Materials

Bonding between Atoms

Attraction

Coulombic force between particles

$$F_A = q_1 q_2 / 4\pi\epsilon_0 r^2$$

q1,q2 – electric charge of the two ions

E_0 – permittivity of vacuum

r – distance between particles

More simply

$$F_A = A'/r^2$$

Work done by F_a for pulling particle from infinity to position r

$$E_A = \int_r^\infty F_a dr = -\frac{A}{r}$$

Repulsion

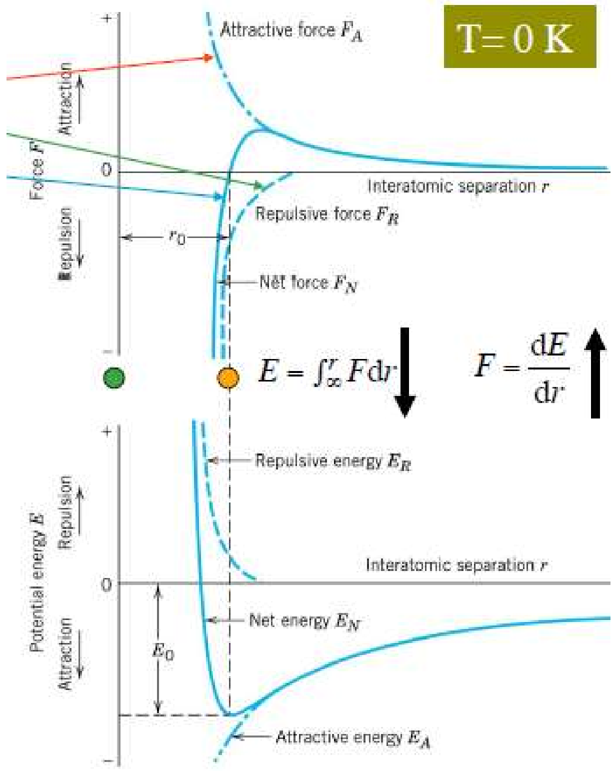
$$F_R = -\frac{B'}{r^{n+1}}$$

$$E_R = B/r^n$$

Total

$$F_N = \frac{dE_N}{dr} = F_A + F_R = \frac{A'}{r^2} - \frac{B'}{r^{n+1}} \cong \frac{A'}{r^{m+1}} - \frac{B'}{r^{n+1}}$$

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n} \cong -\frac{A}{r^m} + \frac{B}{r^n}$$



Covalent bonding

Sharing electrons, strong primary bonds

m<n

Metallic bonding

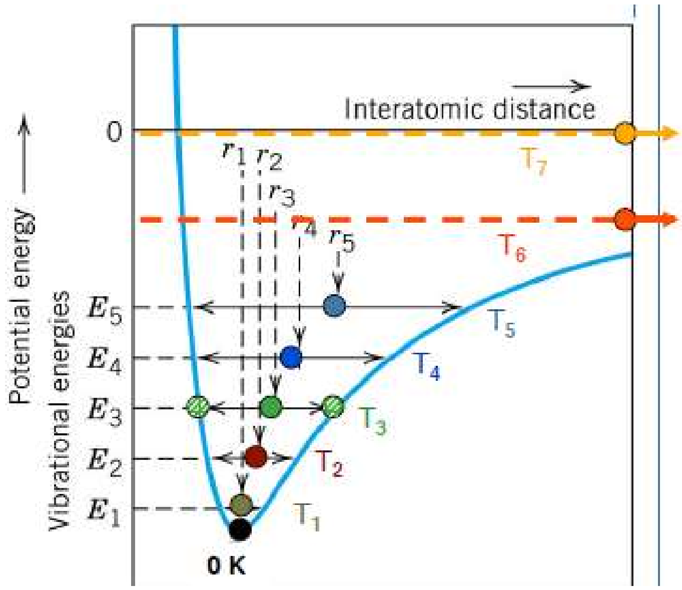
Valence elecrons can move freely from atom to atom – not localised

m<n

van der Waals bonding

Dipoles form and go at all times, attraction between oppositely charged poles, weak secondary bonds

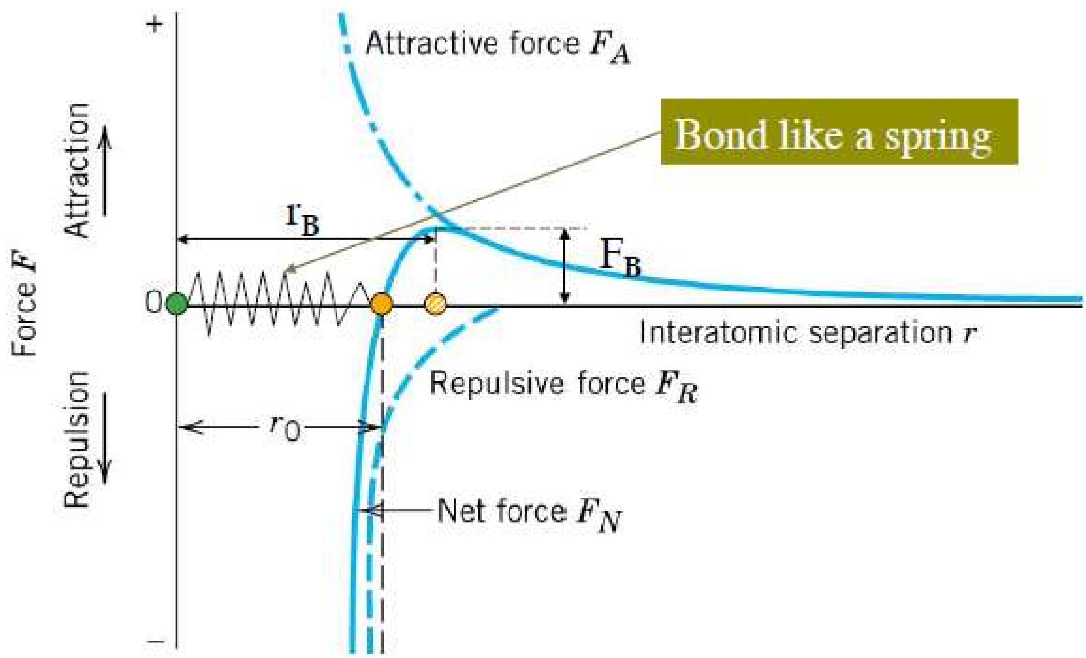
Effect of Temperature



T1 < T2 < T3 < T4 < T5

As temperature increases, r increases – thermal expansion

Effect of Force



rB: breaking distance

FB: breaking force

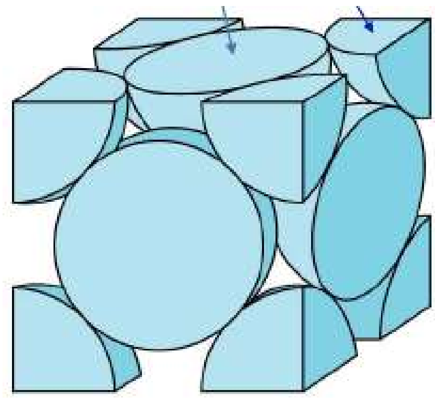
Once you have passed the breaking distance/force it becomes easier to pull the atom away

Structure of Crystalline Solids

General

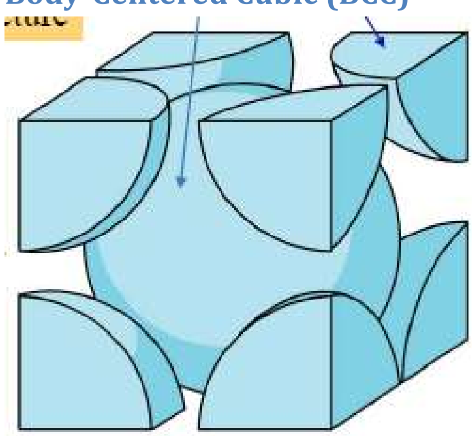
- Amorphous solids – packing of atoms is random
- Crystalline – periodic packing of atoms
- Unit cell – repeating unit in crystal
- Materials take certain structures so that the lowest potential is achieve

Face-Centered Cubic (FCC)



Equivalent atoms	4
Length of a	$2\sqrt{2} * \mathrm{R}$
Total volume of unit cell	$16\sqrt{2}R^3$
Total volume of atoms	$\frac{16}{3}\pi R^3$
Atomic packing factor (APF)	0.74
Packing type	AB

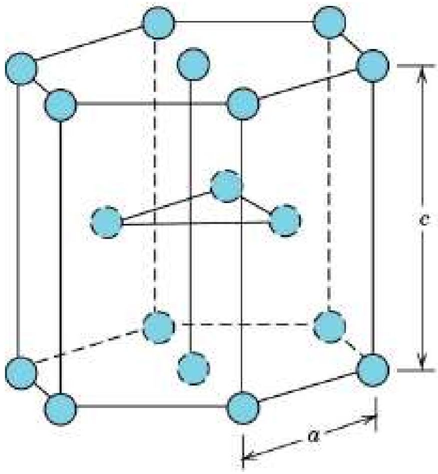
Body-Centered Cubic (BCC)



Equivalent atoms	2
Length of a	$\frac{4\mathrm{R}}{\sqrt{3}}$

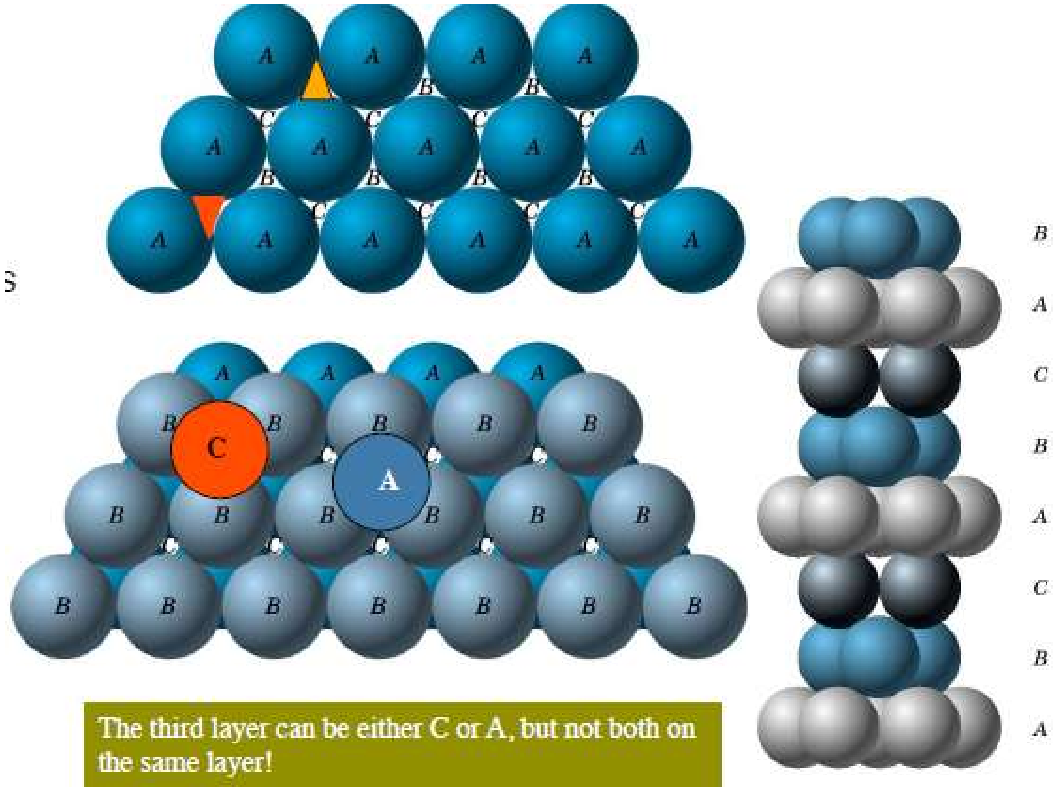
Total volume of unit cell	$\frac{64R^3}{3\sqrt{3}}$
Total volume of atoms	$\frac{8}{3}\pi R^3$
Atomic packing factor (APF)	0.68

