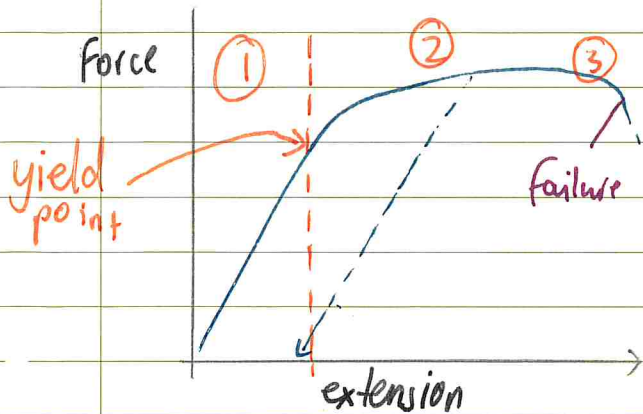


E. Mechanical Behaviour

No. 1

Date 23.2.19

- A material of known dimensions can be examined via **tensile testing**, in which it is stretched.

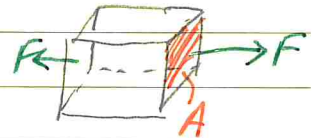


- ① **Elastic region** - deformation is linear and fully recoverable
- ② **Plastic deformation** - permanent shape change even when external load has been removed
- ③ **Necking** - sample gets thinner so less force needed to extend.

- Force and extension depend on a material's dimensions. It is more useful to have quantities that depend only on the material.

- The **normal stress** σ is the outward force per unit area on a cuboid: $\sigma = F/A$

↳ by definition, $\sigma > 0 \Leftrightarrow$ stretching
 \Leftrightarrow **tensile stress**



↳ $\sigma < 0 \Rightarrow$ **compressive stress**

- Stress on a material leads to **normal strain** ϵ , the relative change in the linear ~~direction~~ dimension in the direction of the force.

$$\int \epsilon = \frac{\delta L}{L} \Rightarrow \epsilon_{true} = \int_{l_0}^{l_i} \frac{dl}{l} = \ln(l_i/l_0)$$

↳ this can be approximated by the **engineering strain** ϵ_{eng} , which is the % change in length, when ϵ_{true} is small.

- The **engineering stress** assumes that the area of the cross-section remains the same even when strained, i.e. $\sigma_{eng} = F/A_0$.

↳ reasonable approximation when strain $< 2\%$ because most engineering focuses on the elastic region.

- In reality, a cuboid under tension will contract laterally

- **Poisson's ratio** ν is the ratio of ~~axial~~ lateral contraction to axial elongation: $\epsilon_x = \epsilon_y = \nu \epsilon_z$

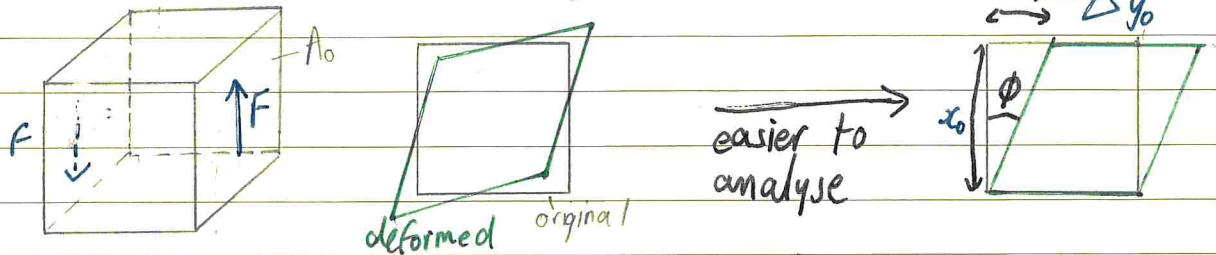
- most materials have ν in the range 0.2-0.5

- cork has $\nu \approx 0$; when forced into bottle it doesn't expand.

- A force applied parallel to a surface results in a **shear stress**

$$\tau = \frac{F}{A_0}$$
 ← sign of τ has no physical meaning.

- Shear stress causes one diagonal axis to shorten and one to lengthen.

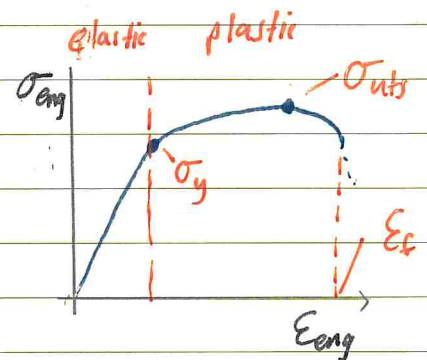


- The **shear strain** is the distortional deviation:

$$\gamma = \frac{\Delta y_0}{x_0} = \tan \phi \quad \leftarrow \text{angle of shear}$$

- The stress-strain curve can be plotted:

- **yield stress** σ_y is the maximum stress before plastic deformation (a.k.a strength).
- **ultimate tensile strength** σ_{uts} represents the maximum load a material can bear
- **strain to failure** ϵ_f is the strain a material can sustain before failing.



Elastic deformation

- In the elastic region, the strain is directly proportional to stress.
- For normal stress, the constant of proportionality is **Young's Modulus** E

$$\sigma = E \epsilon$$
- For shear stress, the equivalent is the **shear modulus** G : $\tau = G \gamma$
- Both E and G are measured in pascals
- Most structural materials have $E \sim 100 - 200 \text{ GPa}$
- Composite materials are more complex, and can have moduli that depend on the axis being tested.
- In the elastic region, behaviour is exactly analogous to a spring.

- Because elastic deformation is recoverable, the energy must be stored somewhere.
- Stretching a sample by dL requires work to be done:

$$dW = FdL = (\sigma A)(L d\varepsilon)$$

i.e. $dW = VE\varepsilon$, assuming $V \equiv AL$ is constant.

$$\therefore W = \int_0^{\varepsilon_{\max}} VE\varepsilon d\varepsilon$$

\Rightarrow work done per unit volume = $\frac{1}{2} E \varepsilon^2$

- Likewise, the work/volume for a shear stress is $\frac{1}{2} G \gamma^2$

- At an atomic level, elasticity is the result of a near-quadratic potential.

- for very small separations, (neutral) atoms experience a **Pauli repulsion**
- however, in general there is the **Van der Waals attraction**.
- there will be some equilibrium separation r_0 that minimises the energy.

- Can be modelled by the **Lennard-Jones potential**:

$$U_{LJ} = U_0 \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^6 \right]$$

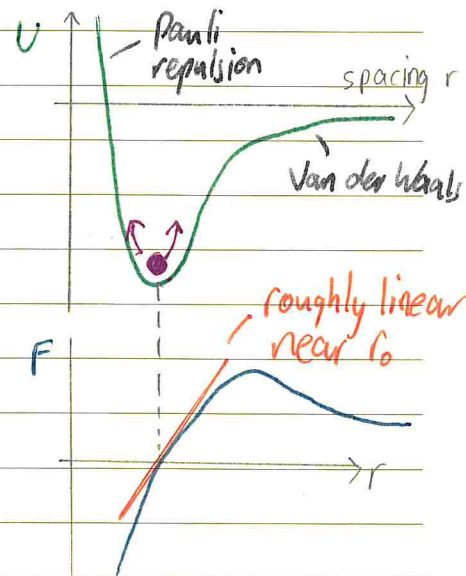
\hookrightarrow If we model each bond as having area r_0^2 :

$$\sigma = \frac{F}{r_0^2} = \frac{1}{r_0^2} \frac{dU}{dr}$$

\hookrightarrow combined with $d\varepsilon = dr/r_0$:

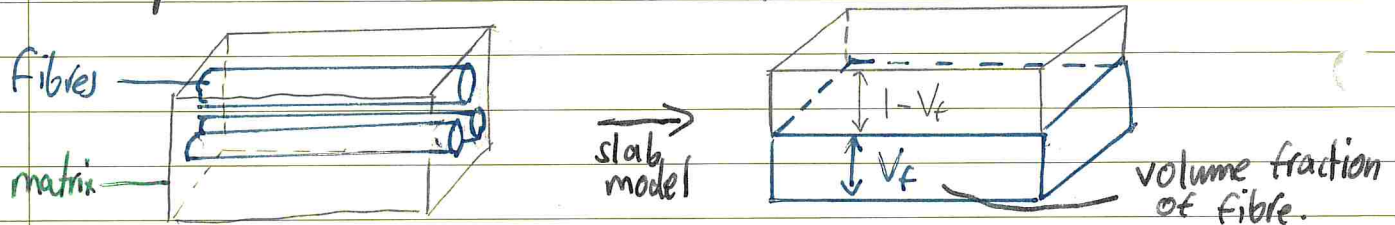
$$E \equiv \frac{d\sigma}{d\varepsilon} = \frac{d\sigma}{dr} \frac{dr}{d\varepsilon} \quad \Rightarrow \quad E = \frac{1}{r_0} \left. \frac{d^2U}{dr^2} \right|_{r=r_0}$$

\hookrightarrow i.e. Young's modulus is equal to the curvature of the potential well about equilibrium.



