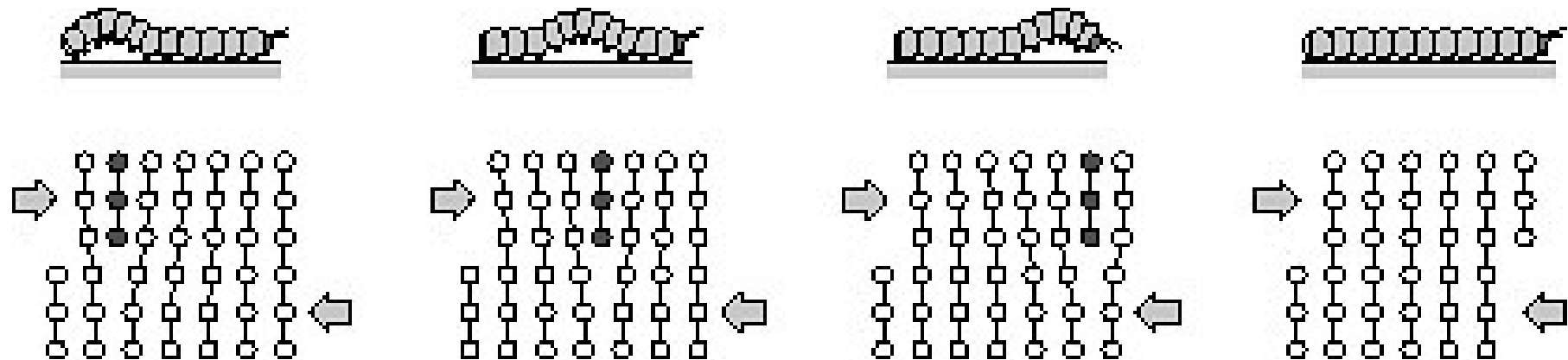
- Shear must act in direction of **Burgers vector** $b$

- Edge
  - Positive & negative
- Screw
  - Right-hand & left-hand
- Analogies for motion
  - Caterpillar crawling
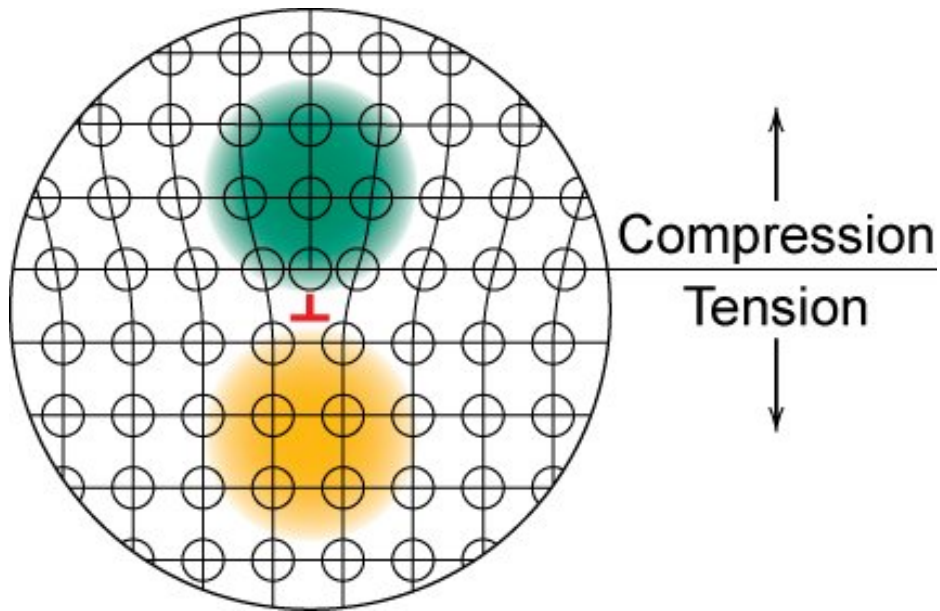
# Interfacial Defects - Planar

- **2-Dimensional in extent**
- **External surfaces**
  - **Do not bond to maximum nearest neighbors $\Rightarrow$ high surface energy**
- **Grain Boundaries**
  - **Boundary separating two grains (crystals)**
  - **Atoms bonded less regularly along these boundaries**
  - **Larger grains have lower total interfacial energy**
  - **High angle (more energy) vs. low angle boundaries**



