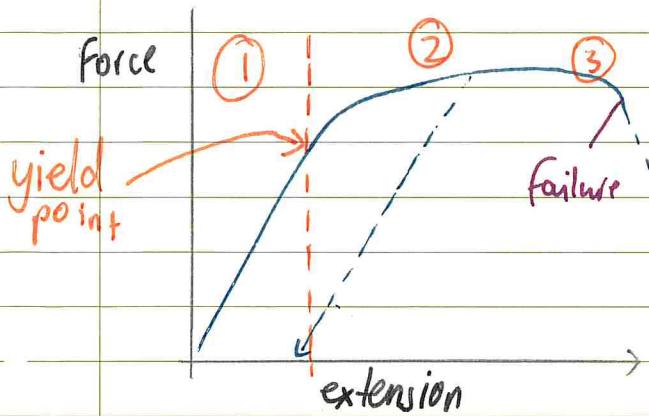


E. Mechanical Behaviour

No. |

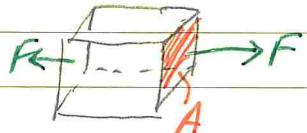
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- A material of known dimensions can be examined via tensile testing, in which it is stretched.



- 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
 - $\Leftrightarrow \sigma < 0 \Rightarrow$ compressive stress



- stress on a material leads to normal strain ϵ the relative change in the linear dimension in the direction of the force.

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

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

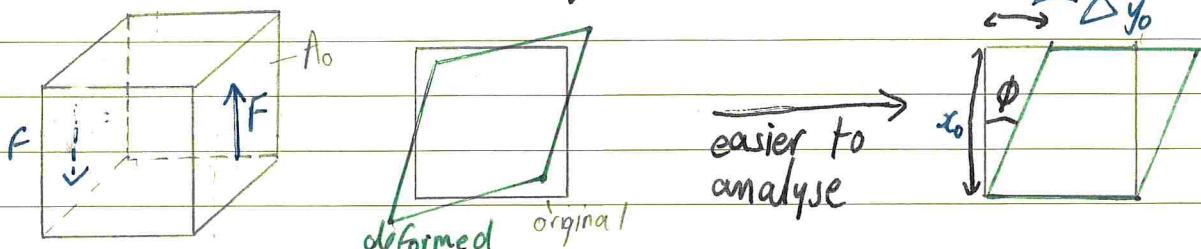
- The engineering stress assumes that the area of the cross-section remains the same even when strained, i.e. $\sigma_{\text{eng}} = F/A_0$.
 - reasonable approximation when strain $< 2\%$ because most engineering focuses on the elastic region.

- In reality, a cuboid under tension will contract laterally
 - Poisson's ratio ν is the ratio of 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

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

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



- The shear strain is the distortional deviation:

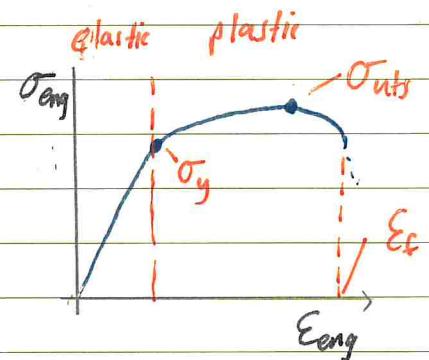
$$\gamma = \frac{\Delta y_0}{x_0} = \tan \phi \leftarrow \text{angle of shear}$$

- 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:

$$dW = F dL = (\sigma A)(L d\epsilon)$$

i.e. $dW = V E \epsilon$, assuming $V \equiv AL$ is constant.

$$\therefore W = \int_0^{E_{\max}} V E \epsilon d\epsilon$$

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

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**:

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

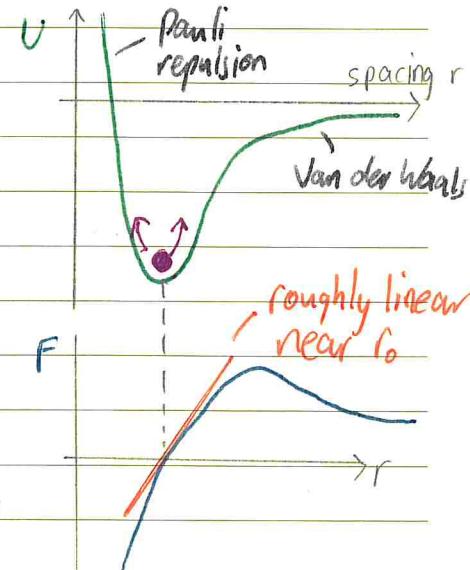
\hookrightarrow if we model each bond as having area r_0^2 :

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

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

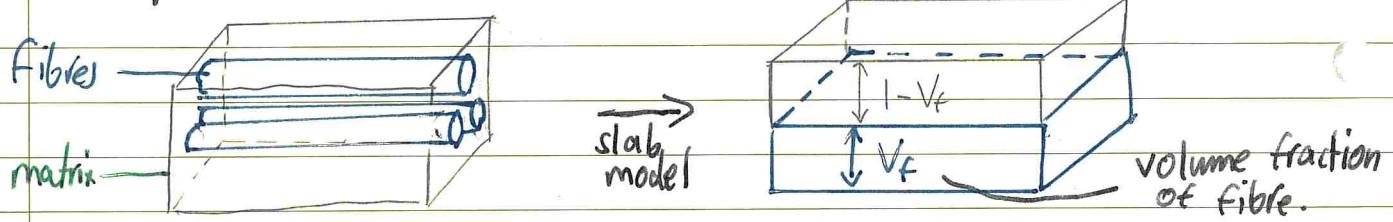
$$E = \frac{d\sigma}{d\epsilon} = \frac{d\sigma}{dr} \frac{dr}{d\epsilon} \Rightarrow E = \frac{1}{r_0} \frac{d^2 U}{dr^2} \Big|_{r=r_0}$$

\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



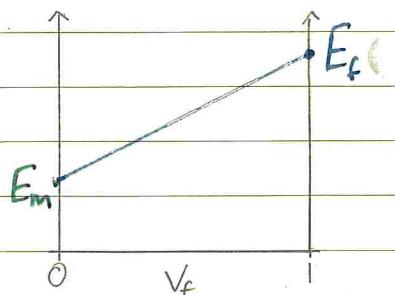
- The axial modulus can be approximated by the Voigt Model, which assumes that each slab experiences the same normal strain.