Composite materials

- Combining materials can result in 'best of both worlds' properties
- Typically, a ceramic fibre is embedded in a polymer matrix, e.g. glass/carbon/aramid fibres in epoxy.
- These are strongest when fibres are parallel and aligned, but this leads to highly anisotropic elastic behaviour, so in practice **plies** of aligned fibre are stacked in different directions.
- Composites can be modeled as slabs of fibre/matrix



- The **axial modulus** can be approximated by the **Voigt Model**, which assumes that each slab experiences the same normal strain.

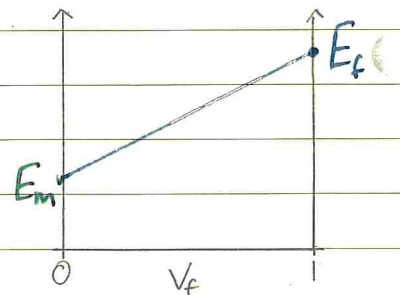
stress on composite

$$\rightarrow \sigma_c = \sigma_f V_f + \sigma_m V_m = \sigma_f V_f + \sigma_m (1 - V_f)$$

$$\therefore \boxed{E_c = E_f V_f + E_m (1 - V_f)} \quad \text{using the Voigt assumption}$$

i.e. $E_c = \epsilon_f = \epsilon_m$.

- This results in a linear rule of mixture (i.e. weighted average) that provides reasonable estimates of E_c .



- In the case of the **transverse modulus**, we assume that the slabs are under the same ~~stress~~ stress but can extend differently.

$$\epsilon_c = \epsilon_f V_f + \epsilon_m V_m \quad \Rightarrow \quad \frac{1}{E_c} = \frac{V_f}{E_f} + \frac{(1 - V_f)}{E_m}$$

- This model produces inaccurate values \rightarrow lower bound estimate only.
 - \hookrightarrow parts of the matrix near the fibres are shielded from stress because the fibres are very stiff vertically
 - \hookrightarrow model overestimates matrix extension, underestimates E_c .

Thermal strains

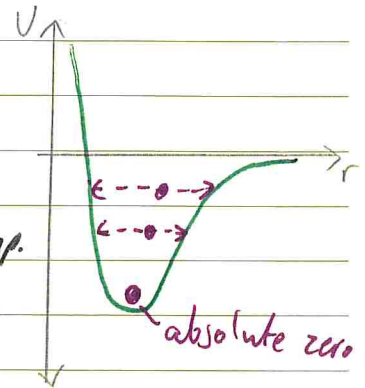
- The temperature measures the mean KE of atoms:

$$\frac{3}{2} kT = \left\langle \frac{1}{2} m v^2 \right\rangle$$

- Thus at higher temperatures, atoms are no longer stationary at the equilibrium position.
- The asymmetry of the potential well means that the mean ~~position~~ separation increases with temp.
 - ↳ materials expand when heated.
- This results in a near-linear relationship between **thermal strain** and temperature:

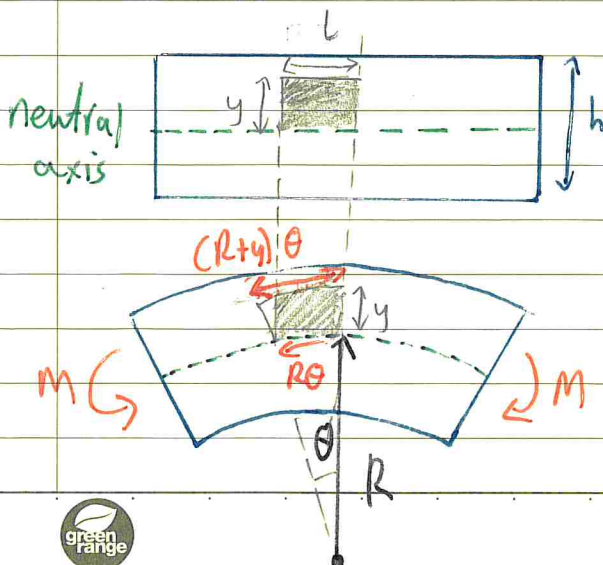
$$\epsilon_T = \alpha \Delta T, \text{ where } \alpha \text{ is the coefficient of thermal expansion.}$$

- Materials with stronger inter-atomic bonds have deep sharp potential wells \Rightarrow high E , low α . e.g. ceramics.
- Polymers have shallow potential wells \Rightarrow low E , high α .
- α itself has a small increasing trend with temperature, but this rate of change depends on the specific potential well.
- As temp \uparrow , the average d^2V/dr^2 decreases $\Rightarrow E \downarrow$.
- Thermal strain can be applied in **bimetallic strips**



Beam theory

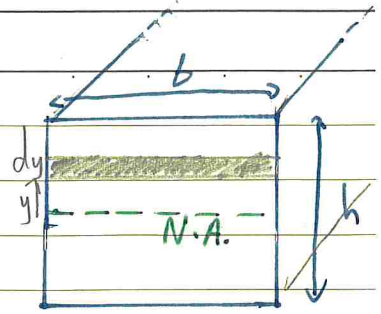
- Consider a uniform beam subject to pure bending (i.e. no shear)



- The top will be subject to tension and the bottom to compression, but there will be some undeformed **neutral axis**
- This helps us define the radius of curvature, $R = l/\theta$.

$$\epsilon_{\text{axial}} = \frac{(R+y)\theta - R\theta}{R\theta} = \frac{y}{R} \Rightarrow \sigma_{\text{axial}} = \frac{E y}{R}$$

- The force on a cross-sectional element (looking down the beam) is $F = \sigma A = \frac{E y}{R} \cdot b dy$



↳ in general, $b = b(y)$ for non-cuboids.

- Moment about the neutral axis:

$$M_y = y \left(\frac{E y}{R} \right) \cdot b(y) dy \quad \leftarrow \text{force} \times \text{distance.}$$

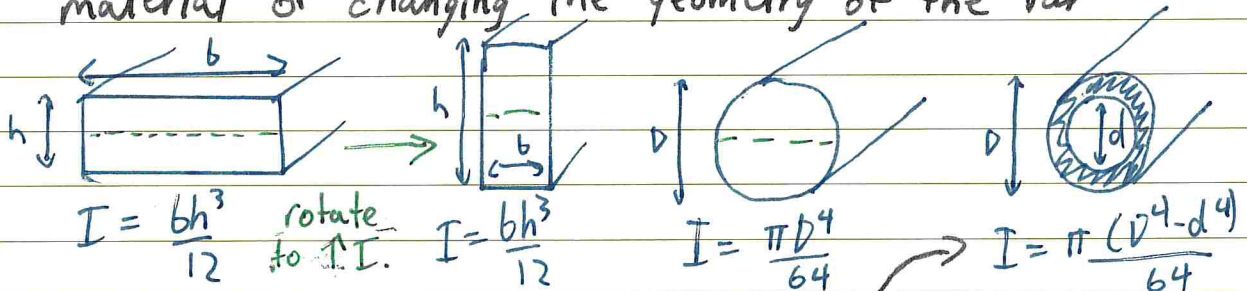
- Total bending moment found by integrating:

$$M = \frac{E}{R} \int_{-h/2}^{h/2} y^2 b(y) dy \quad \leftarrow \text{second moment of area (I)}$$

- Can be written in terms of E , I , and curvature $\kappa = 1/R$

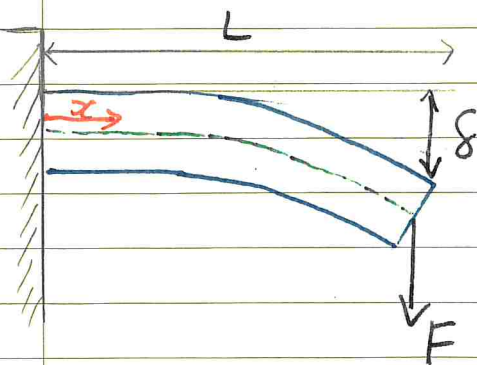
$$M = \kappa EI \quad \leftarrow EI \text{ is the flexural rigidity (i.e. beam stiffness).}$$

- Flexural rigidity can thus be increased by using a stiffer material or changing the geometry of the bar



- Using the principle of superposition, $I_{\text{hollow}} = I_{\text{solid}} - I_{\text{void}}$

Cantilever beams



- Bending moment is function of x :

$$M = F(L-x)$$

- Consider a small segment:

$$R d\theta \approx dL \approx dx \Rightarrow \frac{d\theta}{dx} = \frac{1}{R}$$

- But $\theta \sim dy/dx$

$$\therefore \kappa = \frac{1}{R} = \frac{d^2 y}{dx^2}$$

- Thus the equation for cantilever loading:

$$M = EI \frac{d^2 y}{dx^2} = F(L-x)$$

- This equation can be solved for y using $y'(0) = y(0) = 0$ as boundary conditions (horizontal at $x=0$).