Angle of misalignment

High-angle grain boundary

Small-angle grain boundary

Angle of misalignment
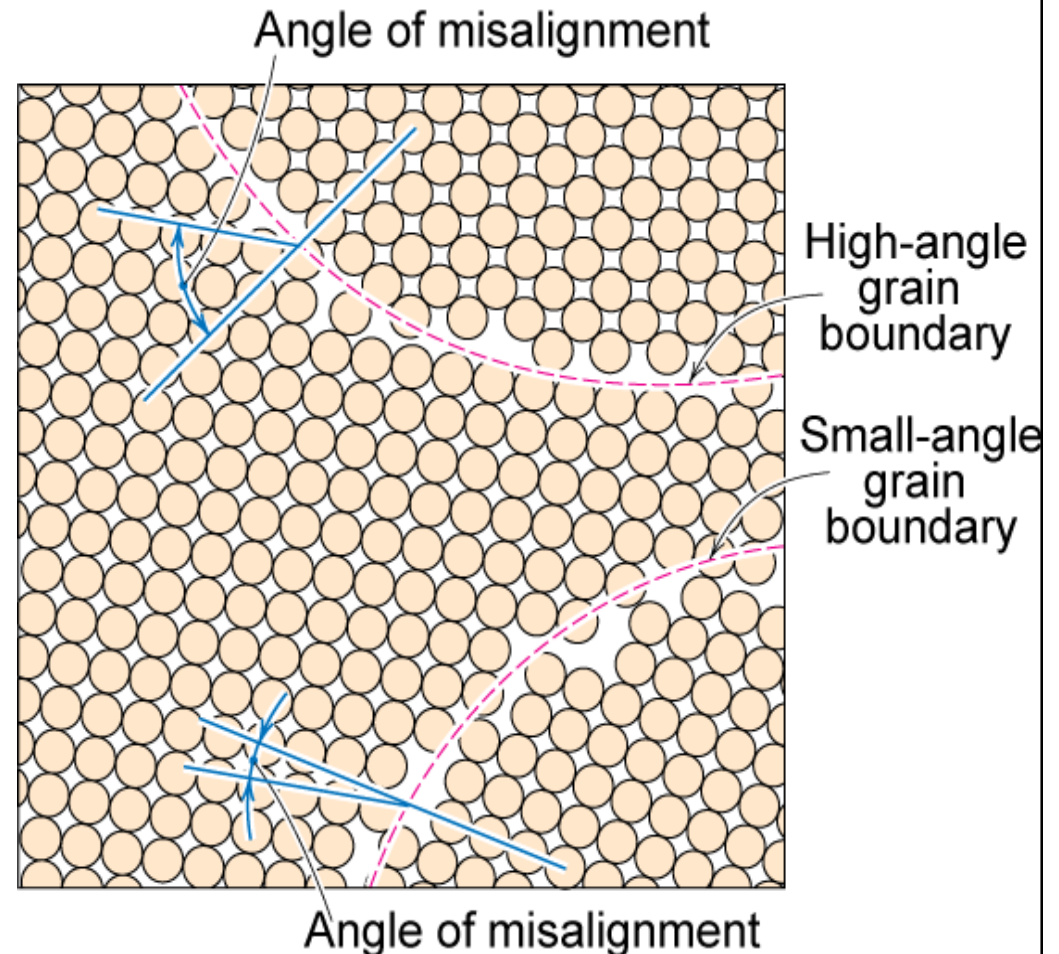
**From**: Callister, p.79, 84.