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

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

i.e. $E_c = E_f = E_m$.

- 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 but can extend differently.

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

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

Thermal strains

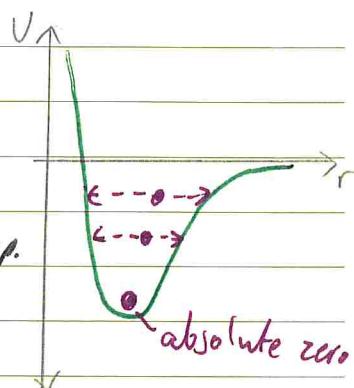
- The temperature measures the mean KE of atoms:

$$\frac{3}{2} kT = \langle \frac{1}{2} mv^2 \rangle$$

- 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:

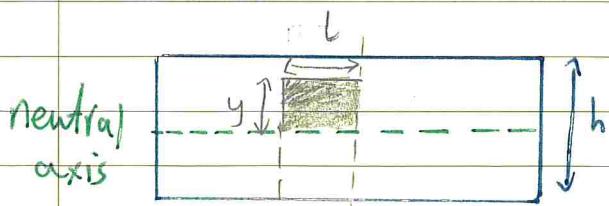
$\epsilon_T = \alpha \Delta T$, where α is the coefficient of thermal expansion.

- Materials with stronger inter-atomic bonds have deep sharp potential wells ⇒ high E, low α . e.g. ceramics.
- Polymers have shallow potential wells ⇒ 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 ↑, the average dV/dr^2 decreases ⇒ E↓.
- Thermal strain can be applied in bimetallic strips



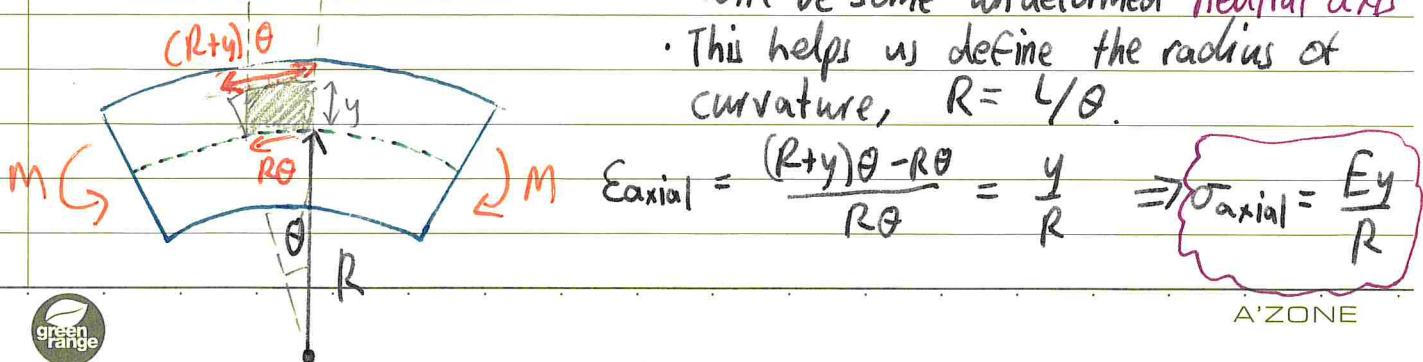
Beam theory

- 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, $R = l/\theta$.



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

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

- Moment about the neutral axis:

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

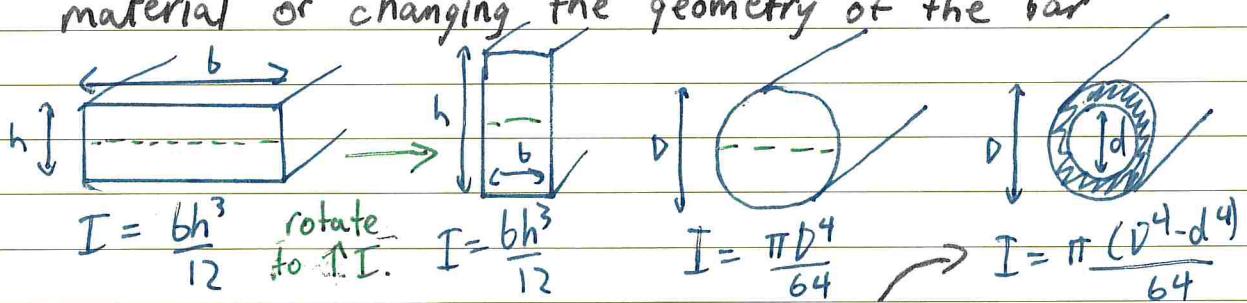
- Total bending moment found by integrating:

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

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

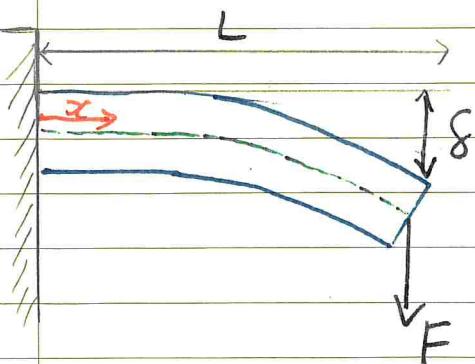
$$M = \kappa EI \quad \rightarrow \text{EI is the flexural rigidity (ie beam stiffness).}$$

- 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 $\theta \sim dy/dx$

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

- Thus the equation for cantilever loading:

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

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

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

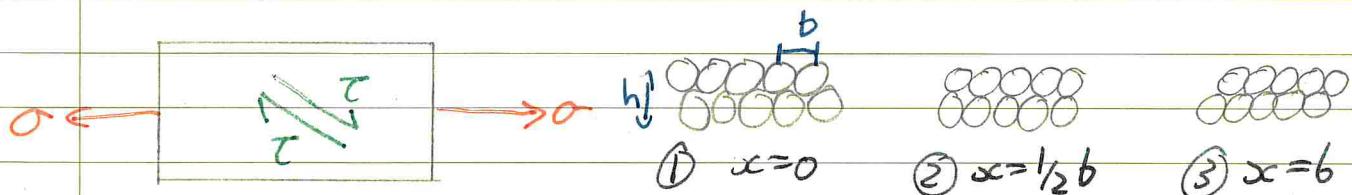
- The max deflection is obviously at the end of the beam ($x=L$)

$$\Rightarrow S_{\max} = \frac{FL^3}{3EI}$$

higher flex rigidity \Rightarrow lower S .

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

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

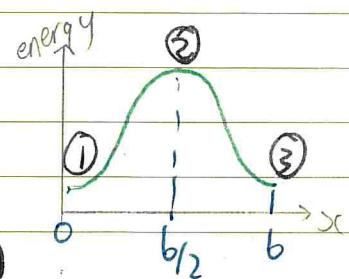
$$\tau \approx C \left(\frac{2\pi h \gamma}{b}\right), \text{ but } \frac{\tau}{\gamma} = G \Rightarrow C = \frac{Gb}{2\pi h}$$

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

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

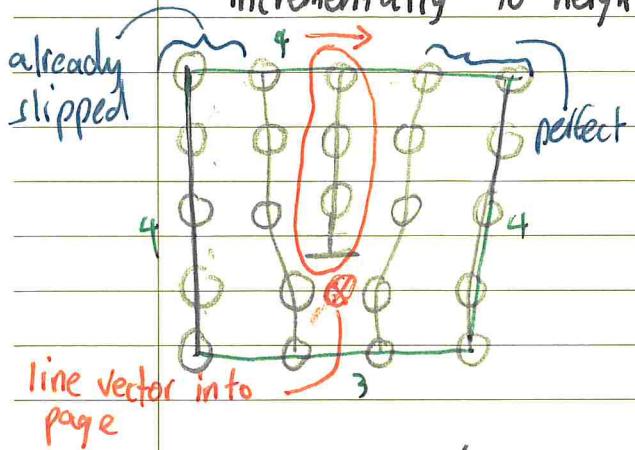
- This model overestimates τ_{crit} by a factor of ten

↳ 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.

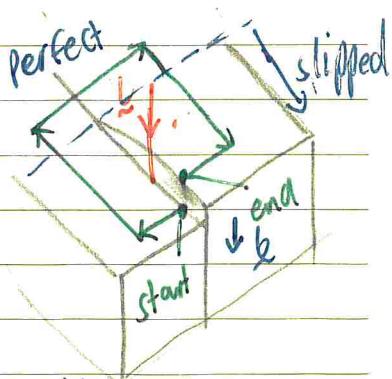
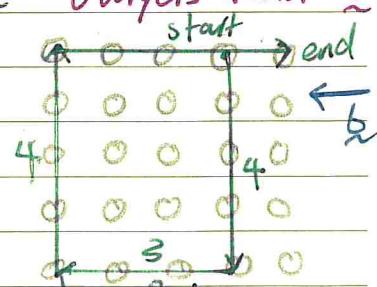
This line separates the slipped and perfect parts of the crystal and defines the **line vector ℓ** for an edge dislocation.

- The magnitude and direction of the lattice displacement caused by a dislocation is described by the **Burgers vector 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: 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 b** through the middle.

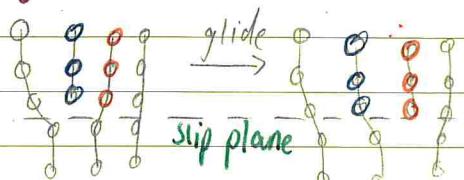
The relationship between ℓ and b determines the character of the dislocation:

$$\begin{cases} b \perp \ell \iff \text{edge dislocation} \\ b \parallel \ell \iff \text{screw dislocation} \end{cases}$$