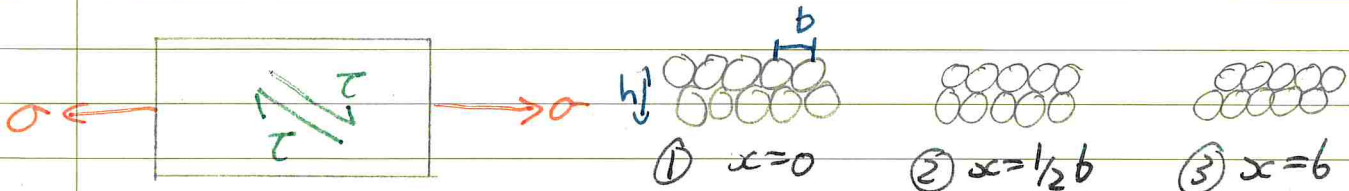
$$\therefore y = \frac{Fxc^2}{6EI} (3L-x)$$

- The max deflection is obviously at the end of the beam ($x=L$)

$$\Rightarrow \delta_{\max} = \frac{FL^3}{3EI} \leftarrow \text{higher flex rigidity} \Rightarrow \text{lower } \delta.$$

Plastic deformation

- Plastic deformation involves a change at the atomic level which is irreversible.
- Viewing a plastically deformed substance under a microscope shows fine parallel lines at an angle to the applied stress
- The simplest model considers planes of atoms which only move when a critical value of the shear stress has been applied.



- Clearly, energy is lowest in (1) and (3) (stablest) and maximal at (2)
- Thus the shear stress must be sinusoidal

$$\text{i.e. } \tau = C \sin\left(\frac{2\pi x}{b}\right)$$

\hookrightarrow using small $\frac{x}{b}$ and $\gamma = \frac{dx}{h}$ (shear strain)

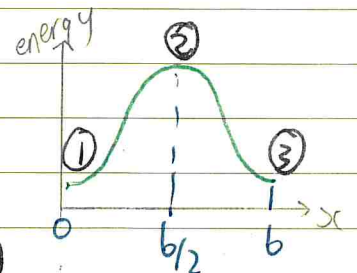
$$\tau \approx C \left(\frac{2\pi h \gamma}{b}\right), \text{ but } \frac{\tau}{\gamma} = G \Rightarrow C = \frac{Gb}{2\pi h}.$$

$\hookrightarrow C$ is the maximum value, i.e. $\tau_{\text{crit}} = C$

$$\Rightarrow \tau_{\text{crit}} = \frac{Gb}{2\pi h}$$

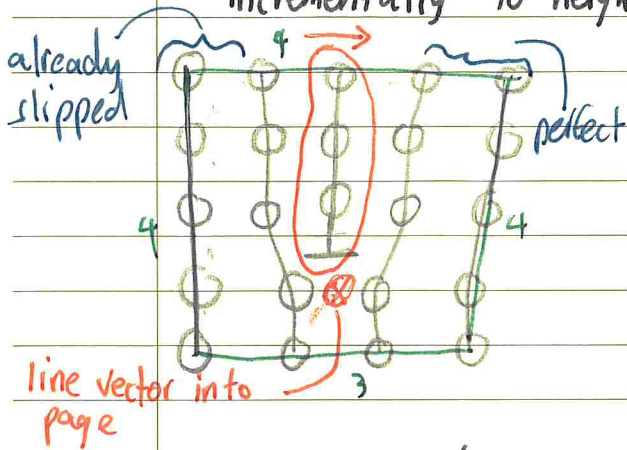
- This model overestimates τ_{crit} by a factor of ten

\hookrightarrow i.e. there must exist an easier way for planes to slip.



Dislocations

- An alternative theory models slip as the movement of local structural defects called **dislocations**.
- When sufficient stress is applied, the dislocation can move incrementally to neighbouring atoms

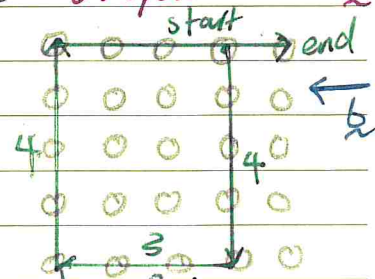


- Consider an extra half-plane of atoms moving to the right - this is an **edge dislocation**, i.e. there is a line going into the page which joins dangling bonds.

- This line separates the slipped and perfect parts of the crystal and defines the **line vector \underline{l}** for an edge dislocation.

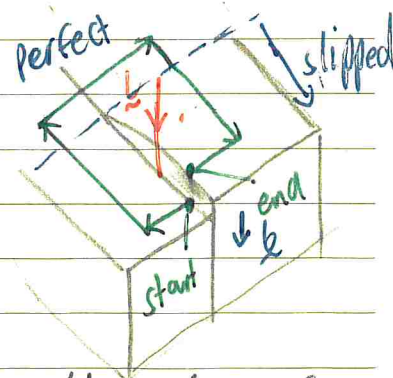
- The magnitude and direction of the lattice displacement caused by a dislocation is described by the **Burgers vector \underline{b}**

- Found by constructing a **Burgers circuit** around the dislocation core then repeating the integer steps in a perfect crystal
- there will be a closure failure: \underline{b} goes from the finish to start of the path



- Dislocation lines cannot end arbitrarily - they either terminate at a boundary or form a closed loop.

- **Screw dislocations** involve a partial shear of the crystal: the Burgers circuit is now a 3D path \rightarrow can be thought of as tracing a square helix with the **line vector** through the middle.



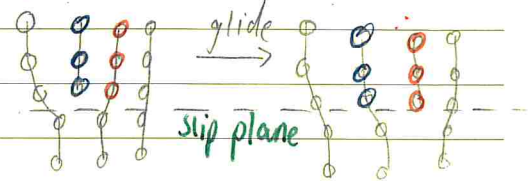
- The relationship between \underline{l} and \underline{b} determines the character of the dislocation:

$\underline{b} \perp \underline{l} \iff$ edge dislocation

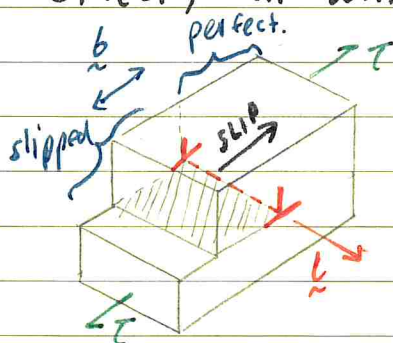
$\underline{b} \parallel \underline{l} \iff$ screw dislocation

Dislocation motion

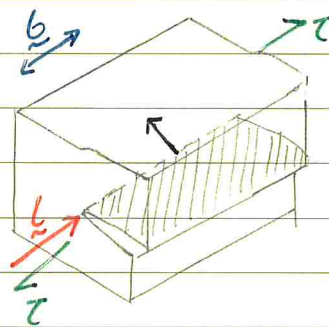
- Only small shifts of some atoms are required for dislocation movement.
 - when a critical shear stress τ_{crit} is applied, the half plane is displaced such that it is favourable to glide one increment
 - glide occurs on a slip plane, which contains both Burgers and line vectors.
 - the slip direction is parallel or antiparallel to \underline{b} , and atoms are displaced by $|\underline{b}|$
 - the original crystal structure is restored after passage.



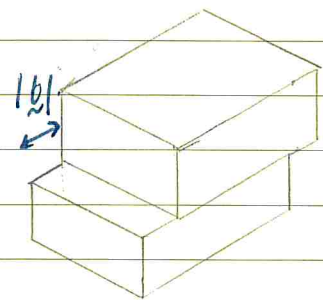
- Both edge and screw dislocations lead to the same macroscopic effect, but with a different mechanism.



EDGE



SCREW



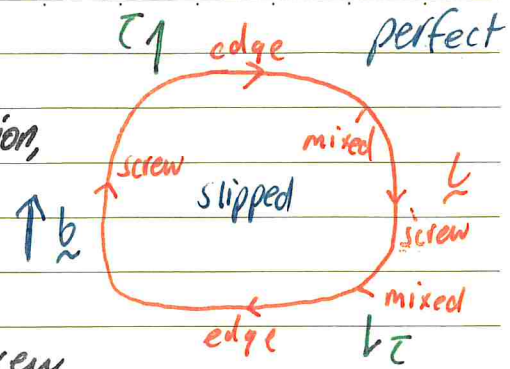
Result

- If the shear stress is aligned with \underline{b} and $\tau \geq \tau_{crit}$, slip occurs parallel to the Burgers vector and the dislocation moves perpendicular to its line vector.
 - for an edge dislocation, there is only one slip plane (because it must contain \underline{b} and \underline{l} , with $\underline{b} \perp \underline{l}$).
 - but there are many possible slip planes for screw dislocations.