Compression

Tension

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

- Extra half plane of atoms cause lattice distortions
- Result in *tensile*, *compressive*, and *shear* strains in neighboring atoms
  - Magnitude decreases with distance
  - Pure compression and tension directly above and below slip line
  - Over most of the effected region combination of stresses
- Screw dislocation
  - Pure shear
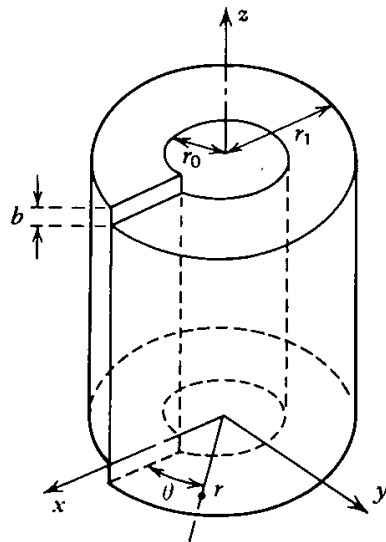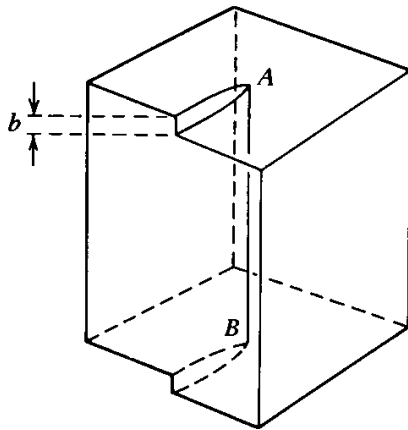
**For small strains**

Shear strain:
$$\gamma_{\theta z} = \frac{b}{2\pi r}$$

From Hooke's law:
$$\tau_{\theta z} = G\gamma_{\theta z} = \frac{Gb}{2\pi r}$$

Elastic strain energy:

$$E_{screw} = \frac{1}{2}\int_{r_o}^{r_1}\tau_{\theta z}bdr = \frac{1}{2}\int_{r_o}^{r_1}\frac{Gb^2}{2\pi}\frac{dr}{r} = \frac{Gb^2}{4\pi}ln\left(\frac{r_1}{r_0}\right)$$

Similarly for edge dislocation

$$E_{edge} = \frac{Gb^2}{4\pi(1-v)}\ln\left(\frac{r_1}{r_0}\right)$$

For our purposes, use:
$$E_{edge} = \alpha Gb^2$$
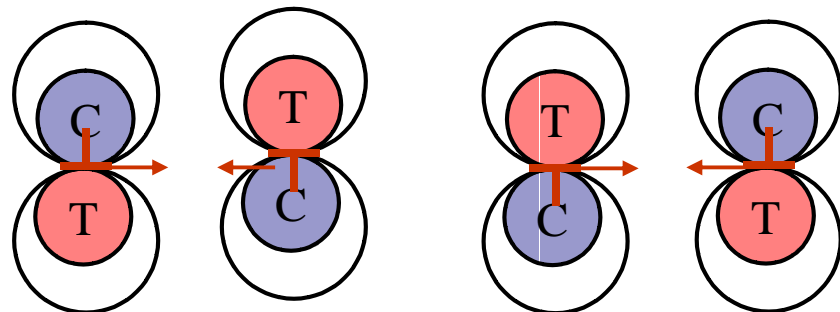
$\alpha$ is geometrical factor

- Want to be in lowest possible energy state
  - When "far" apart, Burger's vectors have no influence on each other
  - When together, there will be interaction between the two
    - Attract each other if Burger's vectors cancel
    - Repel if Burger's vectors are of same sign

Apart

$$E = \alpha Gb^2 + \alpha G(-b)^2 = 2\alpha Gb^2$$
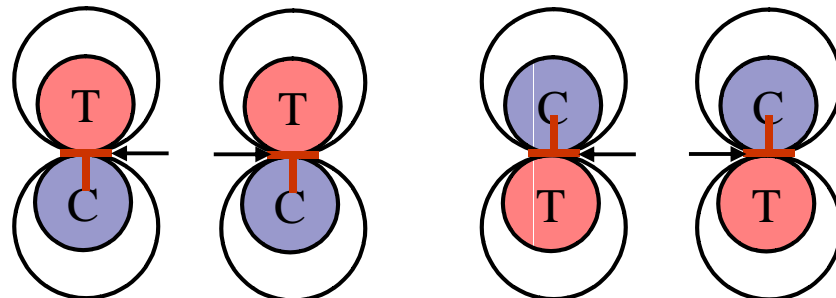
Together