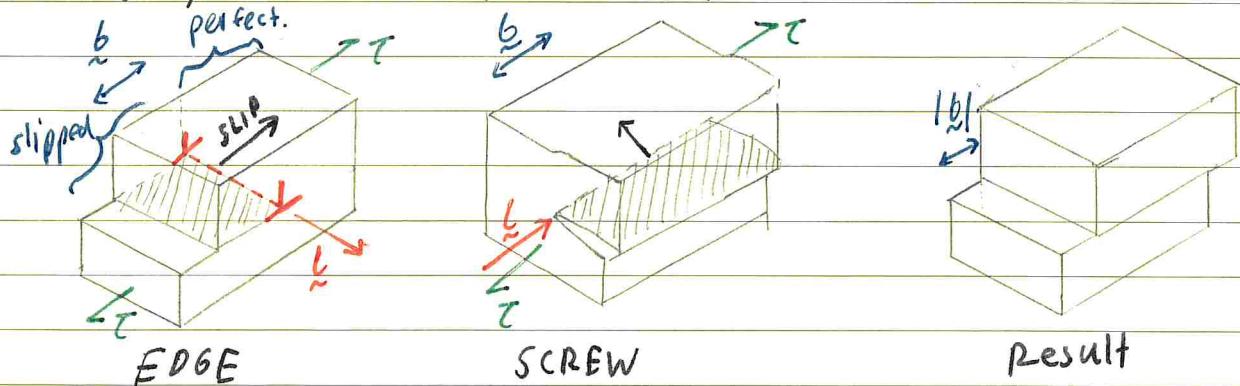


Dislocation motion

- 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 $1\underline{b}1$
 - the original crystal structure is restored after passage.



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

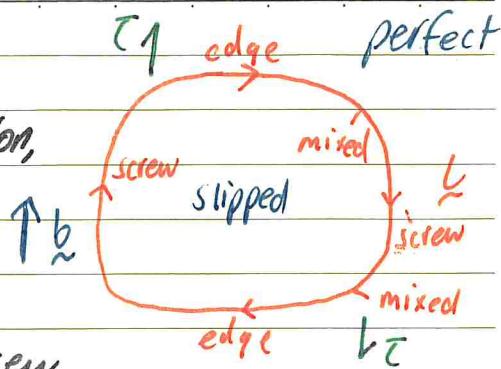


- If the shear stress is aligned with \underline{b} and $\tau \geq \tau_{\text{crit}}$, slip occurs parallel to the Burgers vector and the dislocation moves perpendicular to its line vector.
 - for an edge dislocation, there is only one slip plane (because it must contain \underline{b} and \underline{l} , 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 \underline{L} changing direction
- But because it is still a single dislocation, there is only one Burgers vector \underline{b} ↳ character of dislocation changes around the loop.
- Edge dislocations move $\parallel \underline{L}$, while screw dislocations move $\perp \underline{L}$.
- 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 $\perp L$ 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:

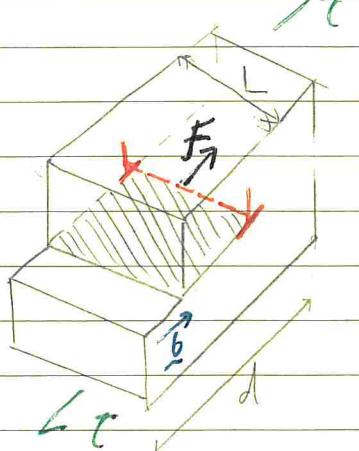
$$\tau_p \approx 3G \exp\left(-\frac{2\pi w}{b}\right)$$

↳ w is the dislocation width, i.e. the distance over which atoms are displaced by more than $\approx \frac{1}{4}b$.
 ↳ 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

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

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

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

↪ 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 .

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

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

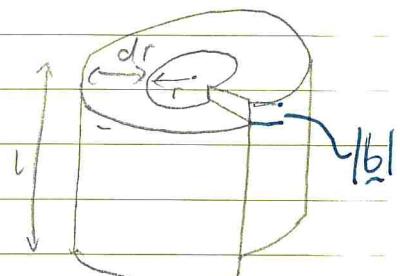
↪ r_0 is chosen to overestimate the energy near r_0 in order to compensate for E_{core} . Empirically, $r_0 \approx |b|/4$

↪ r_∞ is set to half the distance between dislocations.

↪ 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 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	$\{110\} \langle \bar{1}11 \rangle$	$\{111\} \langle \bar{1}\bar{1}0 \rangle$	$\{001\} \langle 100 \rangle$
number	$6 \times 2 = 12$	$4 \times 3 = 12$	$1 \times 3 = 3$
b	$\frac{a}{2} \langle 111 \rangle$	$\frac{a}{2} \langle 110 \rangle$	$a \langle 100 \rangle$

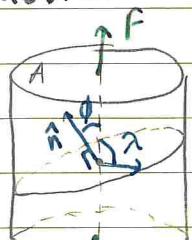
- This explains why hcp metals are stronger but less ductile - there are fewer slip systems. (~~intuitive given ABCABC packing~~)
- fcc-like \rightarrow NaCl structures: $\{110\} \langle \bar{1}10 \rangle$ ($6 \times 1 = 6$)
- bcc-like \rightarrow CsCl structures: $\{110\} \langle 001 \rangle$ ($6 \times 1 = 6$)

- 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:
 - area of plane is $A/\cos\phi$
 - force \parallel to slip direction is $F\cos\lambda$

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

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

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

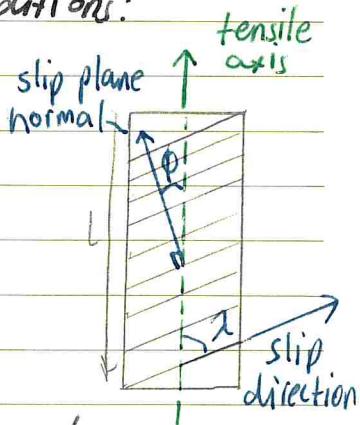


Schmid factor $\in [0, 1]$
because σ_y is the F/A for which dislocations move

- 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 <110> 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 <111> with L sign reversed.