Dislocation loops

- A dislocation loop consists of a central slipped area surrounded by an unslipped region. e.g. formed when the part of the top layer of a crystal is diagonally displaced.

- The dislocation line is thus a loop, with \perp changing direction
- But because it is still a single dislocation, there is only one Burgers vector
 \rightarrow character of dislocation changes around the loop.



- Edge dislocations move $\parallel \tau$, while screw dislocations move $\perp \tau$.
- Because the line vectors on opposite sides of the loop are antiparallel, the segments are of opposite sense, so the loop expands.

Stress and work to move dislocation

- Although \perp movement requires much less stress than block slip, we must apply enough to move it through a high energy state.
- This is described by the **Peierls-Nabarro stress** which is associated with the Peierls-Nabarro energy. τ_p is hard to calculate exactly, but can be modeled as:

$$\tau_p \approx 3G \exp\left(-\frac{2\pi w}{b}\right)$$

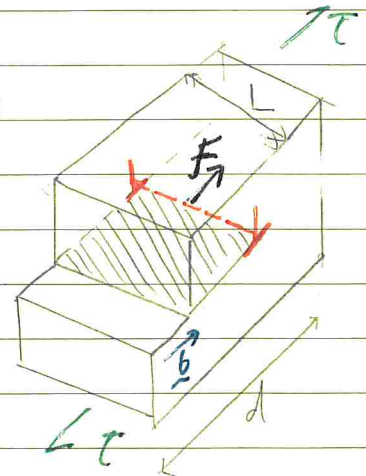
\rightarrow w is the **dislocation width**, i.e. the distance over which atoms are displaced by more than $\approx |b|/4$.

\rightarrow w has a lower bound of $|b|$, so τ_p is maximised when $w = b$. Much less stress is required for wide dislocations (high w/b).

- The work done to shear a crystal a distance $|b|/d$ is given by $W = \tau L d |b|$
- We can use this to define a **glide force**, the force per unit length to move a dislocation.

$$\tau L d |b| = F L d$$

$$\Rightarrow F = \tau |b|$$



Energy of a dislocation

• Dislocations create elastic strain in a crystal, which has an associated strain energy.

• This can be analysed for screw dislocations by considering an annular cylindrical element

$$dV = 2\pi r l dr$$

$$\gamma = b/2\pi r \quad (\text{unwrap into cuboid})$$

$$\hookrightarrow dU = \frac{1}{2} G \gamma^2 dV = \frac{1}{2} G \left(\frac{b}{2\pi r}\right)^2 (2\pi r l dr)$$

\hookrightarrow at the core of the dislocation, energy will be too great to be treated as an elastic strain energy. Hence we call it E_{core} and only integrate from some r_0 .

$$\hookrightarrow U = \int dU = E_{\text{core}} + \frac{Gb^2l}{4\pi} \int_{r_0}^{r_{\infty}} \frac{1}{r} dr$$

$$\Rightarrow U = \frac{Gb^2l}{4\pi} \ln\left(\frac{r_{\infty}}{r_0}\right) + E_{\text{core}}$$

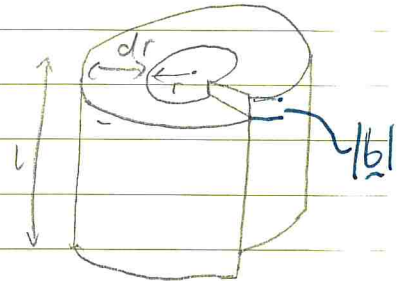
$\hookrightarrow r_0$ is chosen to overestimate the energy near r_0 in order to compensate for E_{core} . Empirically, $r_0 \approx |b|/4$

$\hookrightarrow r_{\infty}$ is set to half the distance between dislocations.

\hookrightarrow together, this gives the strain energy per unit length Λ

$$\Lambda \approx \frac{1}{2} G |b|^2 \quad \text{i.e. favours shorter } |b| \text{ and thus prefers close-packed slip.}$$

• The energy for edge dislocations is always greater than for screw (but harder to derive).



Slip in real crystals

- For slip to occur, the Burgers vector must correspond to a lattice vector. Smaller $|b|$ preferred, favouring slip in close-packed directions.
- Lower \uparrow width \Rightarrow less stress to slip. Thus slip is favoured on low index close-packed planes, which have large interplanar spacings and are densely packed.
- A slip system is the combination of a slip plane and direction.
- The number of slip systems is determined by crystal structure.

| | bcc | fcc | hcp |
|-------------|-------------------------------------|-------------------------------------|-------------------------------|
| Slip system | $\{110\} \langle \bar{1}11 \rangle$ | $\{111\} \langle \bar{1}10 \rangle$ | $\{001\} \langle 100 \rangle$ |
| number | $6 \times 2 = 12$ | $4 \times 3 = 12$ | $1 \times 3 = 3$ |
| b | $\frac{a}{2} \langle 111 \rangle$ | $\frac{a}{2} \langle 110 \rangle$ | $a \langle 100 \rangle$ |

- This explains why hcp metals are stronger but less ductile - there are fewer slip systems. (~~intuitive given ABCABC packing~~)

fcc-like \Rightarrow NaCl structures: $\{110\} \langle \bar{1}10 \rangle$ ($6 \times 1 = 6$)

bcc-like \Rightarrow CsCl structures: $\{110\} \langle 001 \rangle$ ($6 \times 1 = 6$)

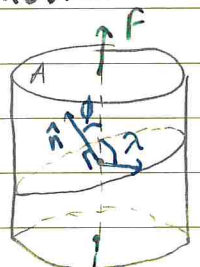
- For slip to occur, there must be a component of stress parallel to the Burgers vector. Thus not all dislocations are mobile.

- Consider a stress applied to a single crystal:

\hookrightarrow area of plane is $A / \cos \phi$

\hookrightarrow force \parallel to slip direction is $F \cos \lambda$

$$\tau_n = \frac{F \cos \lambda}{A / \cos \phi} = \frac{F}{A} \cos \phi \cos \lambda \quad (\text{Schmid's law})$$



- The critical resolved shear stress is the value of τ_n at which slip occurs:

$$\tau_c = \sigma_y \cos \phi \cos \lambda$$

\rightarrow Schmid factor $\in [0, 1]$
because σ_y is the F/A for which dislocations move

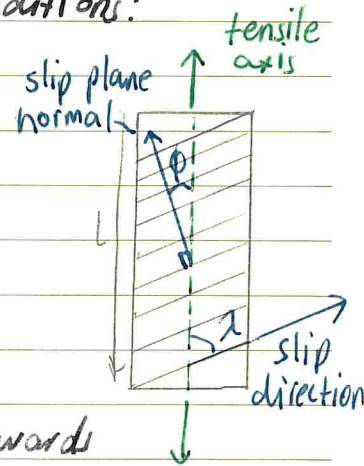
- Slip will first occur for the system with the highest Schmid factor.
- For bcc and fcc, we can use the OILS rule as a shortcut
 1. Write down tensile axis $[UVW]$
 2. Find Highest, Intermediate, Lowest indices (ignoring sign)
 3. If fcc:
 - slip is $\langle 110 \rangle$ with 0 in position of I index
 - else if bcc:
 - slip plane is $\{110\}$ with 0 at I.
 4. If fcc: slip plane is $\{111\}$ with L sign reversed
 - else if bcc: slip $\langle 111 \rangle$ with L sign reversed.

Geometry as slip proceeds

- Slip will encourage lateral displacement in a crystal under tension.
- But if the grips are aligned and fixed, there will be rotation of planes and local bending near the grips.
- This plastic deformation is controlled by two conditions:
 - interplanar spacing remains constant
 - number of planes (N) is conserved.

$$\therefore L = \frac{Nd}{\cos \phi} \quad \text{or} \quad L = \frac{Nd}{\sin \lambda}$$

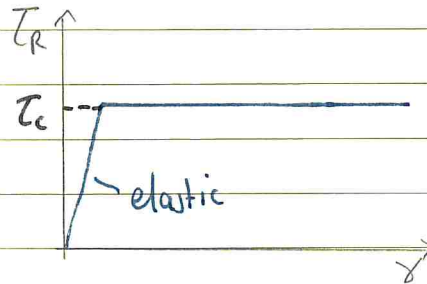
- So any elongation causes $\phi \uparrow$ and $\lambda \downarrow$
 - ↳ Schmid factors change and new slip systems can activate



- In the sample frame, the tensile axis rotates towards the slip direction. After each slip, it rotates closer
 - e.g. after n slips in fcc with original tensile axis $[\bar{2}14]$, the tensile axis will be $[\bar{2}14] + n[011]$
 - when two indices have the same value (ignoring sign), there will be a new slip system with the same Schmid factor
 - e.g. $n=1 \Rightarrow TA = [\bar{2}25]$ so $(111)[\bar{1}01]$ activates
 - $\therefore TA = [\bar{2}25] + n[011] + n[\bar{1}01]$
 - these slips take turns, but eventually $TA \rightarrow [\bar{1}12]$.
 - deformation along $[\bar{1}12]$ is purely elongation. Rotation cancels out.