Hexagonal Close-Packed (HCP)



Equivalent atoms	6
Ratio c/a	1.633
Total volume	
Atomic packing factor (APF)	0.74
Packing type	ABC

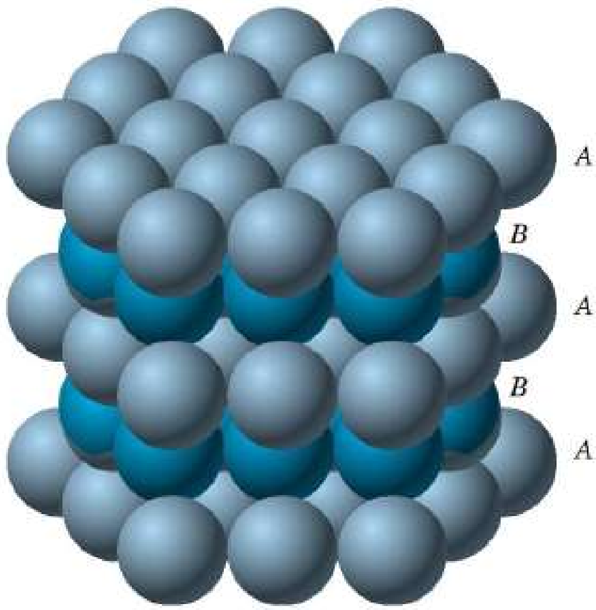
ABC Packing



Close-packed plane (layer A)

Intestitial sites: B(upright triangles), C(upside down triangles)

AB Packing



Miller indices

<uvw> is a family of directions [uvw], every direction has the same arrangement of atoms

{uvw} is a family of planes (uvw)

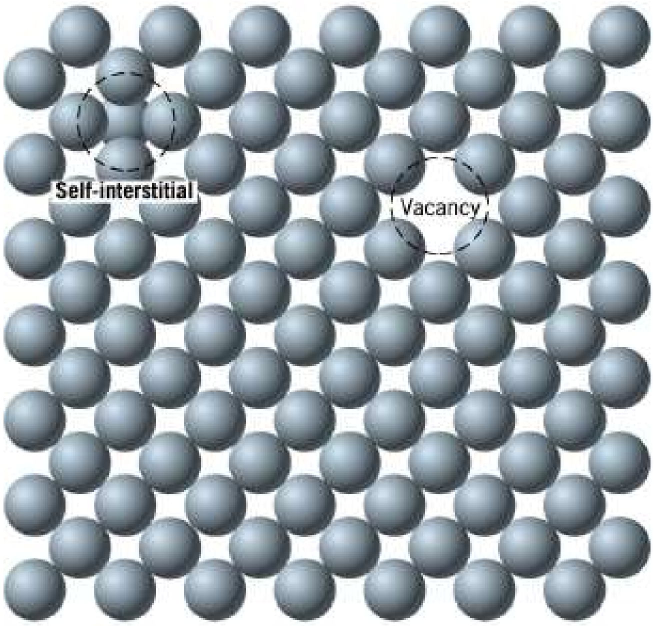
Defects in Crystalline Solids

General

- Perfect crystals have no irregularity
- Defects can give strength and rise to processes like diffusion
- Distortion is deviation of atoms from their sites
- Defects have higher energy

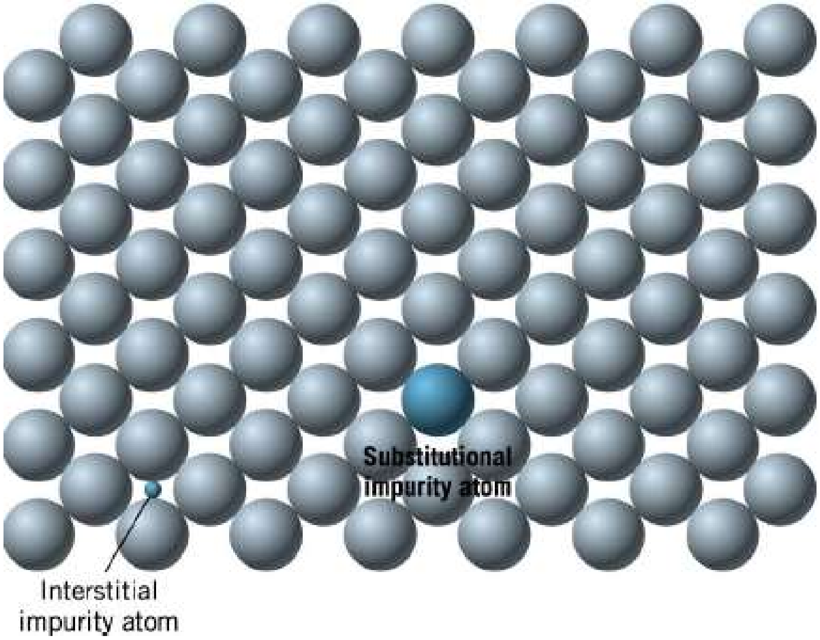
Point defects

Vacancy



- Atoms missing from lattice sites
- $\frac{N_V}{N} = \exp\left(-\frac{Q_v}{kT}\right)$
  N - total number of lattice sites
  Qv – formation energy of one vacncy
  k – Boltzmann's constant
  T – absolute temperature
- Nv = 0 only at T = 0
- Nv = 1 at T = infinity
- Nv increases with T

Impurity (Alloying)

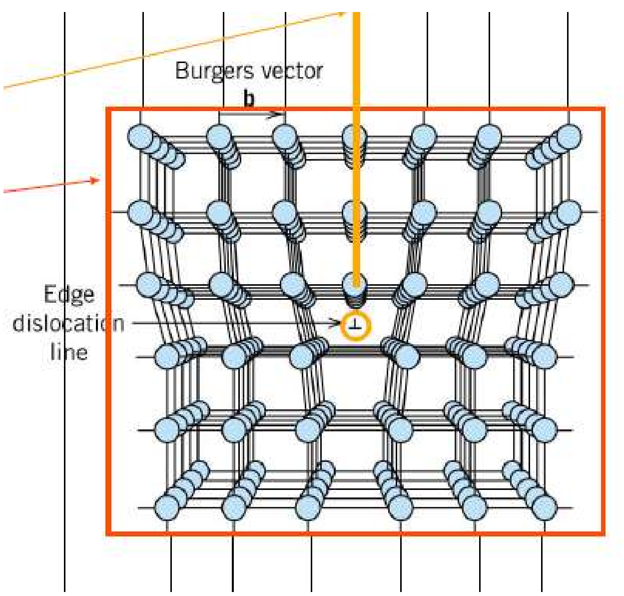


- Substitutional atoms occupy the lattice sites of host atoms
- Interstitial atoms stay between the host atoms

Line defects

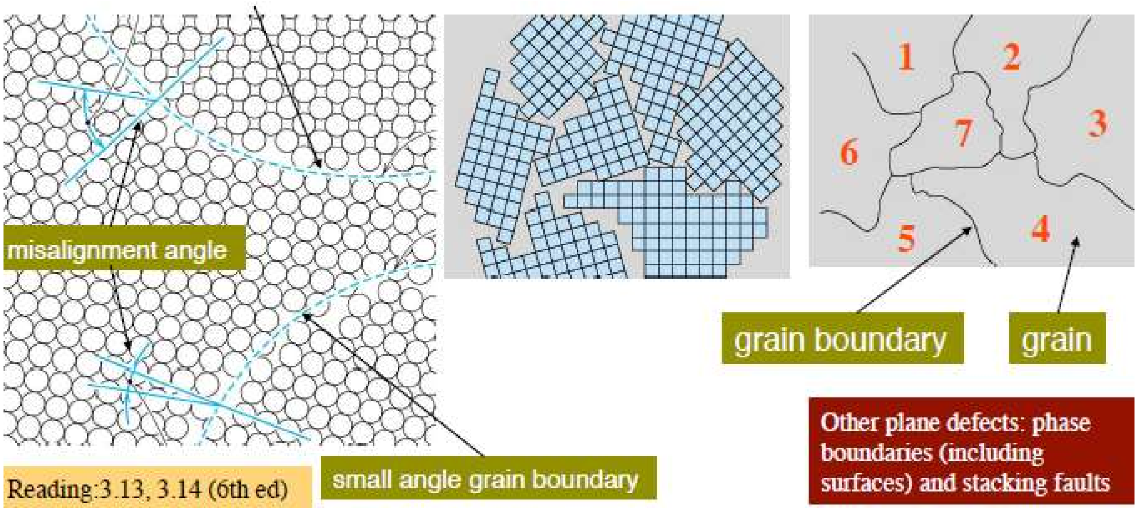
Dislocations

- Edge dislocations: extra half plane of atoms, distortion around dislocation line with associated elastic energy due to changing distance between atoms.
- Screw dislocations: displaced atoms along dislocation line
- Mixed dislocations



Plane defects

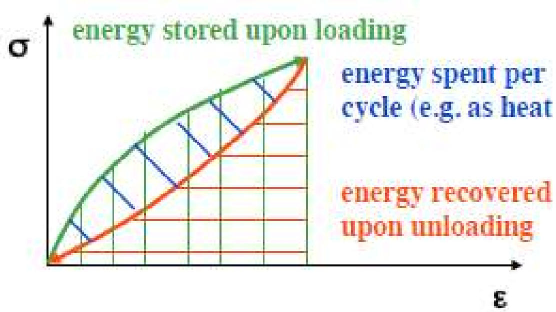
Grain boundaries



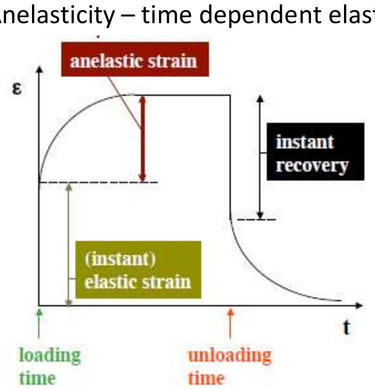
Elastic Deformation

General

- Bonds are being pulled apart, linear relationship for most materials (metal), nonlinear for some (rubber)
- Some materials lose energy during unloading