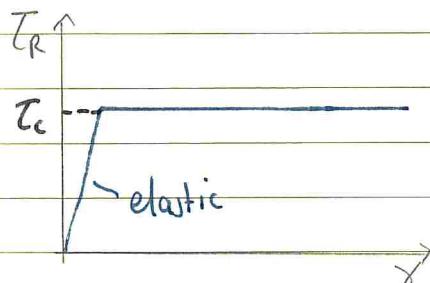
Geometry as slip proceeds

- 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 $\lambda \downarrow$
 \hookrightarrow 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.



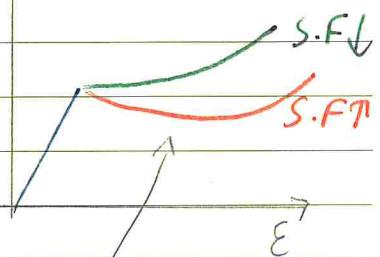
i.e once $T_R = T_c$, it remains there.

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

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

↳ i.e if S.F ↓ $\sigma_y \uparrow$

↳ if S.F ↑, $\sigma_y \downarrow$ - this is geometric softening.



- In FCC metal, initially one slip system operates so T_R is constant (1), though the Schmid factors change: easy glide

$T_R \uparrow$

- In (2), duplex slip occurs. Dislocations move on both slip systems and can interact
 - more T_R needed to move dislocations
 - ⇒ strength increases (work hardening).

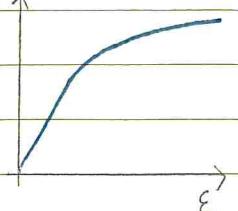
$T_R \uparrow$

- T_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 T_R to reach (3)

\rightarrow

- 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.

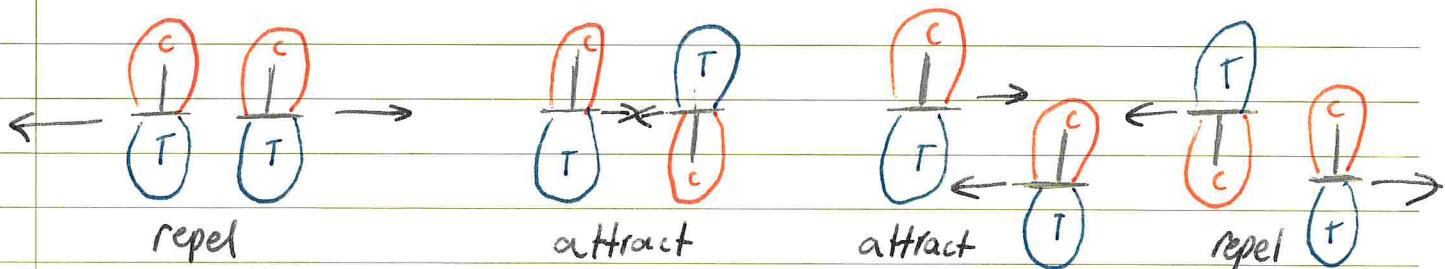
→



- Using the Taylor factor, we expect $\sigma_y \approx 3T_c$ 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, $\bar{z} = G \frac{b}{2\pi r}$.
- Edge Ls are more complex, but can be modelled as causing compression above the slip plane (extra atoms), and tension below.
- Stress fields will interact so as to reduce strain



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

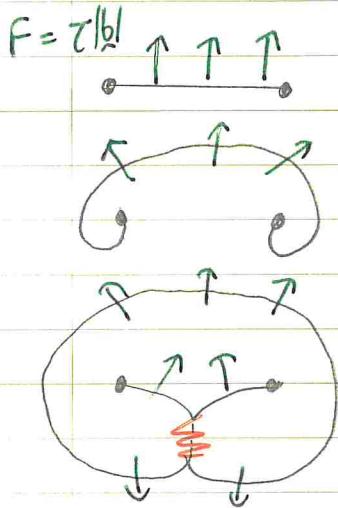
- If two dislocations were to combine, the new Burgers vector would be the vector sum of the individual b . $b_3 = b_1 + b_2$
- The new line vector would be the intersection of both slip planes.
- However, it is only energetically favourable for dislocations to combine if Frank's rule holds:

$$\{b_3^2 < b_1^2 + b_2^2\} \leftarrow \text{because energy } \sim 1/b^2$$

- Using the new b_3 and L_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 L_3
 - ↳ no guarantee that result will be on a valid slip system
 - ⇒ sessile dislocation that blocks other dislocations' movement.

Dislocation generation

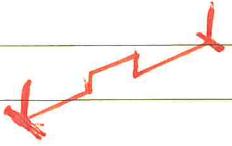
- Once dislocations reach the surface, they no longer participate in deformation \Rightarrow there must be a mechanism for \perp generation.
- A **Frank-Read source** consists of a linear dislocation pinned at both ends (e.g. by a sessile dislocation or point defect).



- 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

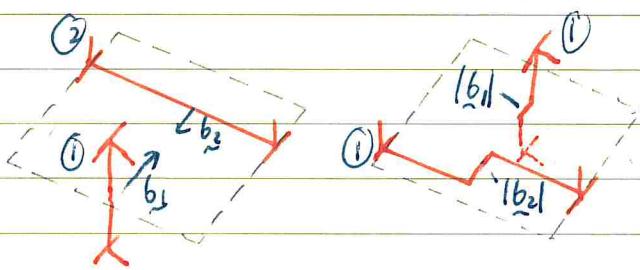
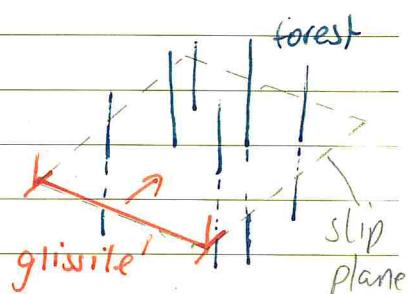
- Edge dislocations, for which glide is confined to a single plane, can bypass obstacles by **climb** - moving to a parallel slip plane
 - \hookrightarrow if a vacancy moves to the \perp core, \perp will move up - **positive climb**
 - \hookrightarrow alternatively, in negative climb, the vacancy at 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 T_R
 - when obstacle encountered, T_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 L separated by L , $\rho = 1/L^2$
 $\hookrightarrow \rho \sim 10^{10} \text{ m}^{-2}$ 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 .
 • Because jogs increase L 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 L s repel
 \hookrightarrow large grains \Rightarrow long piles \Rightarrow more stress \Rightarrow lower yield stress
 \hookrightarrow 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