Plastic deformation of metallic crystals

- For an hcp metal, only one slip system can operate, so the critical resolved shear stress will not vary when deforming.



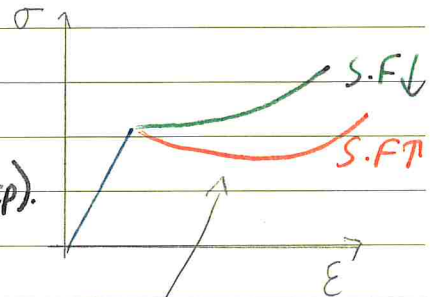
i.e. once $\tau_R = \tau_c$, it remains there.

- But as the TA rotates, ^{the} Schmid factor of the slip system changes (depending on the crystal's initial orientation).

$$\sigma_y = \frac{\tau_c}{\cos\phi \cos\lambda} \quad (\text{because } \tau_c \text{ constant for hcp}).$$

↳ i.e. if S.F ↓ σ_y ↑

↳ if S.F ↑, σ_y ↓ - this is **geometric softening**.



- In fcc metal, initially one slip system operates so τ_R is constant ①, though the Schmid factors change: **easy glide**

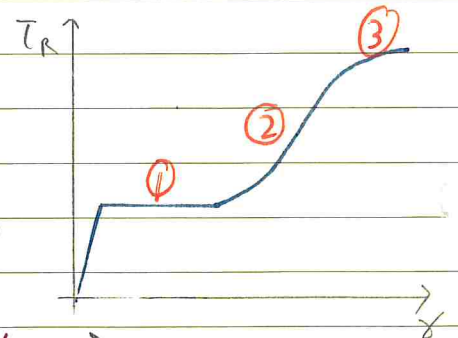
- In ②, **duplex slip** occurs. Dislocations move on both slip systems and can interact

↳ more τ_R needed to move dislocations

⇒ strength increases (**work hardening**).

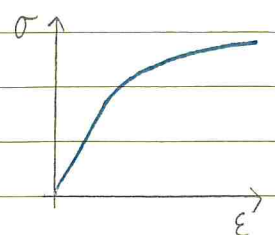
- τ_R is large enough to activate new slip systems - dislocations can now bypass obstacles via **cross slip**.

↳ cross slip easier if stacking fault energy high ⇒ lower τ_R to reach ③



- In polycrystalline metal, crystals are randomly oriented with the mean Schmid factor as 1/3. ← **Taylor factor**

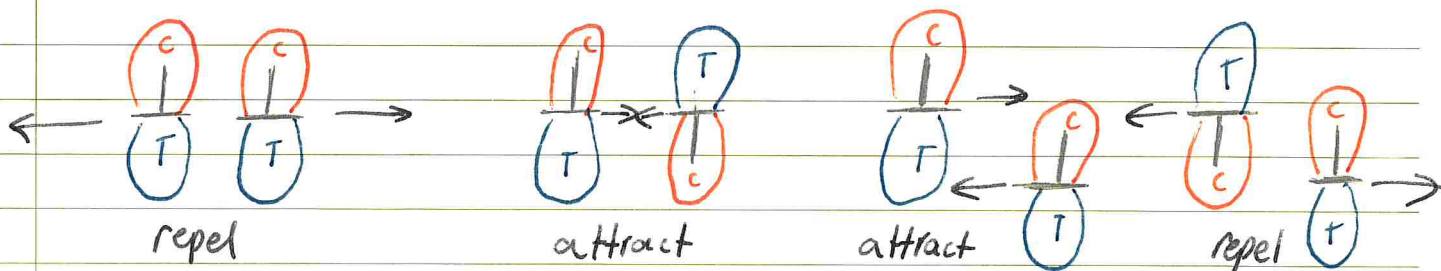
- Hence there is no easy glide, because duplex slip immediately occurs for some of the crystals.



- Using the Taylor factor, we expect $\sigma_y \approx 3\tau_c$ for polycrystalline materials. But this is an underestimate because it ignores grain boundaries.
 - ↳ deformation of a grain must be compatible with neighbours
 - ↳ so multiple slip is required \Rightarrow greater σ_y .

Dislocation interactions

- Dislocations strain the lattice. For screw dislocations, $\tau = G \frac{b}{2\pi r}$.
- Edge \perp s are more complex, but can be modeled as causing compression above the slip plane (extra atoms), and tension below.
- Stress fields will interact so as to reduce strain



- ↳ i.e. if \perp has same sign and same plane, it will repel
- ↳ try to overlay (T) and (C)
- ↳ this can lead to ordered arrays of \perp forming.

- If two dislocations were to combine, the new Burgers vector would be the vector sum of the individual b . $b_3 = b_1 + b_2$
- The new line vector would be the intersection of both slip planes.
- However, it is only energetically favourable for dislocations to combine if Frank's rule holds:

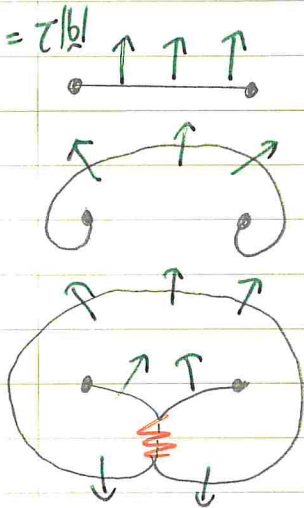
$$\{b_3^2 < b_1^2 + b_2^2\} \quad \leftarrow \text{because energy} \sim |b|^2$$

- Using the new b_3 and \perp_3 , assuming Frank's rule holds and the dislocations combine, we can construct a slip system ~~for~~ plane for the new dislocation
 - ↳ unique for edge dislocation: only one plane contains b_3 and \perp_3
 - ↳ no guarantee that result will be on a valid slip system
 - \Rightarrow sessile dislocation that blocks other dislocations' movement.

Dislocation generation

- Once dislocations reach the surface, they no longer participate in deformation \Rightarrow there must be a mechanism for \perp generation.
- A **Frank-Read source** consists of a linear dislocation pinned at both ends (e.g. by a sessile dislocation or point defect).

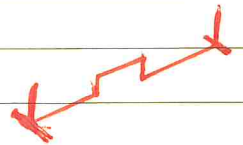
$$F = \tau |b|$$



- initially, \perp is a straight line with b normal
- when τ applied, \perp experiences $F = \tau |b|$
- because it is pinned, it bows out to balance the line tension with the shear force.
- eventually it spirals round the pinned points.
- when the two arms meet below, they annihilate because the segments have opposite sense
- this creates a complete \perp loop and a new \perp .
- if stress is maintained, the \perp loop will propagate outwards and the process repeats for the new \perp .

Out of plane movement

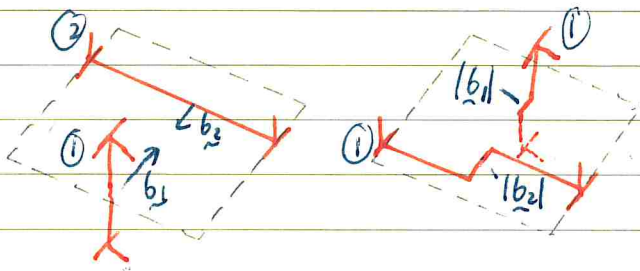
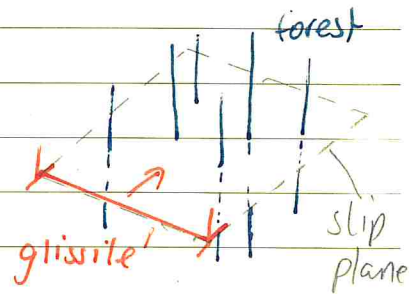
- Edge dislocations, for which glide is confined to a single plane, can bypass obstacles by **climb** - moving to a parallel slip plane
 - \hookrightarrow if a vacancy moves to the \perp core, \perp will move up - **positive climb**
 - \hookrightarrow alternatively, in negative climb, the vacancy at the \perp core moves downwards (i.e. replaced by atom), so \perp moves down.
 - \hookrightarrow this produces **jogs**, steps in the \perp line that are not in the slip plane.
 - \hookrightarrow climb requires significant diffusion and is thus thermally activated.
- Screw dislocations can easily **cross slip** with sufficient τ_R
 - when obstacle encountered, τ_R builds until new slip system activates.
 - at this point, the screw dislocation can continue on the rotated plane. It may double cross slip back to the original plane if the Schmid factor is greater.