- Anelasticity – time dependent elastic deformation



Formulas

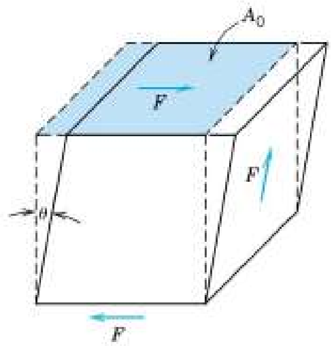
$$Stress: \sigma = \frac{F_n}{A_0}$$

$$Shear\ stress: \tau = \frac{F_s}{A_0}$$

$$Strain: \epsilon = \frac{l - l_0}{l_0} = \frac{\delta l}{l_0}$$

$$Poissons: \nu = -\frac{\epsilon_w}{\epsilon}$$

$$Shear\ strain: \gamma = tan\theta$$



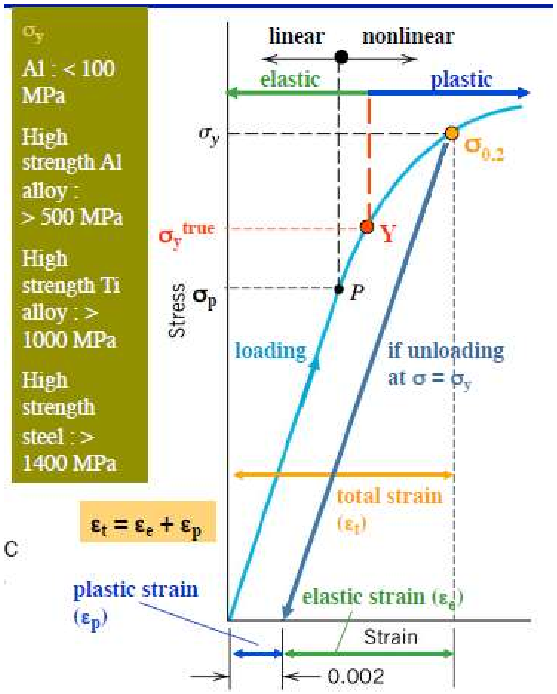
$$Elastic\ modulus: E = \frac{\sigma}{\epsilon}\ (Represents\ stiffness\ of\ bonds)$$

Plastic Deformation

General

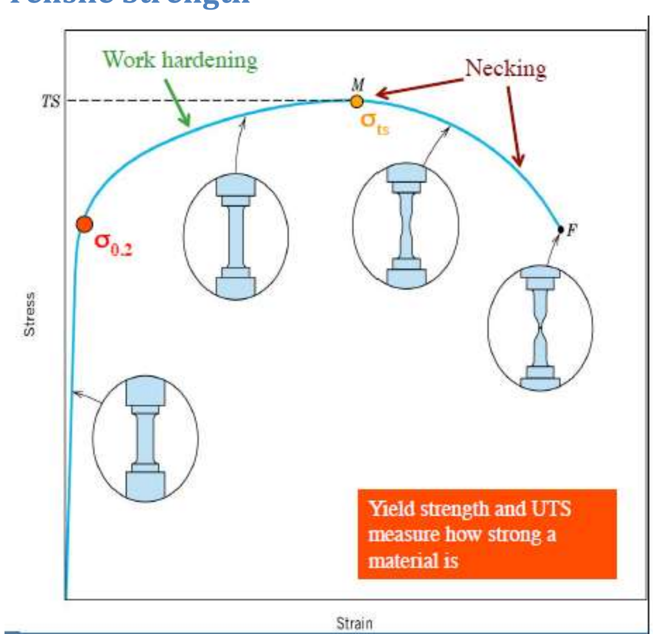
- Movement of dislocations
- Permanent deformation

Yielding



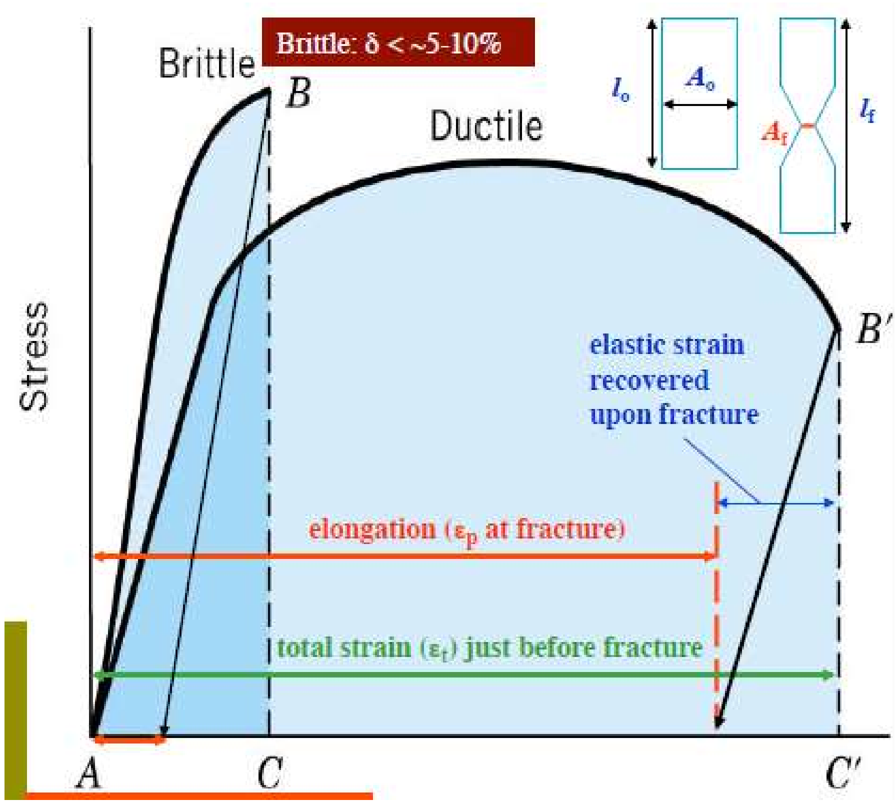
- Yield point – divides between elastic/plastic
- Proportional limit – divides between linear and nonlinear behaviour
- 0.2% proof stress – Approximates yield point with line parallel to linear region drawn from 0.2% strain

Tensile Strength



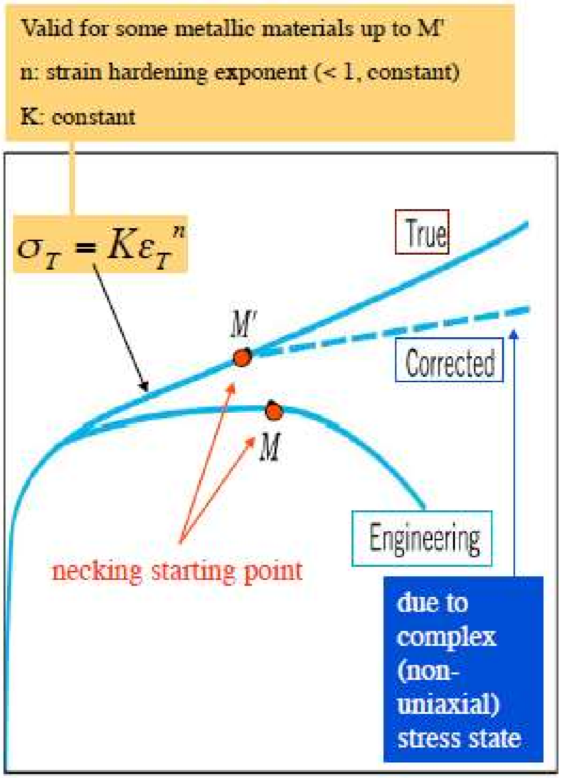
- Maximum stress material can withstand
- Higher than yield stress due to work hardening
- Necking happens after this point until fracture

Ductility



- $Total\ plastic\ strain\ at\ fracture: \delta = \frac{l_f - l_0}{l_0}$
- $Reduction\ in\ area: RA = \frac{A_0 - A_f}{A_0}$

True Stress and Strain

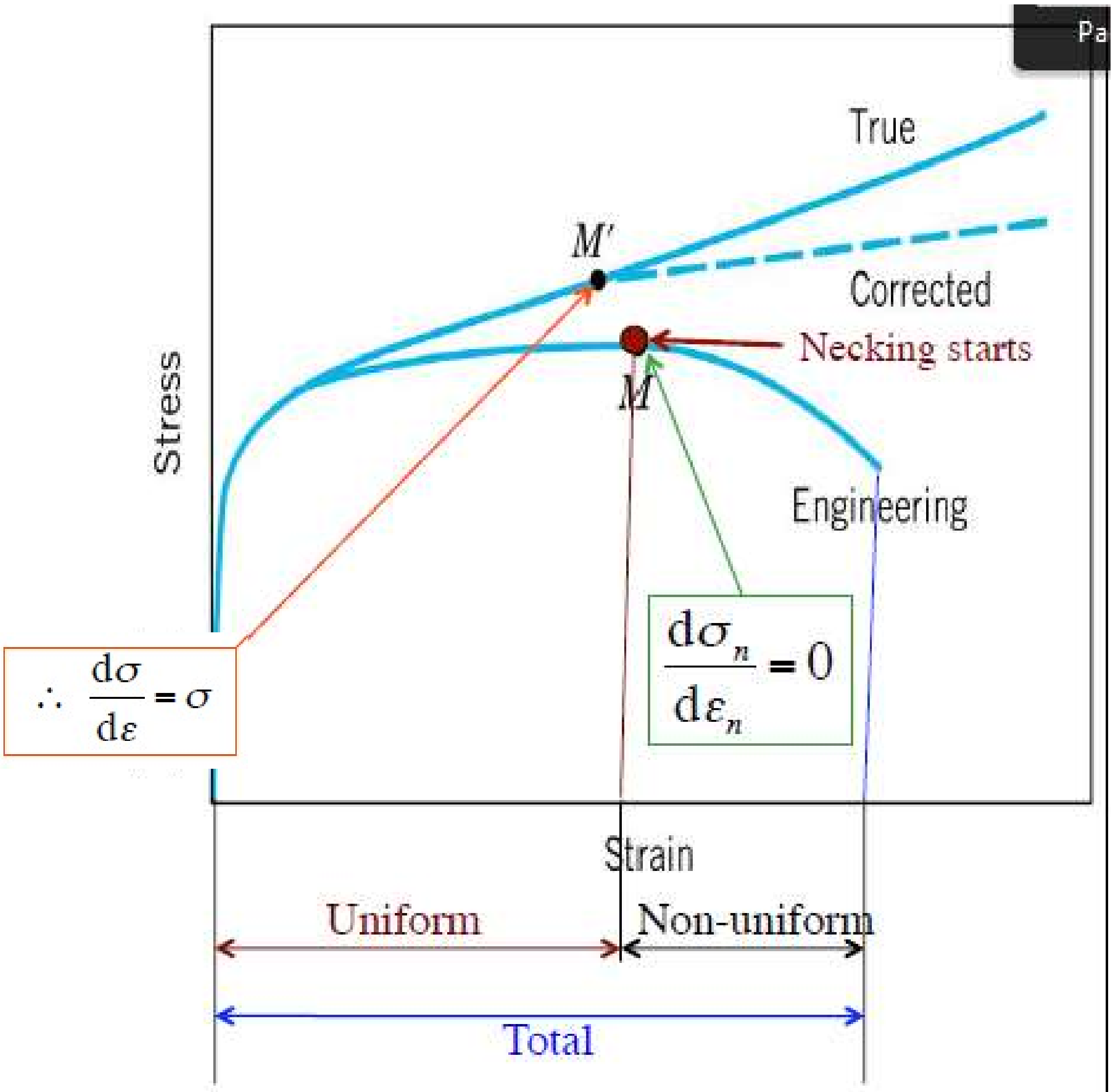


- Area/Length change as material is deformed
- $\sigma_T = \frac{F}{A_i}$
- $\epsilon_T = \int d\epsilon = \int_{l_0}^{l_f} \frac{dl_i}{l_i} = \ln\left(\frac{l_f}{l_0}\right)$
- In plotting the true stress vs true strain curve

  $$\sigma_T = \sigma(1+\epsilon)$$
  $$\epsilon_T = \ln(1+\epsilon)$$

  After necking, use actual force area and length to calculate true stress and strain as these equations are no longer valid