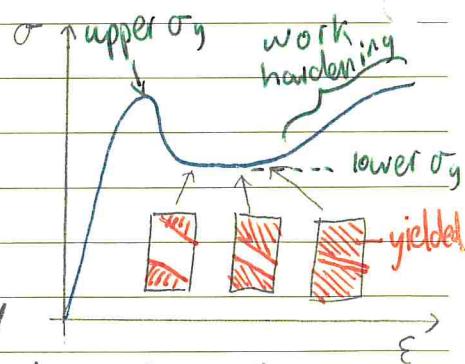
- Alloying tends to increase strength because it introduces solute atoms that interact with dislocations.
- **Substitutional defects** are when the solute atom replaces the original
 - produces a spherically symmetric stress field: compressive if solute atom is larger, tensile otherwise.
 - no shear 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↑).
 - 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 $\alpha\text{-Fe}$
 - smaller size means rapid diffusion towards the dislocation.
 - C atoms can surround the dislocation line: **Cottrell atmospheres** form along

\perp
C atom

low-carbon steel

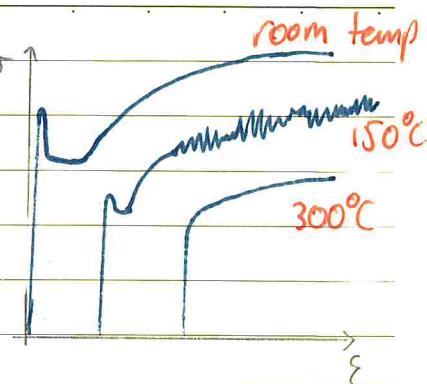
- Cottrell atmospheres provide strengthening because it is expensive to move them.
- Plastic deformation begins at the sample ends
 - no longer pinned by Cottrell atmospheres so continue to deform \rightarrow but they also work harden, so the unyielded regions start to yield
 - the boundaries are **Lüders 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
 - \hookrightarrow at high temp C atoms are very mobile and move with the \perp s so there is no strengthening effect until work hardening occurs.



- At intermediate temp, C and L move at comparable speeds.

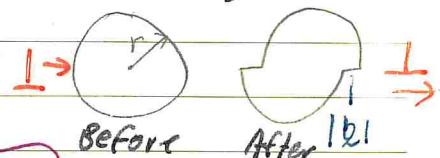
↳ dislocations can escape Cottrell atmospheres only to be repinned

↳ 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.



- 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:

$$\tau |b| L = 2(G|b|^2) \quad (\text{incoherent ppt})$$

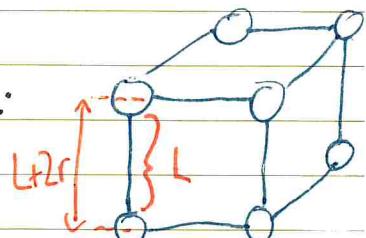
↳ L is surface-surface separation

- Thus the Orowan stress required to bow a dislocation is

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

- Assuming the ppt's have a cubic arrangement:

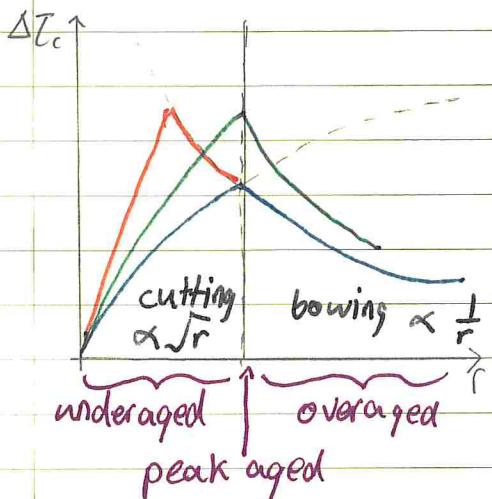
$$V_F = \frac{V_{\text{ppt}}}{V_{\text{cube}}} = \frac{\frac{4}{3}\pi r^3}{(L+2r)^3}$$



- 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**:

- ↑ cutting resistance
- no effect on bowing
- ∴ ↑ peak stress but at lower t

- With **greater fraction of precipitates**:

- ↑ cutting resistance (more to cut)
- ↑ bowing resistance because L_b
- ∴ ↑ peak stress.

- But there are other factors that affect the yield strength.

- Initially after quenching, we will have a supersaturated solid solution

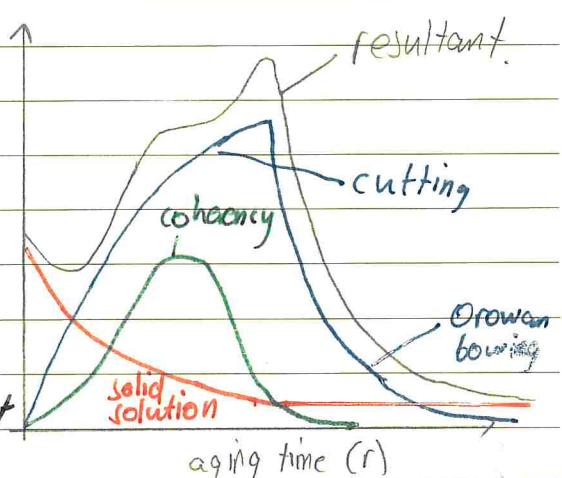
- i.e. **solid solution strengthening** from substitutational/interstitial solute atoms
- this decreases as solute precipitates out.