Strengthening single-phase metals

- Strengthening requires processing that reduces dislocation mobility, such that more stress is required for plastic deformation.
- The **dislocation density** ρ is the number of dislocations intersecting a unit area (total dislocation line length / unit volume).
- Assuming a cubic array of \perp separated by L , $\rho = 1/L^2$
 $\rightarrow \rho \sim 10^{10} \text{ m}^{-2}$ annealed, $\sim 10^{16} \text{ m}^{-2}$ for plastically deformed.

- Primary slip planes will be threaded with sessile dislocations (**forest dislocations**)
- Thus a **glissile dislocation** will have to intersect all the forest dislocations to traverse



- When the dislocations cut they form **jogs** whose lengths are equal to the intersecting b_2 .
- Because jogs increase \perp length, it requires energy to cut.

- If the jogs are sessile, there will be strengthening as a result of further barriers to slip \Rightarrow **forest hardening** (a mechanism for work hardening).

Grain boundaries

- Dislocations cannot simply pass from one grain to the next: they accumulate at the boundary in a **dislocation pile** - yield only occurs when applied stress is significant
- But the pile itself causes stress because \perp s repel
 \rightarrow large grains \Rightarrow long piles \Rightarrow more stress \Rightarrow lower yield stress
 \rightarrow smaller grains \Rightarrow higher yield stress
- Related by **Hall-Petch**: $\sigma_y = \sigma_0 + k/\sqrt{d}$ — constant — diameter

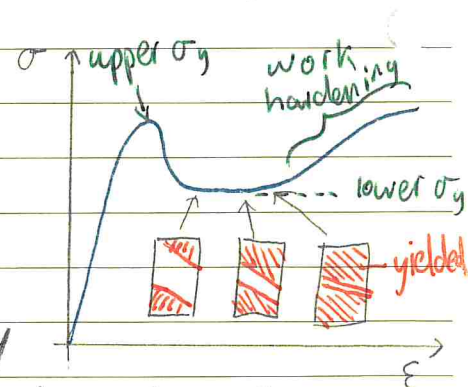
intrinsic yield stress

Solid solution strengthening

- Alloying tends to increase strength because it introduces solute atoms that interact with dislocations.
- Substitutional defects** are when the solute atom replaces the original
 - produces a spherically symmetric stress field: compressive if solute atom is larger, tensile otherwise.
 - no shear stress component so don't interact with screw dislocations.
 - they will attract and repel edge dislocations, e.g. large (compressive) defects will attract the tensile part of \perp
 - once an arrangement of defect/ \perp is formed, it will tend to persist, inhibiting further movement of dislocations (strength \uparrow).
 - but solute atoms are essentially static, so this will only happen if they are close to a slip plane.
 - thus substitutional solutes provide a weak strengthening effect.
- Interstitial defects** cause large compressive distortions, with asymmetric stress fields that interact with edge and screw dislocations.
 - e.g. C atoms in octahedral interstice of α -Fe
 - smaller size means rapid diffusion towards the dislocation.
 C atoms can ~~surround~~ form along the dislocation line: **Cottrell atmospheres**

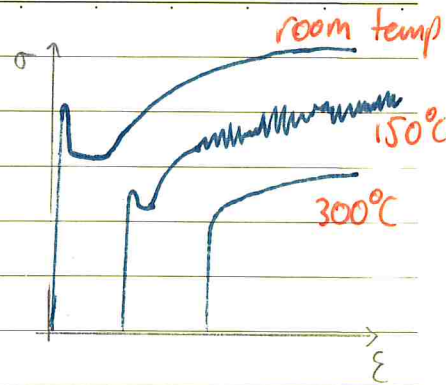


- Cottrell atmospheres provide strengthening because it is expensive to move them.
- Plastic deformation begins at the sample ends
 - no longer pinned by Cottrell atmospheres so continue to deform \rightarrow but they also work harden, so the unyielded regions start to yield
 - the boundaries are **Lüders bands**, lying at $\sim 50^\circ$ to the tensile axis and moving towards each other.
 - when the bands meet, the entire sample work hardens as expected.
- This strengthening is highly temperature-dependent
 - \rightarrow at high temp C atoms are very mobile and move with the \perp s so there is no strengthening effect until work hardening occurs.



low-carbon steel

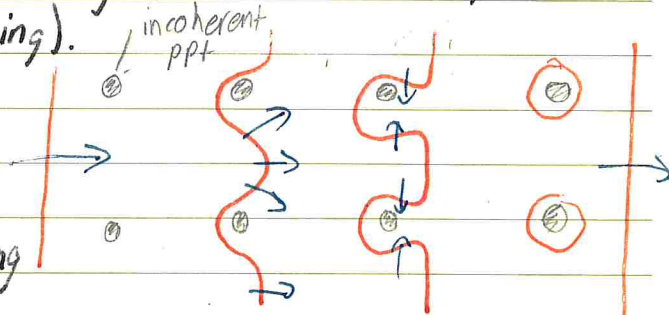
- At intermediate temp, C and L move at comparable speeds.
 - ↳ dislocations can escape Cottrell atmospheres only to be re-pinned
 - ↳ this is the **Portevin-Le Chatelier** effect and leads to a serrated stress-strain curve.



Precipitate strengthening

- Small precipitates tend to be coherent with the surrounding matrix → dislocations can pass through by **precipitate cutting**, but clearly this is harder than gliding through the matrix.
 - ↳ This is illustrated by a diagram showing a dislocation line (red) approaching a circular precipitate (grey) with radius r . 'Before' shows the dislocation approaching, and 'After' shows the dislocation line has cut through the precipitate, leaving a step on the surface.
- Thus there is a strengthening effect: $\Delta \tau \propto \sqrt{r}$

- But beyond a certain radius, ppt is likely to be incoherent, so L cannot pass through (no cutting).
- Instead, they can pass around precipitates by **Orowan bowing**.
- By considering the peak energy situation (semicircle) and equating the vertical force with the line tension from each dislocation:



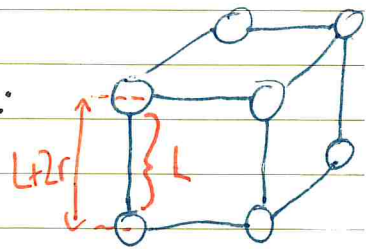
$$\tau |b| L = 2 \left(\frac{G |b|^2}{2} \right)$$

- ↳ L is surface-surface separation
- Thus the **Orowan stress** required to bow a dislocation is

$$\tau = \frac{G |b|}{L}$$

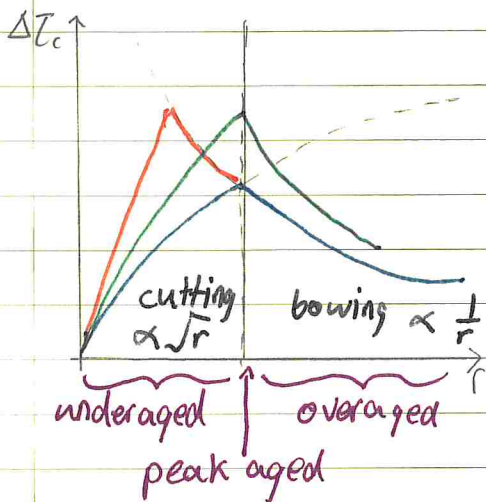
- Assuming the ppts have a cubic arrangement:

$$V_f = \frac{V_{ppt}}{V_{cube}} = \frac{\frac{4}{3} \pi r^3}{(L+2r)^3}$$



- So for a constant volume fraction, $L \propto r$
- Thus greatest τ (i.e. strongest) when many small ppt particles.

- As a sample is aged, ppt radius will increase. There will be some ideal radius that has maximum resistance to cutting, before Orowan bowing becomes significant.



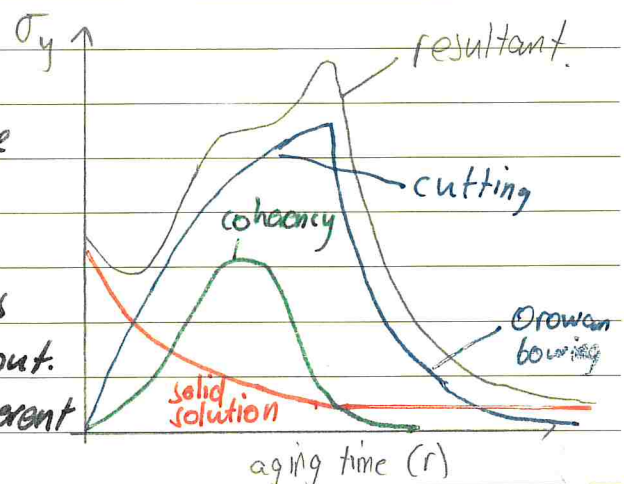
- With stronger precipitates:
 - \uparrow cutting resistance
 - no effect on bowing
 - $\therefore \uparrow$ peak stress but at lower r
- With greater fraction of precipitates:
 - \uparrow cutting resistance (more to cut)
 - \uparrow bowing resistance because $L \downarrow$
 - $\therefore \uparrow$ peak stress.