$$E = \alpha G(b + (-b))^2 = 0$$
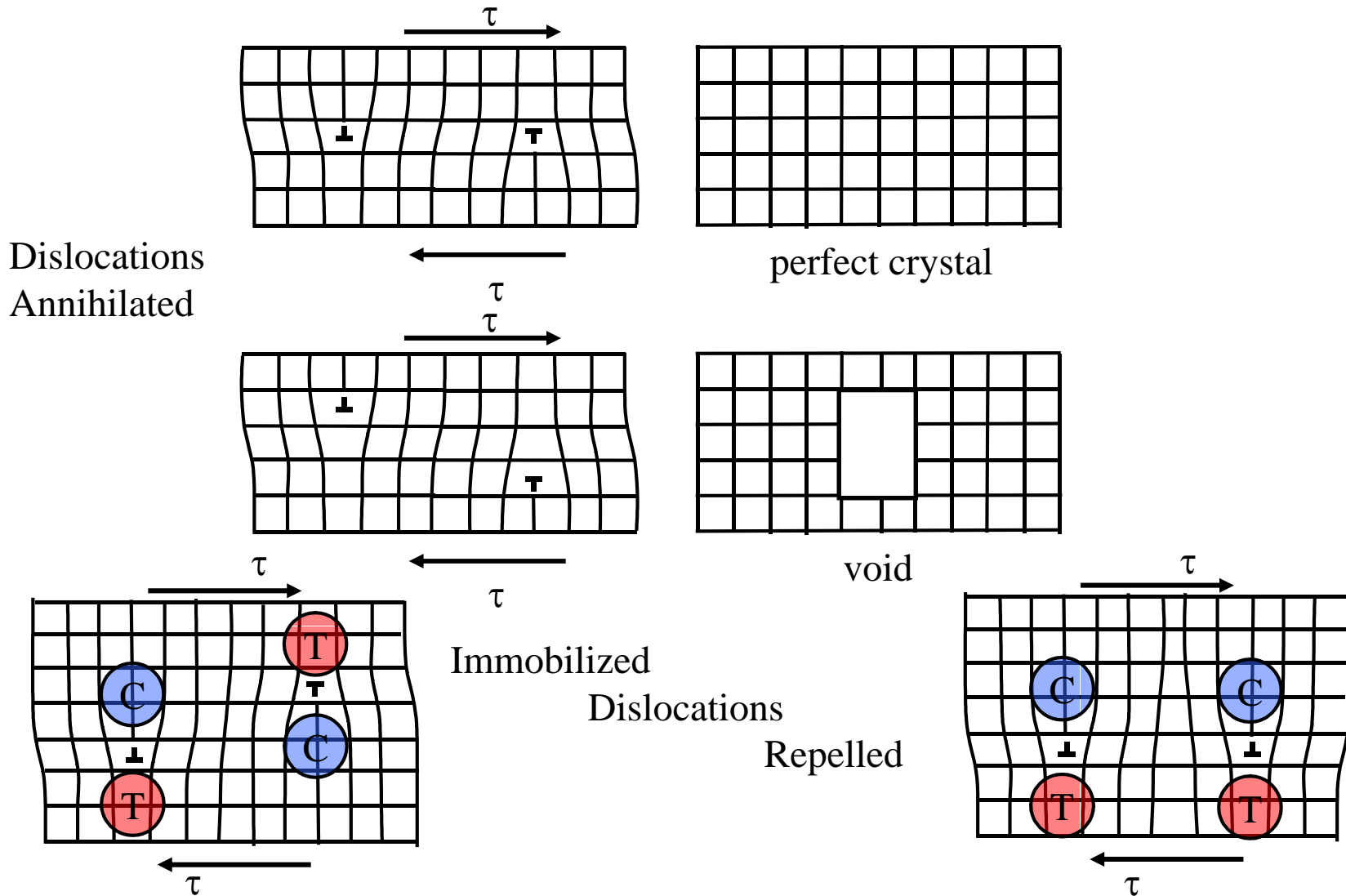
Apart