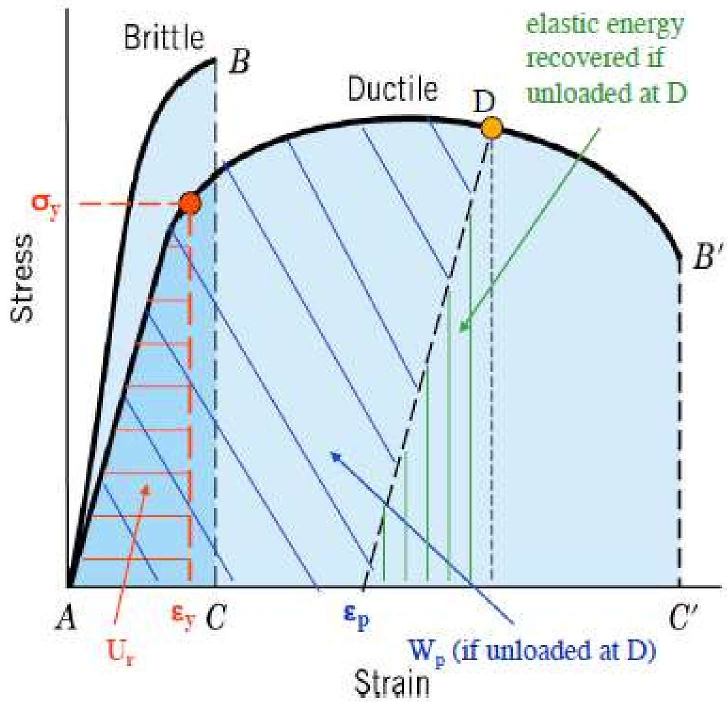
Plastic Instability



- Before UTS plastic deformation is uniform
- At UTS, necking starts and deformation becomes non-uniform (becomes localised at neck)
- Want to maximise uniform deformation
- Flow stress is the stress needed to cause flow (plastic deformation)

  Flow force = $A\sigma_T$ (A is the real area at the moment)
  - in tension: $A \downarrow$; $\sigma_T \uparrow$(work hardening)
  - if $\sigma_T \uparrow$ more than $A \downarrow$ so that $A\sigma_T \uparrow$, flow not localised
  - if $\sigma_T \uparrow$ less than $A \downarrow$ so that $A\sigma_T \downarrow$, flow localised = instability (necking)
-

Resilience and plastic work



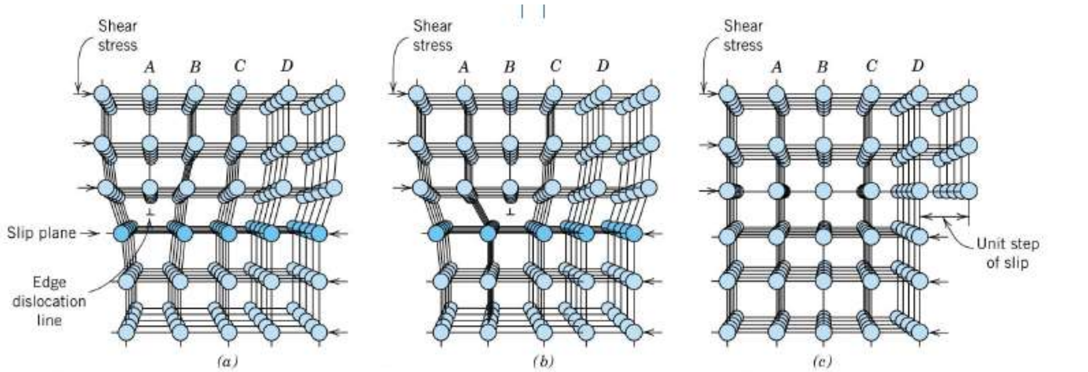
- Modulus of resilience is the elastic strain energy per volume stored in the material at point of yielding

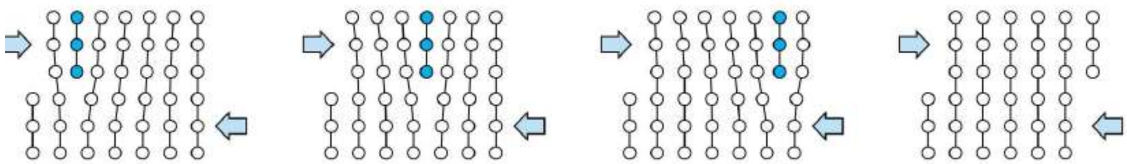
$$U_r = \int_0^{\epsilon_y} \sigma d\epsilon$$
$$When\ Hooke's\ law\ applies$$
$$U_r \cong \frac{1}{2}\sigma_y \epsilon_y = \frac{\sigma_y^2}{2E}$$

- Plastic work per volume Wp – work done to cause a plastic strain of ϵ_p

Dislocations & Plastic Deformation

Movement of dislocations

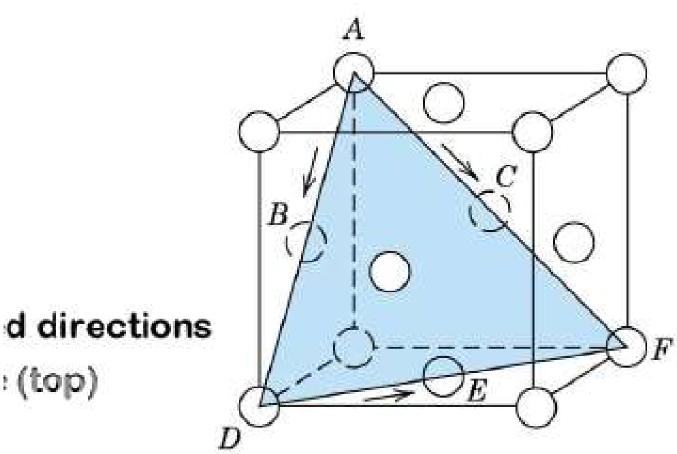


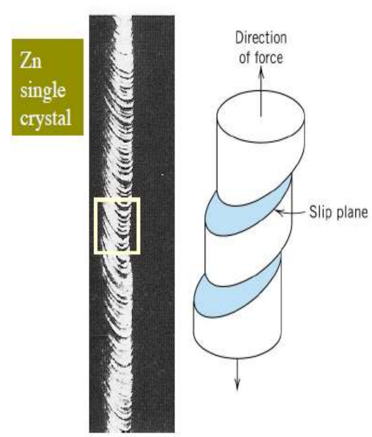


- Dislocation shifts across

Slip Systems

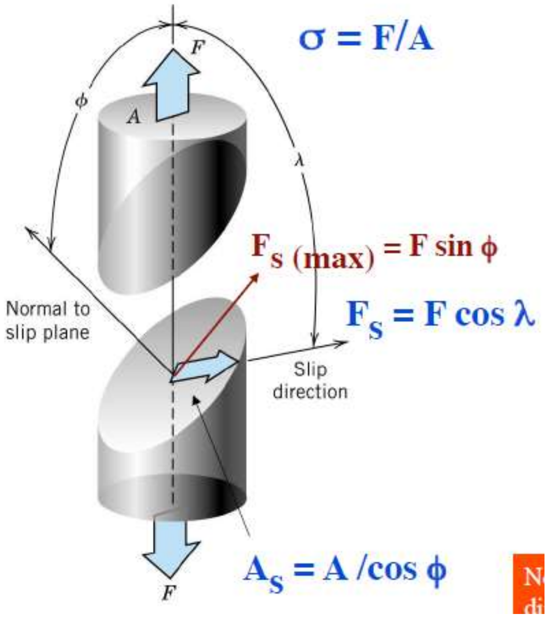
– 12 slip systems in a FCC structure: 4 x {111} planes & 3 <110> directions on each plane





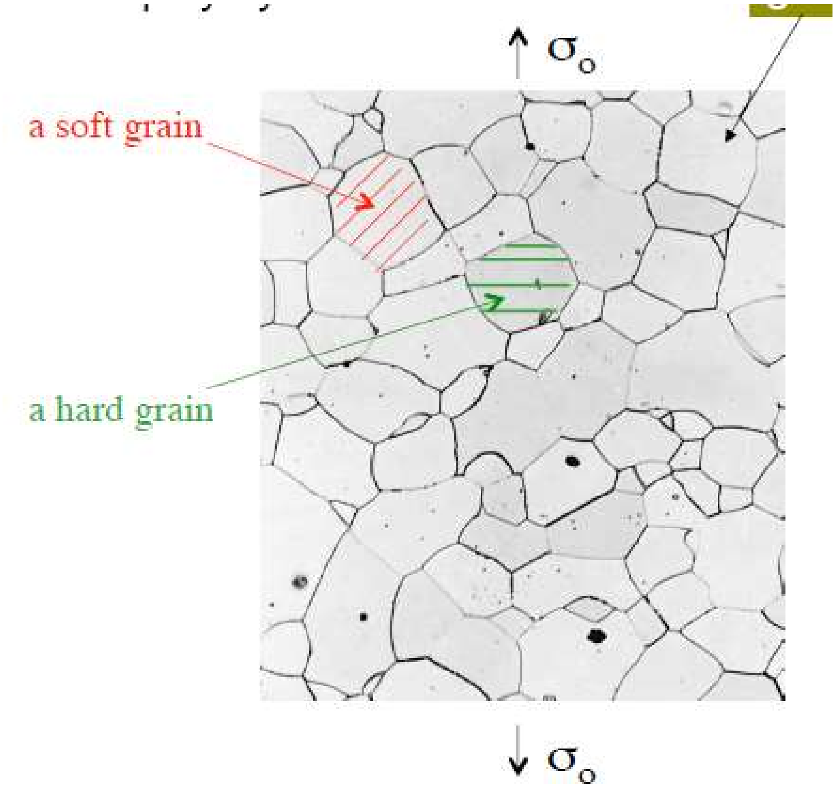
- Dislocation moves on slip plane
- Dislocation density increases with deforming
- Often takes place on close packed planes and directions because they require smallest stress to slip
- One slip plane + one slip direction = slip system