- 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.

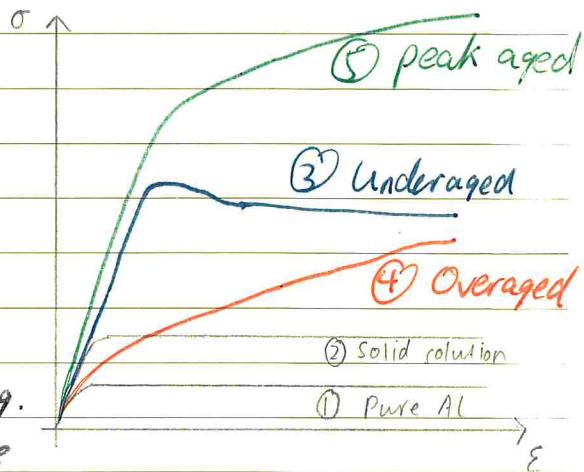
- For example, in the Al-Cu system:

- ↑ Cu ↑ strength (greater ppt fraction)
- ↓ temp ↑ peak stress, because the coherent phases have more time to separate and grow
- but there is a tradeoff because ↓ 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.



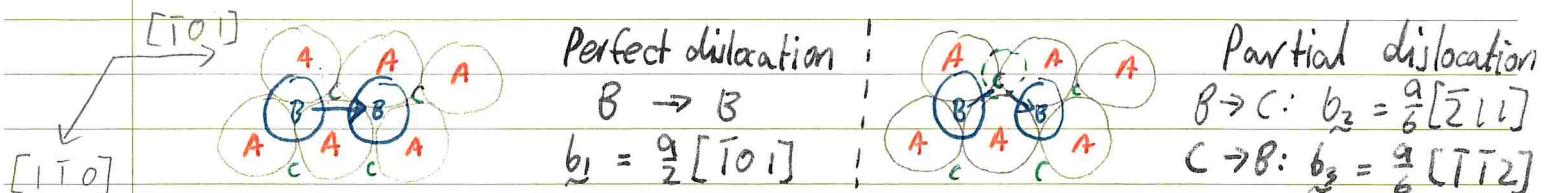
Precipitates and work hardening

- ① Pure Al has a low yield strength and will only have a little work hardening from L 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, L can pass through the entire crystal and shear the GP zones
- ④ Overaged has low σ_y because Ls will bow around ppt. But bowing produces **dislocation debris** (loops and tangles) that inhibit further L 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



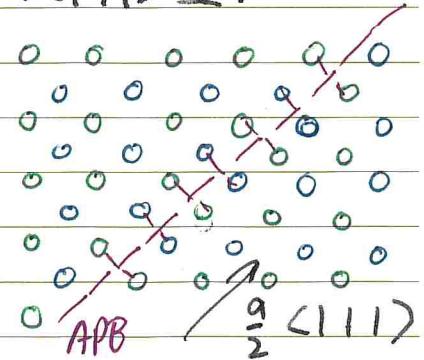
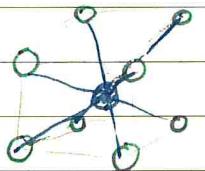
- Instead of a perfect dislocation, an alternative path involves two partial dislocations (which aren't lattice vectors).
- A perfect L will dissociate if it is energetically favourable (Frank's rule). Partial Ls are always mixed.
- Note that after passage of the first partial L, the stacking sequence has changed: initial: $A B C A B C A B C$
 after b_2 : $A B C A B C A B C$

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.

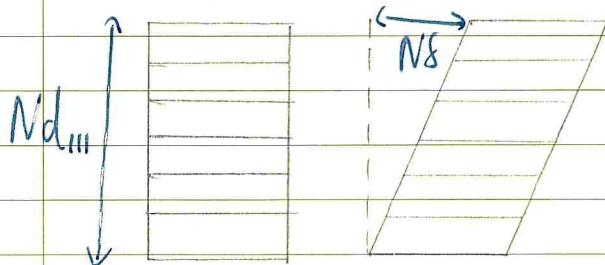
Order hardening

- At low temperatures, β brass has an ordered CsCl structure (cubes of Cu with Zn in centre).
 - ↳ we would expect slip with $\mathbf{b} = \frac{9}{2}\langle 111 \rangle$ 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 $\mathbf{b} = \frac{9}{2}\langle 111 \rangle$ 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 $\frac{9}{2}\langle 111 \rangle$ \perp s to give a perfect $a\langle 111 \rangle \perp$.
 - passage of $\frac{9}{2}\langle 111 \rangle$ 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).

$$d_{111} = \frac{a}{\sqrt{3}} \text{ and } s = \frac{a\sqrt{6}}{6} \leftarrow \frac{a_0}{6} \text{ equivalent}$$

- ∴ maximum shear:

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

- Thus, twinning can facilitate significant deformation ($\gamma \approx 70\%$).

- 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 (~ 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 minimizes 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.