$$E = \alpha Gb^2 + \alpha Gb^2 = 2\alpha Gb^2$$
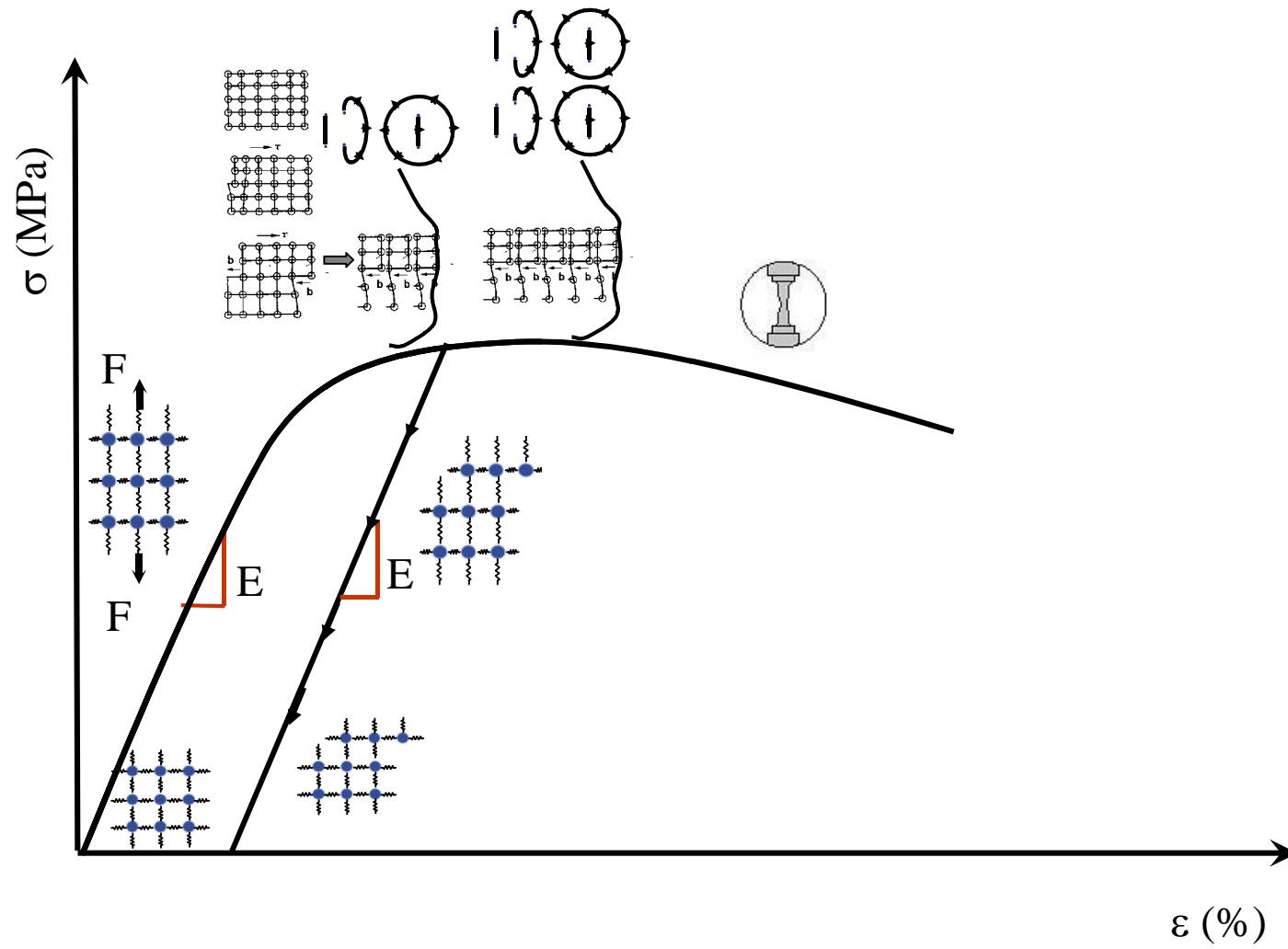
Together