Slip in single crystals



- ϕ is angle between normal to slip plane and force
- λ is angle between force and slip direction
- $Schmidt\ factor = \ cos\phi cos\lambda$
- $\tau_R = \frac{F_s}{A_s} = \sigma cos\phi cos\lambda$
- $\tau_{R(MAX)} = \ \sigma cos\phi cos\lambda = \ \ \sigma cos\phi sin\phi\ , \lambda = \frac{\pi}{2} - \phi$
- The stress required to cause slip is the critical resolve shear stress τ_{CRSS}

Plastic deformation of polycrystalline materials

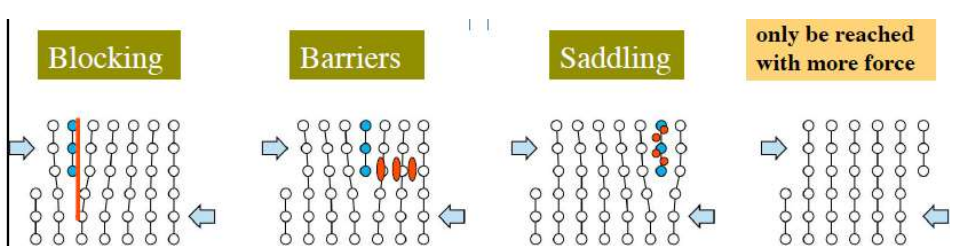


- Grains have their own usually random orientation
- Schmid factor varies, so an average behaviour is observed
- Yield strength is dependent on grain size

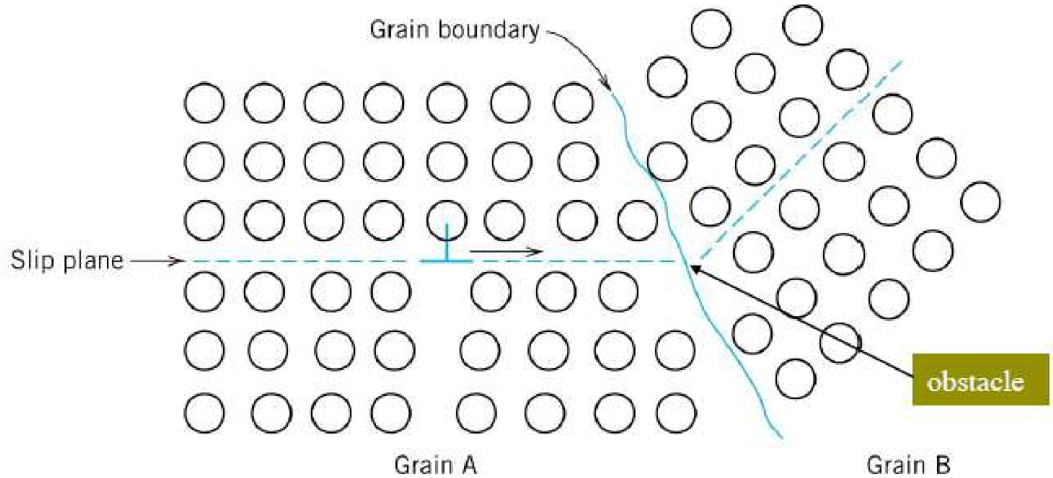
Strengthening and Softening

General

- Alloys typically stronger than pure
- Alloys stronger as more deformed
- Finer grain sizes are stronger
- Metals can be softer after exposure at higher temp
- Strengthening occurs by stopping movement of dislocations/increasing difficulty of movement
- Can be achieved by changing composition

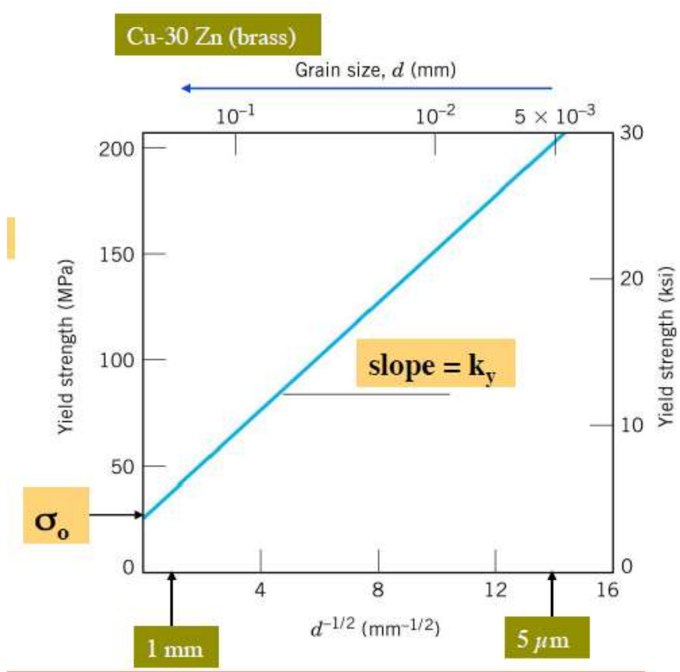


Grain Size Strengthening

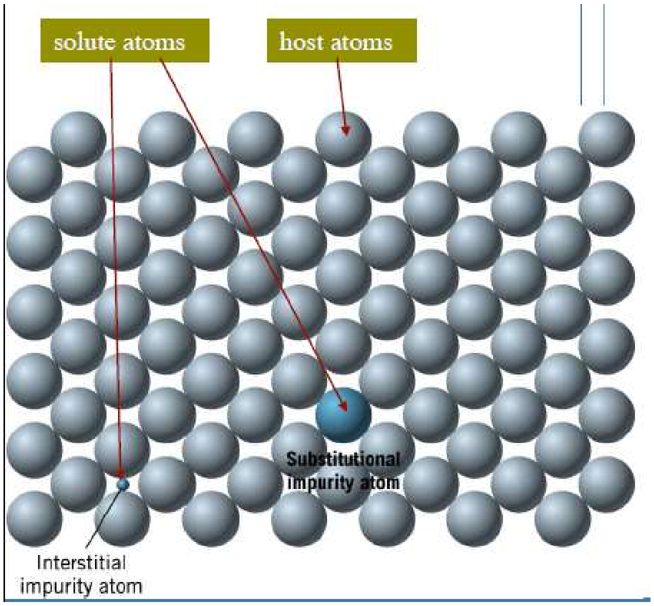


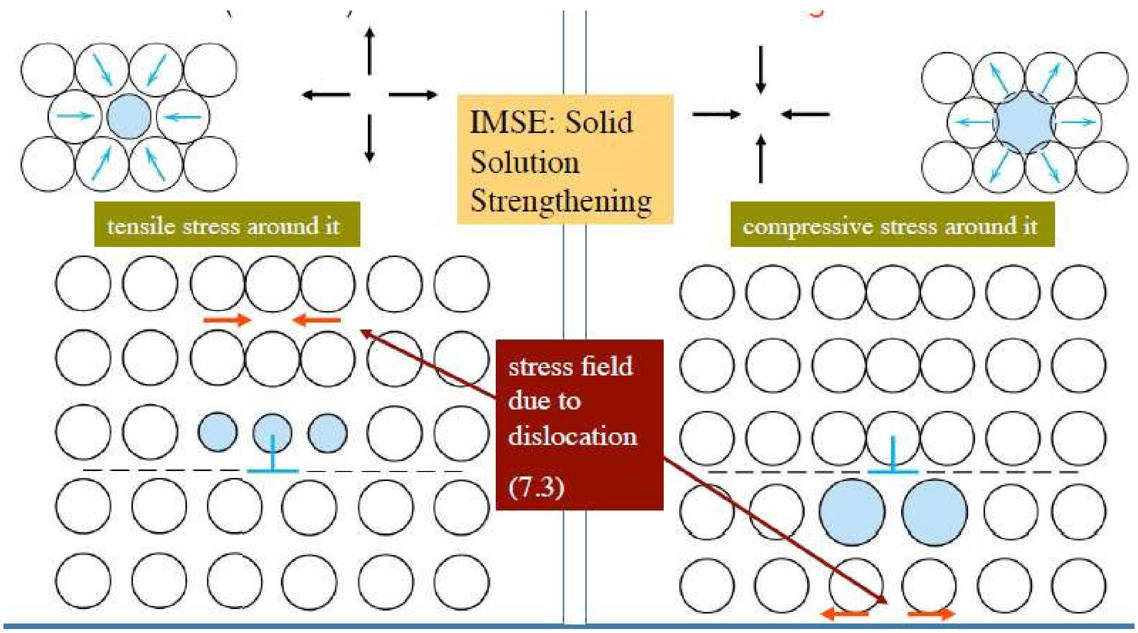
- Grain boundaries can be a barrier to dislocations
- Dislocations may not be able to continue between grains as they are different orientations
- Large angle boundaries are more effective
- Finer grains = more grain boundaries
- Hall-Petch relationship, σ_O, k_y are constants.
  Yield strength increases rapidly with decreasing grain size. May not work at extreme small/large grain sizes.

$$\sigma_y = \sigma_O + \frac{k_y}{\sqrt{d}}$$



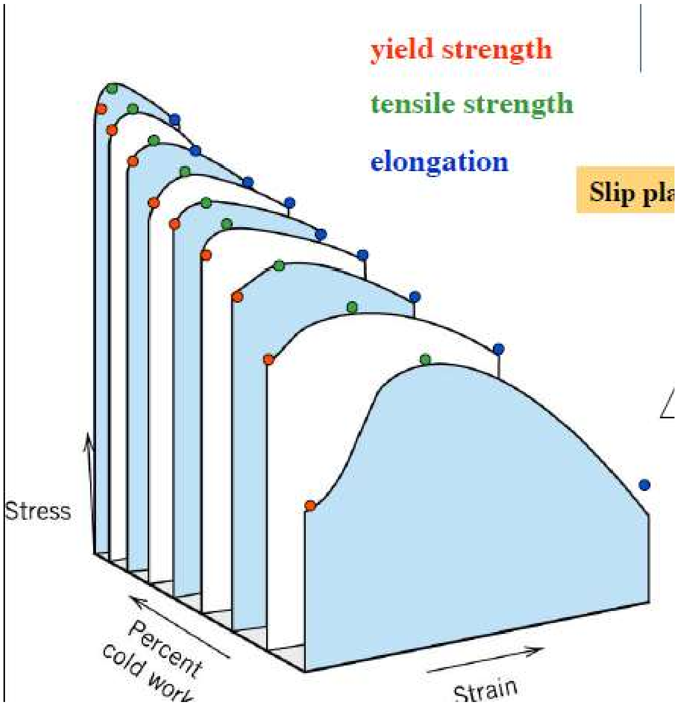
Solid Solution Strengthening





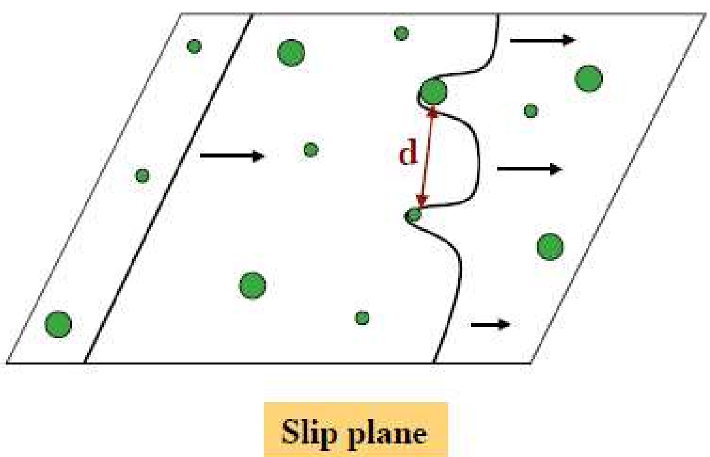
- Smaller/Larger atoms cause compressive/tensile stress fields around them.
- Atoms 'saddle' dislocations
- Makes it harder for dislocations to move
- $\Delta\sigma_y \propto \sqrt{C_{solute}}$, Csolute is the concentration of solute atoms