- But there are other factors that affect the yield strength.
- Initially after quenching, we will have a supersaturated solid solution

- i.e. solid solution strengthening from substitutional/interstitial solute atoms
- this decreases as solute precipitates out.

- Initially, when ppt is coherent/semicoherent it distorts the matrix and inhibits dislocation motion - coherency strain

↳ but once ppt becomes incoherent, they become a dislocation source.

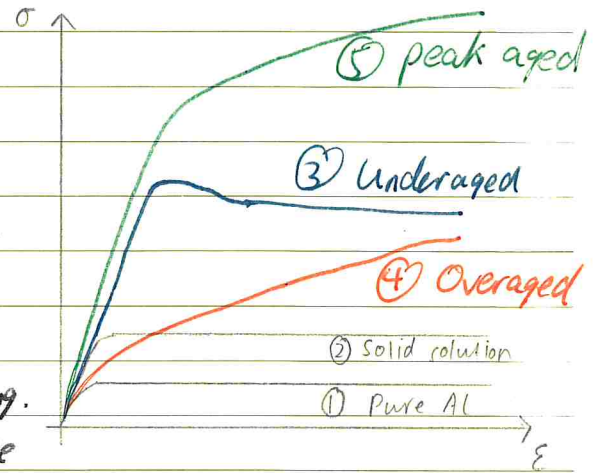


- For example, in the Al-Cu system:

- \uparrow Cu \uparrow strength (greater ppt fraction)
- \downarrow temp \uparrow peak stress, because the coherent phases have more time to separate and grow
- but there is a tradeoff because \downarrow temp requires much longer time to reach peak strength
- the optimal strength sample will have both θ' and θ'' phases, with both cutting and bowing.

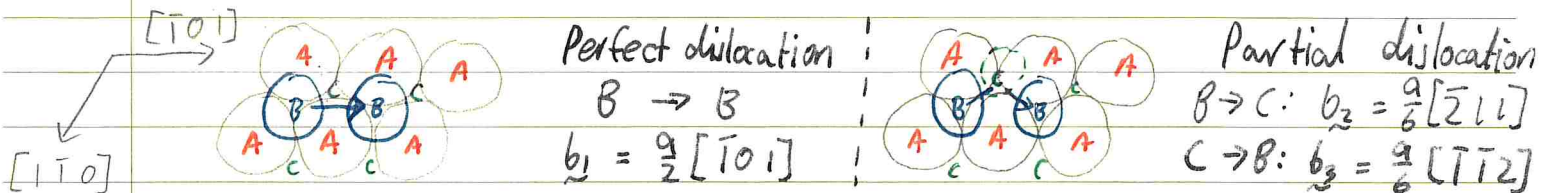
Precipitates and work hardening

- ① Pure Al has a low yield strength and will only have a little work hardening from \perp interactions
- ② A solid solution alloy will have higher σ_y than pure Al but the same hardening.
- ③ Underaged sample will contain GP zones that provide significant strengthening. But once slip starts, \perp can pass through the entire crystal and shear the GP zones
- ④ Overaged has low σ_y because \perp s will bow around ppt. But bowing produces **dislocation debris** (loops and tangles) that inhibit further \perp movement \Rightarrow rapid work hardening
- ⑤ Peak aged material has the best of ③ and ④, having high σ_y due to cutting, and rapid work hardening from bowing.
 \hookrightarrow this is why the best alloys have Θ'' and Θ'



Other deformation mechanisms

Partial dislocations and stacking faults



- Instead of a perfect dislocation, an alternative path involves two partial dislocations (which aren't lattice vectors).
- A perfect \perp will dissociate if it is energetically favourable (Frank's rule). Partial \perp s are always mixed.
- Note that after passage of the first partial \perp , the stacking sequence has changed:

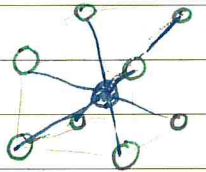
| | | | | | | | | | |
|---------------|---|---|---|---|---|---|---|---|---|
| initial: | A | B | C | A | B | C | A | B | C |
| after b_3 : | A | B | C | A | C | A | B | C | A |

slip stacking fault. A' ZONE

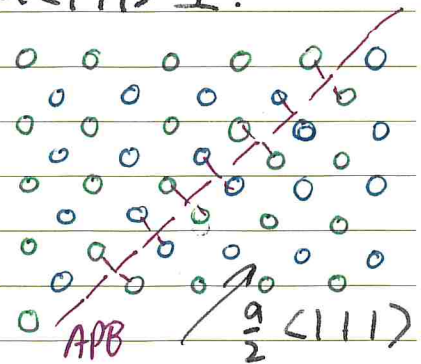
- When a perfect \perp dissociates, the elastic stress fields of the partial \perp s repel, causing them to separate, causing an extended stacking fault region to appear
 - ↳ width determined by **stacking fault energy (SFE)**. If SFE is high, partial \perp s will be close by.
- Partial \perp s cannot cross-slip because they have an edge component - they must recombine before they can change plane.
 - ↳ materials with low SFE (harder to recombine \perp s) will thus work harden rapidly.

Order hardening

- At low temperatures, β brass has an ordered CsCl structure (cubes of Cu with Zn in centre).
 - ↳ we would expect slip with $b = \frac{a}{2} \langle 111 \rangle$ but this is not a lattice vector and would create expensive Cu-Cu bonds.
- But at high temp it is a random solid solution, so $b = \frac{a}{2} \langle 111 \rangle$ corresponds to a perfect \perp
 - ↳ thus there is a large drop in T_c at a particular temp.

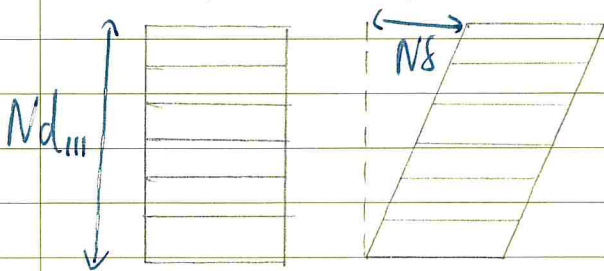


- But if we apply enough stress to low temp β brass it will still have to slip: it does this by passage of two $\frac{a}{2} \langle 111 \rangle$ \perp s to give a perfect $a \langle 111 \rangle$ \perp .
 - passage of $\frac{a}{2} \langle 111 \rangle$ creates an **anti-phase boundary (APB)**, an energetically unfavourable layer of like-like bonds.
 - as with stacking fault regions, the two partial \perp s will repel to form a **superdislocation** (which includes both partial \perp s and the APB).
 - thus order hardening provides significant strengthening, even at relatively high temp (as long as it's below the order \rightarrow disorder temp).



Deformation by cooperative shear

- Cooperative shear is an alternative deformation mechanism that does not involve \perp motion.
- Instead, successive planes are sheared, which can form the same crystal structure but at a different orientation
 - ↳ i.e. **deformation twinning**
 - ↳ each plane is only sheared a small amount, with no changes in bonding.
- The **twinning direction** will be the same as the partial \perp direction, e.g. $\frac{a}{6} \langle 11\bar{2} \rangle$ for fcc.



- the twinning plane for fcc is (111) .

$$d_{111} = \frac{a}{\sqrt{3}} \quad \text{and} \quad \delta = \frac{a\sqrt{6}}{6} \leftarrow \frac{1}{2} \text{ equivalent}$$

- \therefore maximum shear:

$$\gamma = \frac{\delta}{d_{111}} = \frac{1}{\sqrt{2}}$$

- Thus, twinning can facilitate significant deformation ($\frac{1}{\sqrt{2}} \approx 70\%$).

- Twinning is an athermal process, so may be the dominant deformation mechanism at cryogenic temperatures.
- Twinning is more likely for crystal systems with fewer slip systems, for which dislocations are less mobile.
- Twinning is more likely with low SFE, such that regions of a different stacking pattern (i.e. twins) may form
- Deformation twinning can propagate rapidly (\sim speed of sound), so may be the favoured mechanism at high strain rates.
- Deformation twins have a lenticular shape (such that they are compatible at grain boundaries), allowing them to be distinguished from annealing twins.
 - ↳ also, lens shape minimises strain field.

Fracture

- Fracture is the separation of a solid body under the influence of an applied load, involving the creation and propagation of cracks.
- **Toughness** is the resistance of a material to crack propagation.
- Ductile materials undergo plastic deformation before fracture, whereas it is much more sudden for brittle materials.
- We can estimate fracture stress by considering interatomic forces.