$$E = \alpha G(b + b)^2 = 4\alpha Gb^2$$

Dislocations
Annihilated

perfect crystal

Immobilized
Dislocations

void

Dislocations
Repelled

Results from crack propagation

- Griffith Crack

$$\sigma_m = 2\sigma_o \left( \frac{a}{\rho_t} \right)^{1/2} = K_t \sigma_o$$

a stress concentration factor
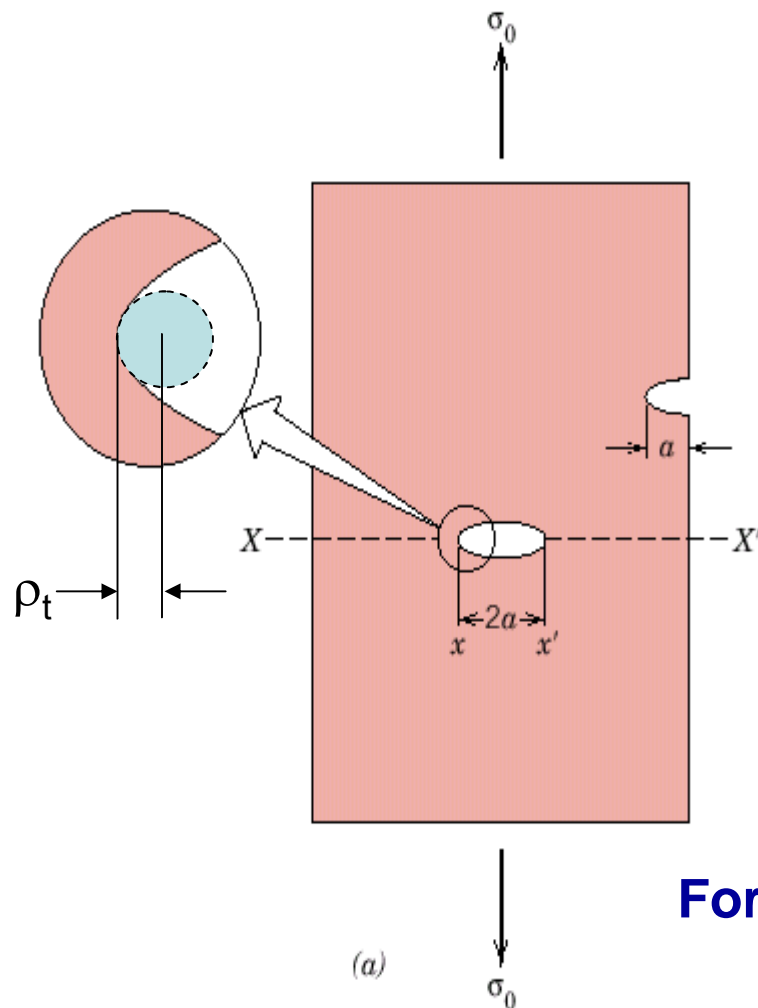
where

$\rho_t$ = radius of curvature

$\sigma_o$ = applied stress

$\sigma_m$ = stress at crack tip

**For a crack, typically have**
**a = 10⁻³m**
**ρ = 10⁻⁹m** $\sigma_{local} = 2000 * \sigma_{applied}$

V

$\Gamma$

$U_T$

a

$U_E$

$a_{crit}$
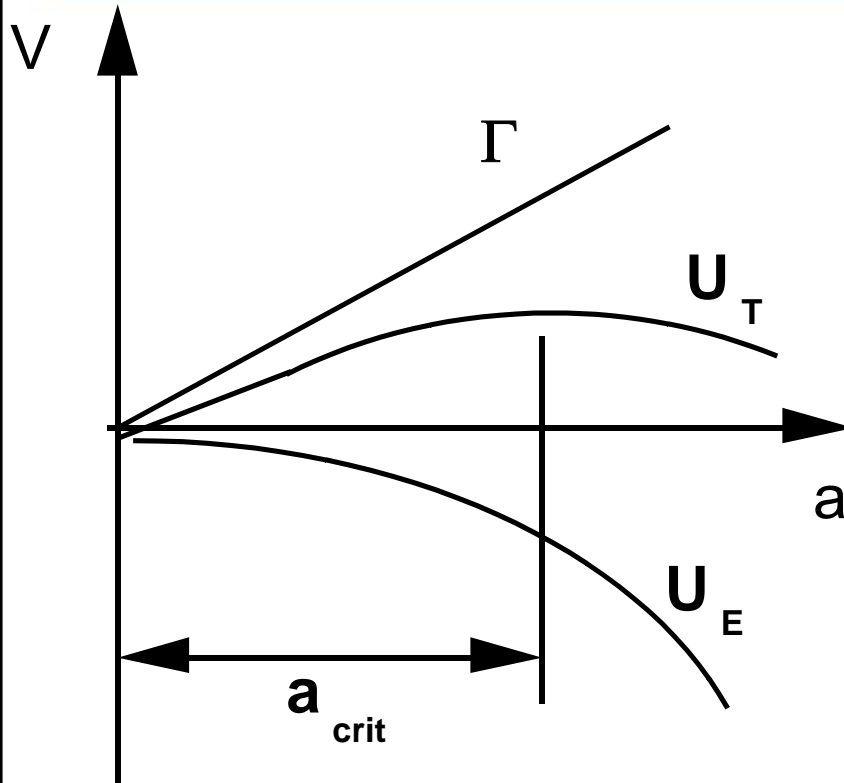
Minimum criterion for stable crack growth:

Strain energy goes into surface energy

$\sigma_{applied}$

$l$

$2a$

$\Delta a$

$2w$

*thickness, t*

$\sigma_{applied}$
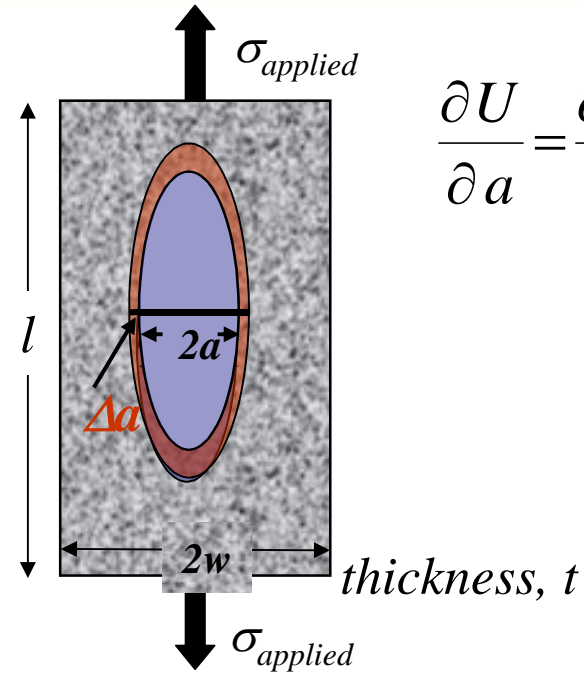
$$\frac{\partial U}{\partial a} = \frac{\partial \Gamma}{\partial a}$$