Strain hardening



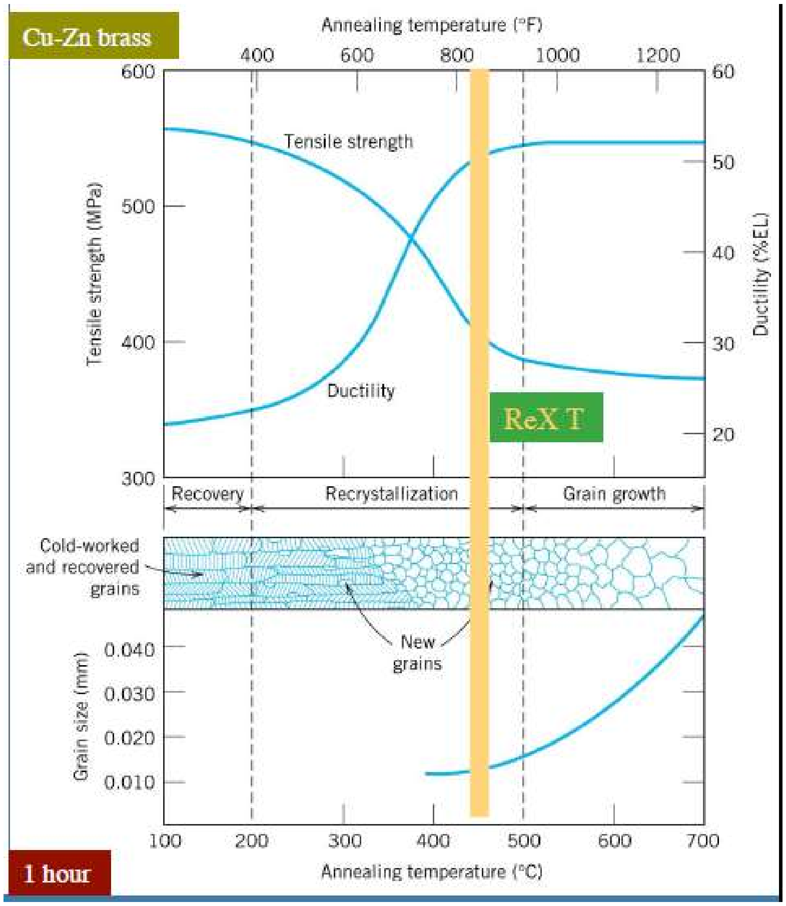
- Cold working (deforming material at low temp) hardens the material
- Yield strength/UTS increased but elongation reduced with increasing strain
- $\%CW = \frac{A_0 - A}{A_0} * 100$, A0 is area before deformation, A is area after deformation
- In cold working the density of dislocations increases and they interact with each other making dislocation movement more difficult
- $\Delta\sigma_y \propto \sqrt{P_{dislocation}}$

Precipitation Strengthening



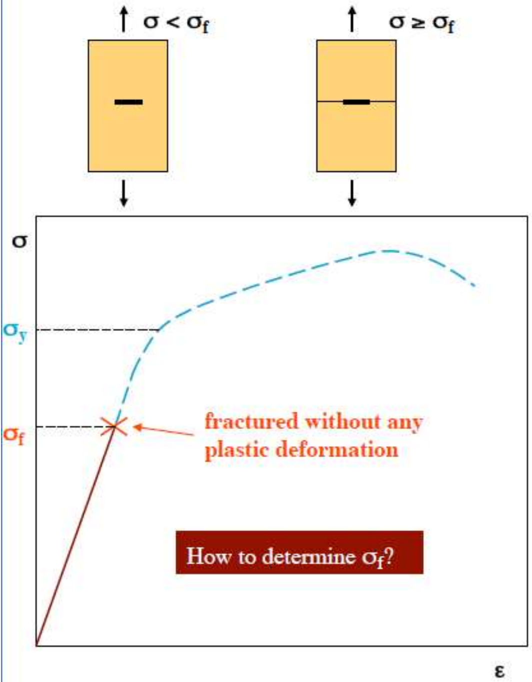
- Fine particles act as obstacles to dislocation
- Dislocations can pass through by looping or cutting through, requires extra stress
- $\Delta\sigma_y \propto \frac{1}{d}$, d is the average interparticle spacing

Softening after cold working



- Recovery
  - Heating a cold worked material with moderately elevated T
  - Dislocations will rearrange themselves reducing amount of dislocations and lower energy configuration
  - Strength lowered
- Recrystallisation
  - Heating to above recrystallization temp creates new grains with low dislocation density from matrix of high strain energy
  - Reduces number of dislocations dramatically
  - Decrease in strength and increase in ductility
- Grain growth
  - Grains will become larger with time at elevated temp
  - Driven by reduction in grain boundary area

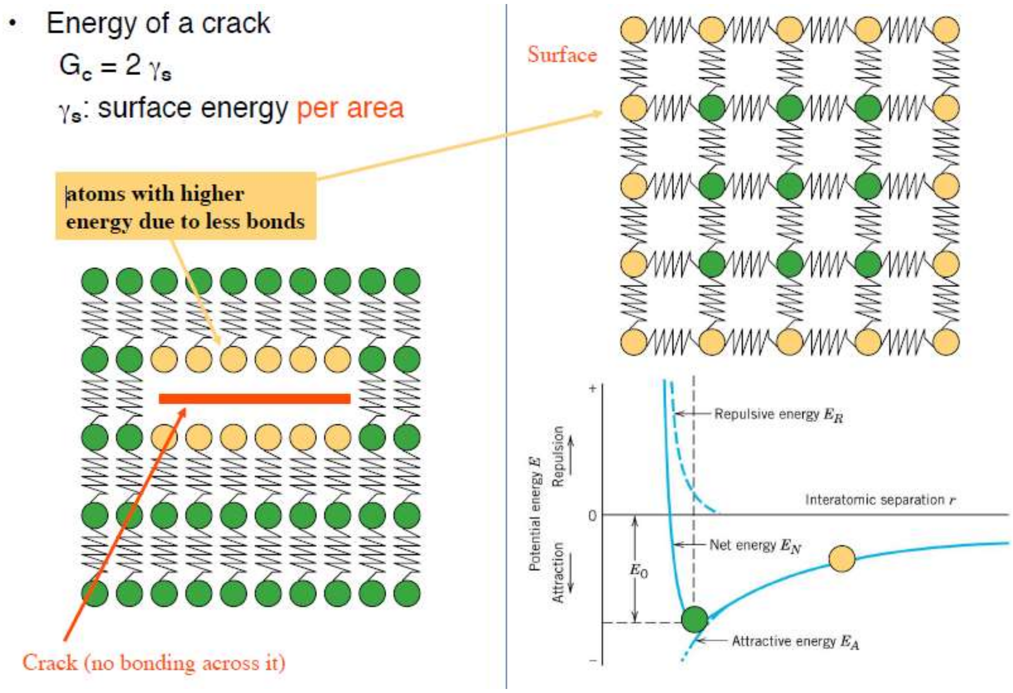
Fast Fracture



General

- Materials may have cracks in them
- Cracks can propagate
  - Very fast: sudden fracture
  - Slow: fatigue and creep failure
- Brittle fracture
  - Happens without plastic deformation first, most dangerous
- Can strengthen by diverting cracks/consuming energy and increase *toughness*

Griffith Criterion



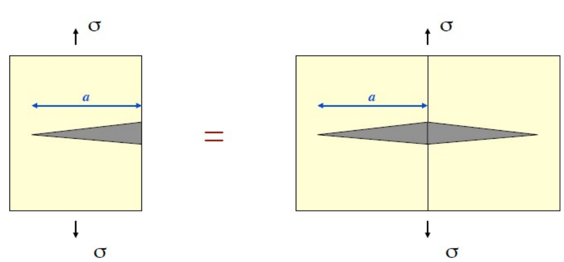
$$G_c = 2\gamma_s$$
$$\gamma_s: surface\ energy\ per\ area$$

- For a piece of material volume V containing a crack with area A with a given stress, total elastic energy stored is $E^e V$, total crack energy is $G_c A$
- For fast propagation, energy released due to cutting bonds > increase in energy of crack due to larger size.
- Griffith Criterion

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

When stress reaches critical value, an internal crack with size of 2a or surface crack with size of a becomes unstable and will propagate fast causing fracture.

- Surface crack is more dangerous



Fracture toughness

- Can rewrite Griffith criterion

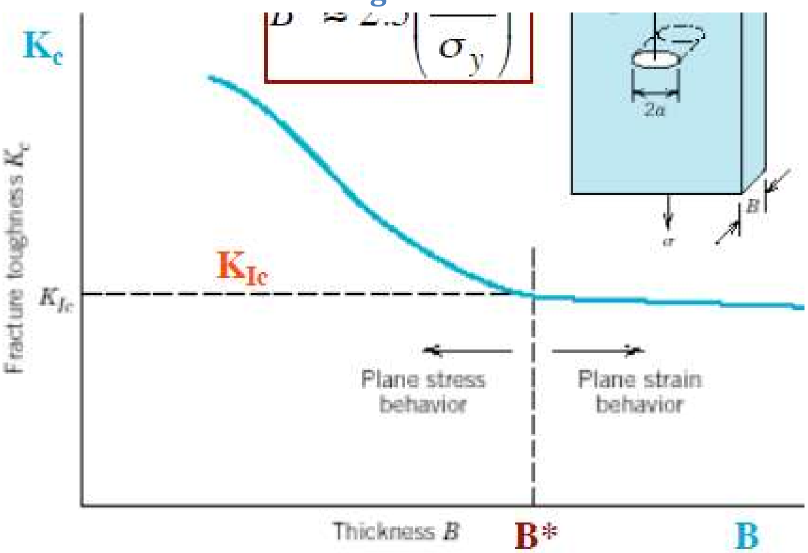
$$\boldsymbol{\sigma\sqrt{\pi a} = \sqrt{2E\gamma_s} = \sqrt{EG_c}}$$