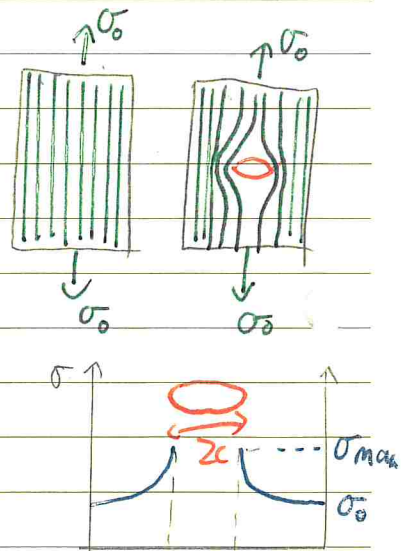
$$E = \frac{1}{r_0} \left. \frac{d^2V}{dr^2} \right|_{r=r_0} = \frac{72V_0}{r_0^3}$$

$$\sigma = \frac{F}{A} = \frac{1}{r_0^3} \frac{dV}{dr} = \frac{E}{6} \left[\left(\frac{r_0}{r} \right)^7 - \left(\frac{r_0}{r} \right)^{13} \right] \Rightarrow \sigma_{\max} \sim 0.04E$$

- ↳ but this model greatly overestimates fracture stress.
- ⇒ failure is controlled by defects in the material.

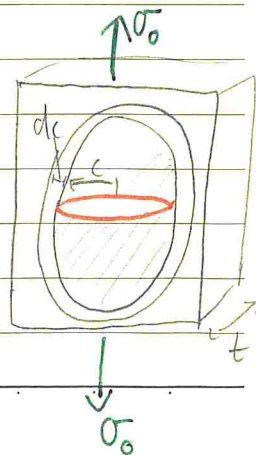
Cracks

- For a defect-free material, stress will be transmitted evenly.
- But if there is a **crack**, the lines of force will have to go around it, creating a **stress-free** region directly above and below the crack, but also a stress conc. at the tips.
- σ_{\max} depends on the crack length and the radius of curvature of the tip



$$\sigma_{\max} = \sigma_0 \left(1 + 2\sqrt{\frac{c}{r}} \right)$$

- When a crack grows, it releases stored elastic strain energy in the surrounding material.
 - if we model the oval as 2x circle of radius c , $dV = (2\pi c dc) \times 2 \times t$ ← thickness
 - elastic strain per unit volume is $\frac{\sigma_0^2}{2E}$



$$\therefore dW = \frac{\sigma_0^2}{2E} \cdot 2 \cdot (2\pi c t dc) = \frac{2\sigma_0^2 \pi c t}{E} dc$$

- The strain energy release rate G is the rate of release of strain energy per unit of new crack area (time-independent).

NOT SHEAR
MODULUS

$$\therefore G = \frac{dW}{\text{new crack area}} = \frac{dW}{4t dc} = \frac{\pi \sigma_0^2 c}{2E}$$

does not agree w/ experiment.
Remove factor of 2 because we assumed constant σ_0

- The constant depends on geometry, but $G \sim \frac{\sigma_0^2 c}{E}$ is general.

↳ $\uparrow G$ if stress \uparrow or if crack length \uparrow

↳ i.e. longer cracks release more energy per unit area

- In order for a crack to propagate, G must exceed some critical value, which will be 2γ if γ is the surface energy of a brittle material

↳ Griffith criterion: $G \geq G_c = 2\gamma$

↳ a.k.a. crack resistance or work of fracture.

- G_c can either be used to find the critical stress for a given crack length, or the critical flaw size for a given stress

$$\sigma^* = \sqrt{\frac{2\gamma E}{\pi c}} \quad \text{or} \quad c^* = \frac{2\gamma E}{\pi \sigma^2}$$

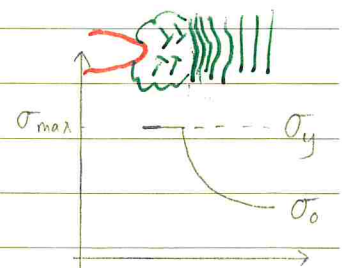
- The fracture stress of a material can be raised by polishing the surface or compressing it, such that cracks become shorter.
- Corrosive environments or fatigue can cause cracks to elongate.

Ductile fracture

- In a ductile material, the stress conc. leads to plastic deformation occurs near the crack tip, blunting it and thus reducing stress.
- Work must be done for plastic deformation, so much higher strain rate required to propagate crack.

↳ use modified Griffith criterion: $G \geq G_c = 2(\gamma + \gamma_p)$

↳ $\gamma_p \gg \gamma$ (by a factor of ~1000).

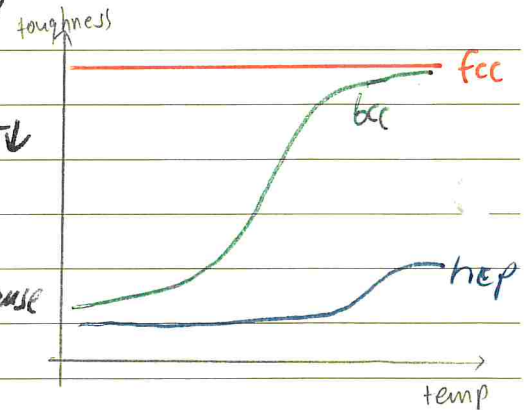


Stress intensity factor

- Because it is very difficult to determine the strain energy release rate G , we introduce the stress intensity factor: $K \equiv \sigma_0 \sqrt{\pi c}$
- When K reaches a critical value (the fracture toughness), fracture occurs. $K_c = \sqrt{G_c E}$ is a material property.
- There are non-destructive testing methods to evaluate K in materials, which can be compared to K_c during audits.

Ductile-brittle transition temperature

- Heating leads to increased plasticity and greater toughness.
- Likewise, cooling makes a sample more brittle.
- Increasing the strain rate also inhibits \perp motion so is similar to cooling, but cooling has a much greater effect.
- The toughness of a material can be measured by impacting the sample with a pendulum. The rebound height tells us the impact energy - a proxy for toughness.
- fcc metals are tough at all temps because of its slip systems \rightarrow mobile \perp s.
- bcc shows a large loss of toughness as $T \downarrow$ because some slip systems require thermal activation and \perp s prone to pinning
- hcp is brittle even at ambient temp because only one slip system can activate.



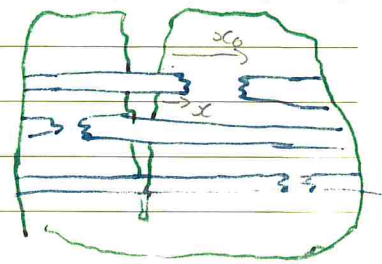
Toughness of composites

- Composites can be tough even when both the matrix and fibres are brittle.
- This is because work must be done on the material to pull fractured fibres out of matrix sockets
- A crack in the matrix can only propagate once embedded fibres are out of their sockets - fibre pull out

- Work is required for **interfacial debonding**, which is a 'friction' that depends on the **interfacial shear stress τ_i^*** :

$$dW = (2\pi r dx) \tau_i^* dx$$

$$\Rightarrow \Delta W = \int_0^{x_0} (2\pi r dx) \tau_i^* dx = \pi r x_0^2 \tau_i^*$$



- The number of fibres per unit area for a volume fraction f is given by $M = f/\pi r^2$
- Hence the **pull-out work of fracture (G_{cp})** is:

$$G_{cp} = M \Delta W = \frac{f \pi r x_0^2 \tau_i^*}{\pi r^2} = 4f s^2 r \tau_i^*$$

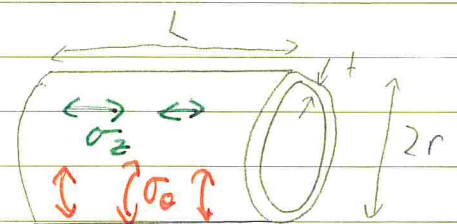
where s is the pull-out aspect ratio $s \equiv x_0/2r$
 $\rightarrow s \sim 20-50$, i.e. 100mm long and 10mm thick.

- The fibres do not tend to break in the crack plane because they are likely to have defects elsewhere.

Pressurised pipes

- Three stress components:

- axial σ_z along pipe
- circumferential (hoop) σ_θ around pipe
- radial σ_r across wall. $\sigma_r \approx 0$ for thin walls.



- The cross sectional area of the walls when cut along the pipe is $2tL$, so if the pressure is P and pipe in equilibrium:

$$\sigma_\theta (2tL) = P(2rL) \Rightarrow \sigma_\theta = \frac{rP}{t}$$

projected area

- Similarly for the axial case:

$$\sigma_z (2\pi r t) = P(\pi r^2) \Rightarrow \sigma_z = \frac{rP}{2t}$$

- Because hoop stress = 2x axial stress, pipes tend to burst longitudinally.