$$\frac{\partial}{\partial a}\left( \frac{\sigma^2}{2E} \pi \, 2 \, a^2 \, t \right) = \frac{\partial}{\partial a}\left( \gamma_s \, 4 \, a \, t \right)$$

$$\sigma = \sqrt{\frac{2 E \gamma_s}{\pi \, a}}$$

# So When Does Crack Propagate?

**Crack propagates rapidly if above critical stress**

$$\text{i.e.,} \quad \sigma_m > \sigma_c$$

$$\sigma_c = \left(\frac{EG_c}{\pi a}\right)^{1/2}$$

$$\sigma_c\sqrt{\pi a} = \sqrt{EG_c} \quad = \text{constant!!}$$

**where**

- *E* = modulus of elasticity
- Gc = specific energy release rate
- *a* = one half length of internal crack

**Measurable (fixed) materials properties**
**Fracture Toughness, K$_c$**

**Brittle:** $\quad G_C = 2\gamma_s$

**Ductile:** $\quad G_C = 2\left(\gamma_s + \gamma_p\right)$

# Additional Reading

- **Callister, Chapter 7&8, in *Materials Science and Engineering*,** 7th Edition, John Wiley, 2007

- NanoHUB resource: "Synthesis & Mechanics of Nanostructures & Nanocomposites" by Rod Ruoff

- Cleland and Roukes, "Noise processes in nanomechanical resonators", JAP, 92(2002)2758