- Criterion for fast fracture

$$Y\sigma\sqrt{\pi a} = K$$
$$K = stress\ intensity\ factor$$
$$Y = constant, Y \cong 1\ for\ small\ cracks$$
$$\sqrt{EG_c} = K_c, Critical\ stress\ intensity\ factor = fracture\ toughness$$

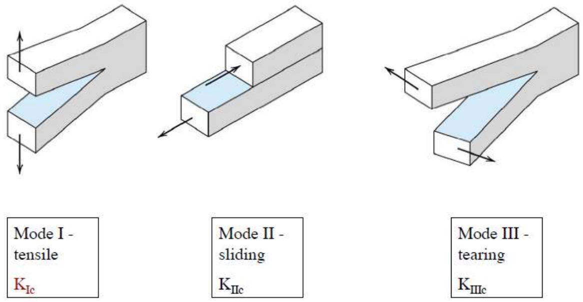
$$\boldsymbol{K = K_c\ for\ fast\ fracture}$$
$$\boldsymbol{Y\sigma\sqrt{\pi a} = K_c}$$
$$\boldsymbol{\sigma = \frac{K_c}{Y\sqrt{\pi a}} = \sigma_c\ Critical\ Fracture\ Stress}$$
$$a = \frac{1}{\pi}\left(\frac{K_c}{\sigma Y}\right)^2 = a_c\ Critical\ Crack\ Size$$

Plane strain fracture toughness

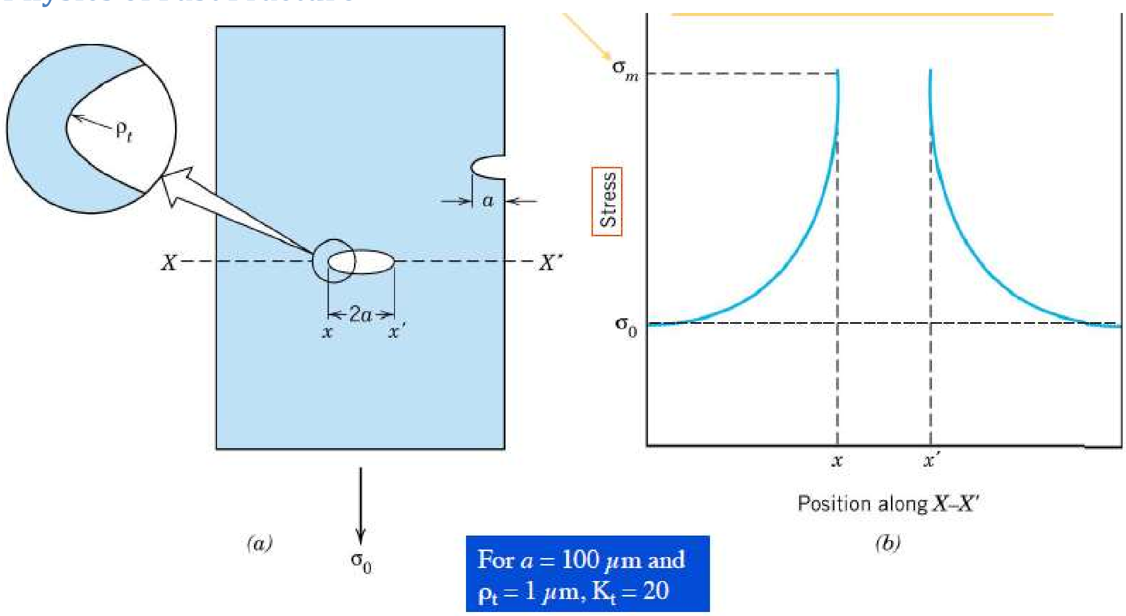


- K_c changes with B (thickness of plate) when B < B*
- When B > B*, $K_c = constant = K_{Ic}$

- $B^* \cong 2.5\left(\frac{K_{IC}}{\sigma_y}\right)^2$

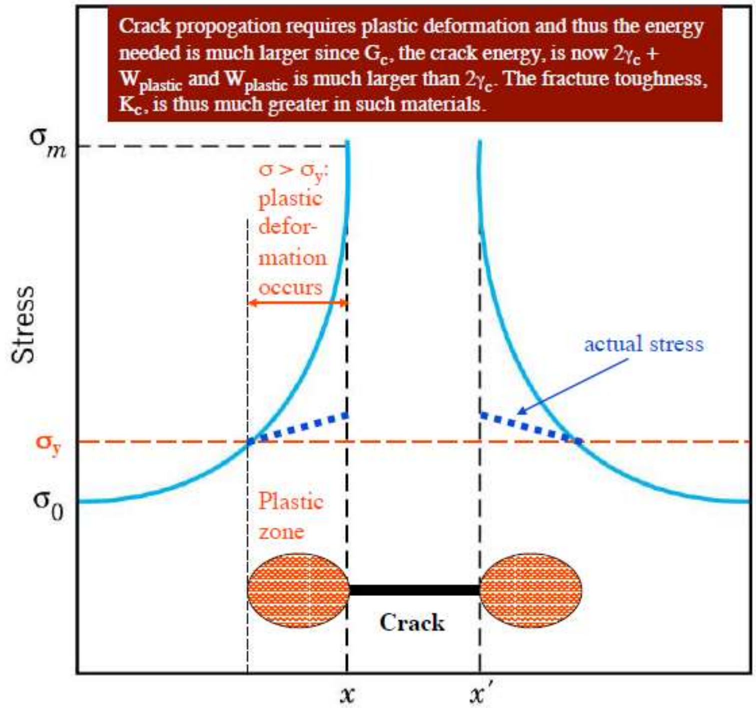


Physics of Fast Fracture



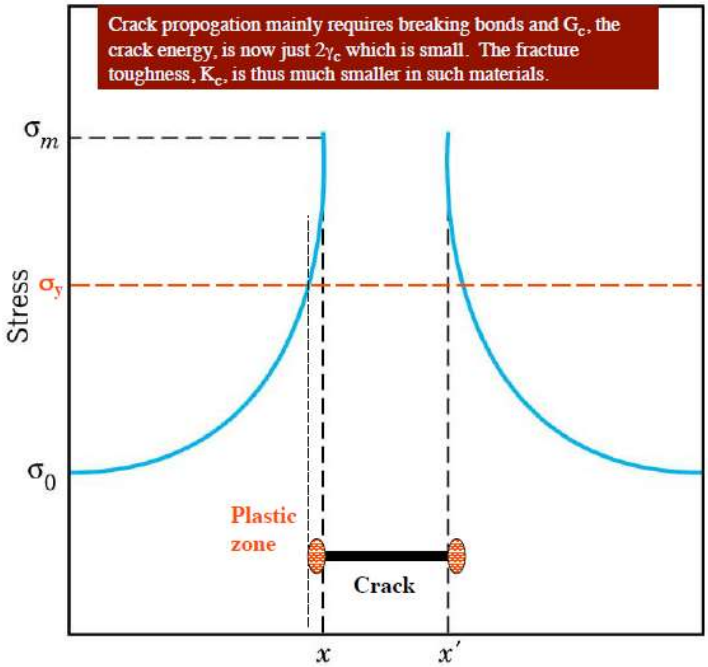
- Smaller the radius of curvature at the crack tip, the sharper the crack.
- Stress concentration factor $K_t = \frac{\sigma_m}{\sigma_o} = 2\sqrt{\frac{a}{\rho_t}}, \sigma_m = 2\sigma_o\sqrt{\frac{a}{\rho_t}}$

Ductile Fracture



- Material with moderate yield strength (metal)
- Plastic zone exists near crack tip
- Role of plastic deformation
    - Stress decreases
    - Radius of tip increases (blunting)
    - Critical stress intensity increases as the plastic work takes a lot of energy
- Higher temperature

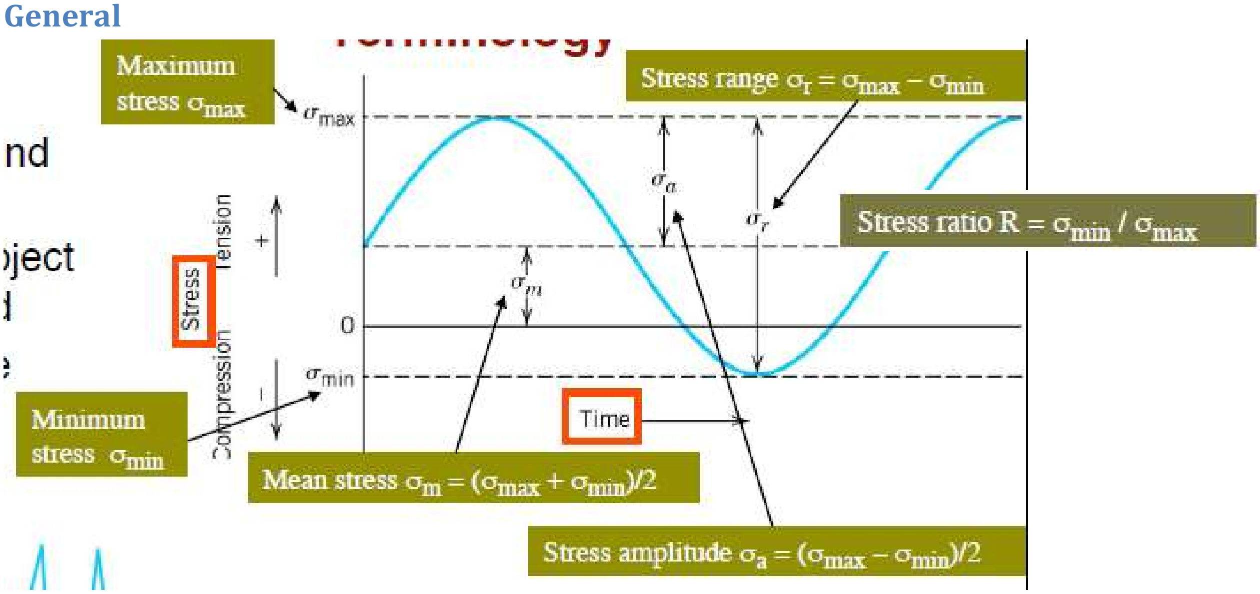
Brittle Fracture



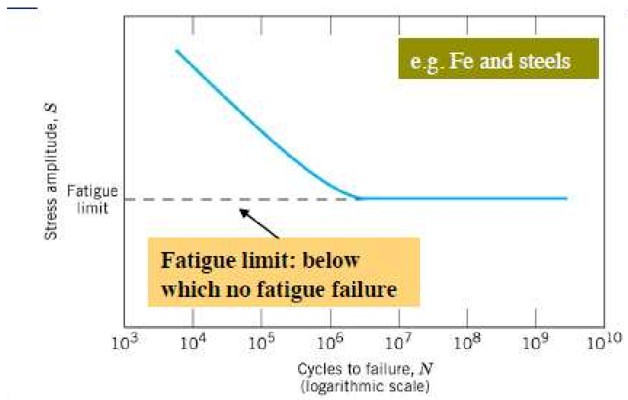
- Material with high yield strength (ceramic)
- Near the crack tip the plastic zone is very small, plastic deformation not significant
- Lower temperature