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

$$\sigma = \frac{F}{A} = \frac{1}{r_0^2} \frac{dV}{dr} = \frac{E}{6} \left[\left(\frac{r_0}{r} \right)^7 - \left(\frac{r_0}{r} \right)^{13} \right] \Rightarrow \sigma_{\max} \approx 0.04E$$

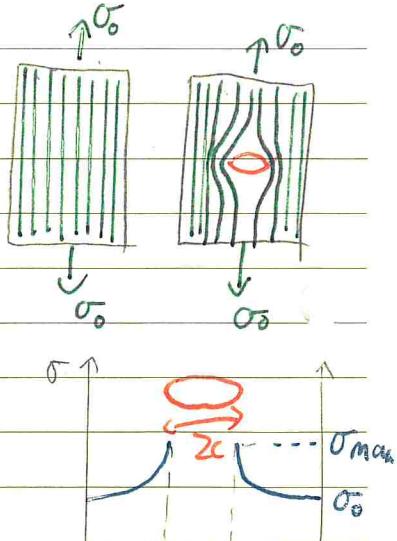
↳ but this model greatly overestimates fracture stress.

⇒ failure is controlled by defects in the material.

Cracks

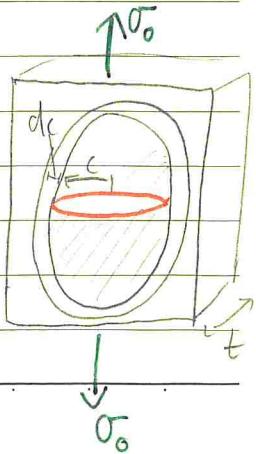
- For a defect-free material, stress will be transmitted evenly.
- But if there is a **crack**, the lines of force will have to go around it, creating a stress-free region directly above and below the crack, but also a stress conc. at the tips.
- σ_{\max} depends on the crack length and the radius of 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 $2\pi c$ circle of radius c , $dV = (2\pi c)dc \times 2\pi t$ ← thickness
- elastic strain per unit volume is $\frac{\sigma_0^2}{2E}$



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

- 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 $\therefore G = \frac{dW}{\text{new crack area}} = \frac{dW}{4tdc} = \frac{\pi\sigma_0^2 c}{2E}$ does not agree w/ experiment. Remove factor of 2 because we assumed constant σ_0

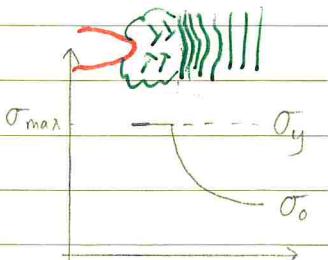
- The constant depends on geometry, but $G \sim \frac{\sigma_0^2 c}{E}$ is general.
 - $\hookrightarrow \uparrow G$ if stress \uparrow or if crack length \uparrow
 - \hookrightarrow i.e. longer cracks release more energy per unit area
- In order for a crack to propagate, G must exceed some critical value, which will be 2γ if γ is the surface energy of a brittle material
 - \hookrightarrow Griffith criterion: $G \geq G_c = 2\gamma$
 - \hookrightarrow 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

$$\sigma^* = \sqrt{\frac{2\gamma E}{\pi c}} \quad \text{or} \quad c^* = \frac{2\gamma E}{\pi \sigma_0^2}$$

- 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

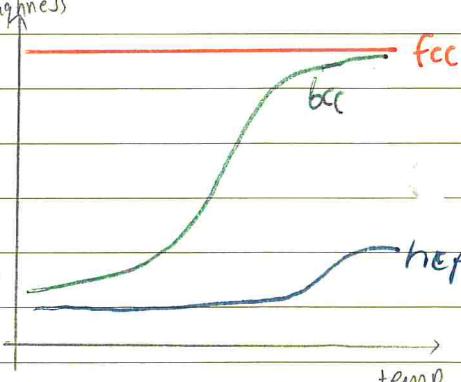
- In a ductile material, the stress conc. leads to plastic deformation occurs near the crack tip, blunting it and thus reducing stress.
- Work must be done for plastic deformation, so much higher strain rate required to propagate crack.
 - \hookrightarrow use modified Griffith criterion: $G > G_c = 2(\gamma + \gamma_p)$
 - $\hookrightarrow \gamma_p \gg \gamma$ (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: $K = \sigma_0 \sqrt{\frac{G}{E}}$
- 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 L 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 Ls. 
- bcc shows a large loss of toughness as T_b because some slip systems require thermal activation and Ls prone to pinning
- hcp is brittle even at ambient temp because only one slip system can activate.

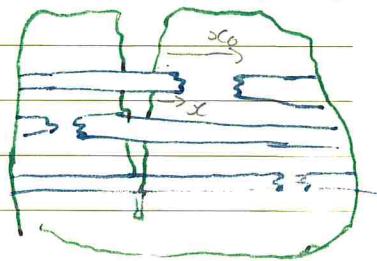
Toughness of composites

- 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^* :

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

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



- 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:

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

where s is the pull-out aspect ratio $s \equiv x_0/2r$

$\hookrightarrow s \sim 20-50$, i.e. 100 μm long and 10 μm 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

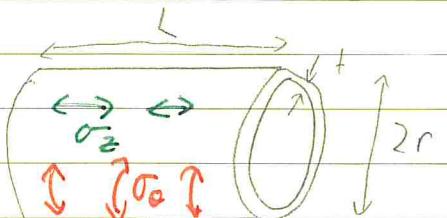
- circumferential (hoop) σ_θ around pipe

- 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 $2\pi r L$, so if the pressure is P and pipe in equilibrium:

$$\sigma_\theta (2\pi r L) = P(2\pi r L) \Rightarrow \sigma_\theta = \frac{P}{t}$$

projected area



- Similarly for the axial case:

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

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