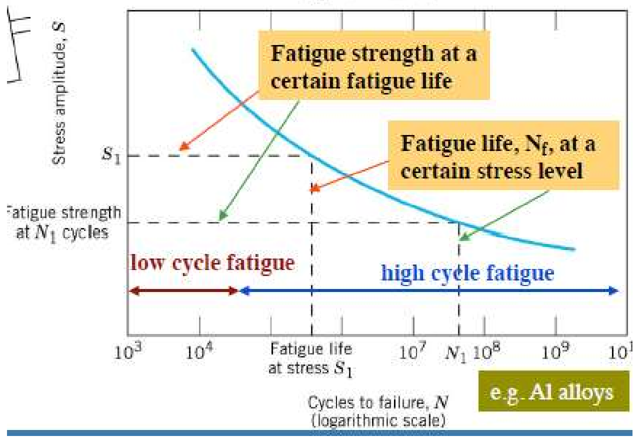
Fatigue

General



- Caused by cyclic stressing which produces slow crack growth resulting in fast fracture
- S-N curve (Stress vs Number of cycles in log scale)
- Cannot fail due to fatigue below a certain fatigue limit



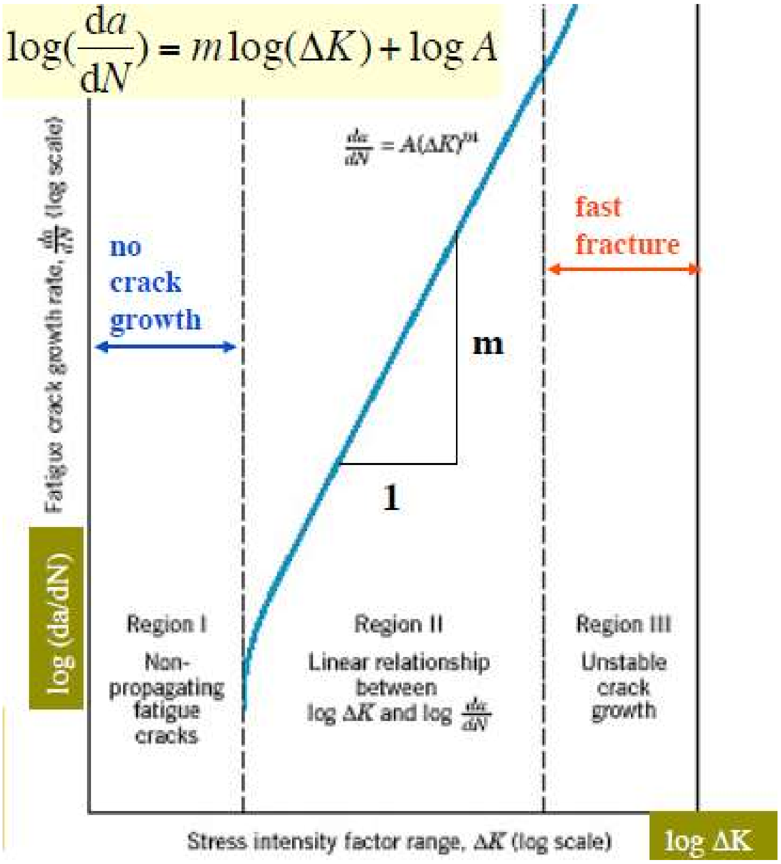


Fatigue process

- Cyclic stressing causes slow crack growth
- Cracks nucleate on surface/defect
- Propagation
  - Stage 1 – Along planes with high resolved shear stress
  - Stage 2 – Perpendicular to applied tensile stress
- Fast fracture

Crack propagation rate

- Applies to high cycle fatigue (>10^4)
- $\frac{da}{dN} = A(\Delta K)^m$
- $\Delta K = Y\Delta\sigma\sqrt{\pi a}$, $\Delta\sigma = \sigma \max - \sigma min$



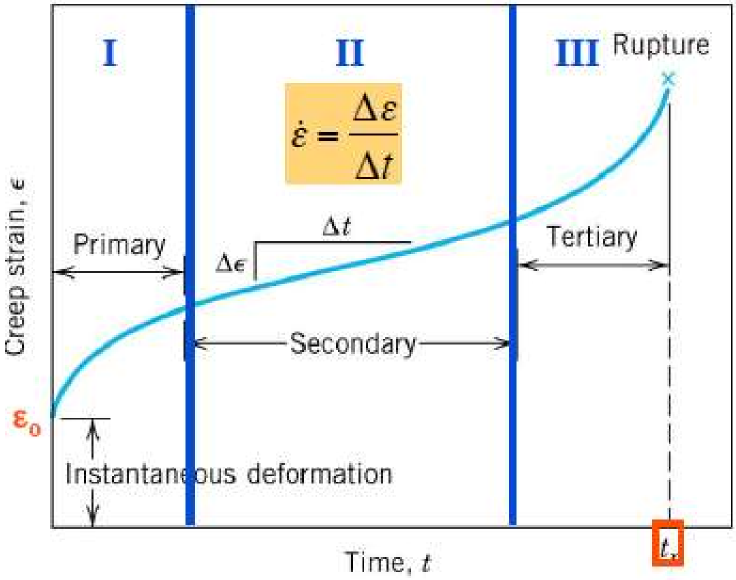
Fatigue life

- Only the life for crack propagation
- Life for crack initiation MAY be significant depending on situation. Assumed to be not needed as there are always existing defects.

$$N_f = \frac{1}{\left(A\pi^{\frac{m}{2}}\Delta\sigma^m\right)} \int_{a_0}^{a_c} \frac{1}{Y^m a^{\frac{m}{2}}} da$$

Creep

General



- Time dependent plastic deformation
- Important at higher temperatures (>0.4 Melting Temp)
- Eventually leads to rupture

Creep Stages

- Three stages
  - Primary – Creep rate decreases
  - Secondary – Creep rate is constant
  - Tertiary – Creep rate increases until fracture
- At a constant T, creep rate increases and creep life decreases with increasing stress
- Second state creep rate dependent on stress, n is stress exponent and K1 is constant.

$$\dot{\epsilon_s} = K_1\sigma^n$$

- At constant stress, creep rate increases and creep life decreases with increasing temperature
- Second state creep rate dependent on temperature, Qc is activation energy for creep and K1 is constant

$$\dot{\epsilon_s} = K_2\exp(-\frac{Q_c}{RT})$$

- Therefore the steady state creep rate is

$$\dot{\epsilon_s} = K\sigma^n\exp(-\frac{Q_c}{RT})$$

- n and Qc are important
  - n=1: diffusional creep
  - n=1-2: grain boundary sliding
  - n=3: viscous glide of dislocations
  - n=4-5: dislocation climb

  - Qc can be compared to activation energies for various diffusion processes that may control creep

Extrapolation methods

- Impractical to test for creep with real temperatures as it may take too long
- Larson-Miller parameter, is constant at a certain stress level (C is a constant)

$$LMP = T(C + \log t_r)$$

Creep resistance

- High melting temp
- High elastic modulus
- Large grain size

Mechanical Properties Summary

Stiffness

- Resistance to elastic deformation
- Elastic modulus (E,G, etc)

Strength

- Resistance to plastic deformation
  - Yield strength
- Limited by fracture
  - Fracture Strength

Ductility

- How much plastic deformation without fracture
- Tensile elongation or area reduction

Toughness

- Resistance to fast fracture
- Fracture toughness (Kc)

Mechanics

$$\epsilon = \frac{du}{dx}$$
$$Strain = Change\ in\ Displacement$$

$$\gamma_{xy} = \frac{du_2}{dx} + \frac{du_2}{dy}$$
$$Shear\ Strain(angle)$$

$$E = \frac{\sigma}{\epsilon}$$
$$Hooke's\ Law$$

$$\epsilon_{xy} = \frac{1+\nu}{E}\sigma_{xy}$$
$$Hooke's\ Law\ (Shear)$$

$$U = \frac{1}{2}\sigma_{xx}\epsilon_{xx}$$
$$Strain\ Energy\ Density$$

$$\int\int \delta U\ dxdy = \int\int P_x\delta u_1 + P_y\delta u_2\ ds + \int\int B_x\delta u_1 + B_y\delta u_2\ dxdy = 0$$
$$Virtual\ Work$$

$$\frac{dV}{dP} = u, \frac{dV}{dM} = \theta$$
$$Castigliano's\ Theorem$$

$$U = \int_0^L \frac{M^2}{2EI}dx,\ \ where\ M = EI\frac{d^2y}{dx^2}$$
$$Strain\ Energy\ in\ beam$$

$$V = \frac{1}{2}P\delta = mg(h+\delta)\ (massless)$$
$$V = \frac{1}{2}P\delta = mgh + (m+m_c)g\delta\ (mass)$$
$$Strain\ energy\ in\ impact\ loading$$

$$P = \sigma A = \frac{EA\delta}{L}, \delta = \frac{PL}{AE}$$
$$V = mgh + (m+m_c)\delta g$$
$$P = mg\left(1 + \sqrt{1 + 2h\left(\frac{EA}{mgL}\right)}\right)$$
$$\delta = \frac{mgL}{EA} + \sqrt{\left[\left(\frac{mgL}{EA}\right)^2 + 2h\left(\frac{mgL}{EA}\right)\right]}$$
$$Mass\ falling\ onto\ massless\ flange$$

$$\delta = \frac{PL^3}{48EI}$$
$$P = mg\left(1 + \sqrt{1 + \frac{96EIh}{mgL^3}}\right)$$
$$Mass\ falling\ onto\ a\ massless\ beam$$

$$P_{cr} = \frac{n^2\pi^2}{L^2}EI$$
$$y = Asin\frac{n\pi x}{L}$$
$$Critical\ load\ and\ buckling\ mode\ (central\ load)$$

$$\delta = e\left[\sec\left(\frac{\pi}{2}\sqrt{\frac{P}{P_{cr}}}\right) - 1\right]$$
$$Deflection\ with\ eccentric\ load$$

$$\sigma_{xmax} = \frac{M_{max}c}{I}$$
$$Flexure$$

$$\sigma_{max} = \frac{P}{A}\left[1 + \frac{ec}{r^2}\sec\left(\frac{L}{2r}\sqrt{\frac{P}{EA}}\right)\right]$$
$$\sigma_{max} = \frac{P}{A} = \frac{\pi^2 E}{\frac{L}{r^2}}, for\ e$$
$$= 0,\ \ failure\ when\ P = P_{cr}$$
$$r = \sqrt{\frac{I}{m}}$$
$$Secant\ Formula$$

$$\sigma_1 - \sigma_3 > \sigma_Y$$
$$\sigma_1 > \sigma_2 > \sigma_3$$
$$Max\ shear\ stress > \frac{\sigma_Y}{2}$$
$$Tresca\ Criterion(more\ conversative)$$

$$\sigma_v = \sqrt{\sigma_1^2 + \sigma_2^2 - \sigma_1\sigma_2}$$
$$Von\ mises\ Criterion\ for\ plane\ stress, (most\ accurate)$$