

Nuclear Fuel Performance

NE-533
Spring 2023

Exam Notes

- Avg 89.5, no curve implemented
- Pretty good all around
- If you have questions or comments, please reach out to me

Last Time

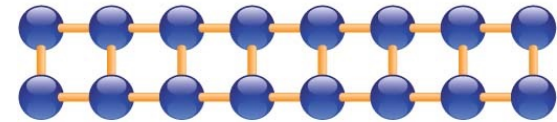
- Temporal and spatial discretization for numerical integration
- Forward and Backward Euler (Explicit and Implicit methods)
 - explicit can be sensitive to the timestep size
 - implicit are harder to implement, but more stable for stiff problems
- Finite difference, volume, and element
 - all three are used in fuel performance codes and have strengths/weaknesses
 - FD is fast, but works on a grid and is discrete
 - FE is most flexible, continuous, utilized in MOOSE
- Started into mechanics with concept of elasticity

MECHANICS

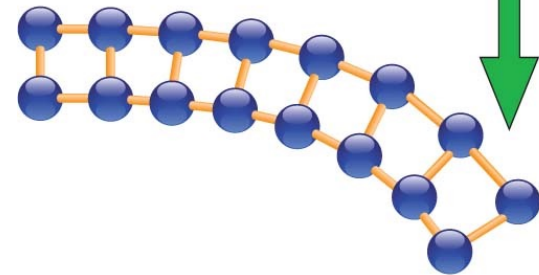
Elasticity

- Elasticity is the ability of a body to resist a distorting influence and to return to its original size and shape when that influence or force is removed
- In elastic deformation, we are stretching the atomic bonds
- The more we stretch the bonds, the more force it takes to stretch
- When we release the load, the atoms spring back into their lattice sites

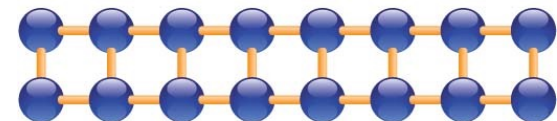
1. Original form



2. Force applied...

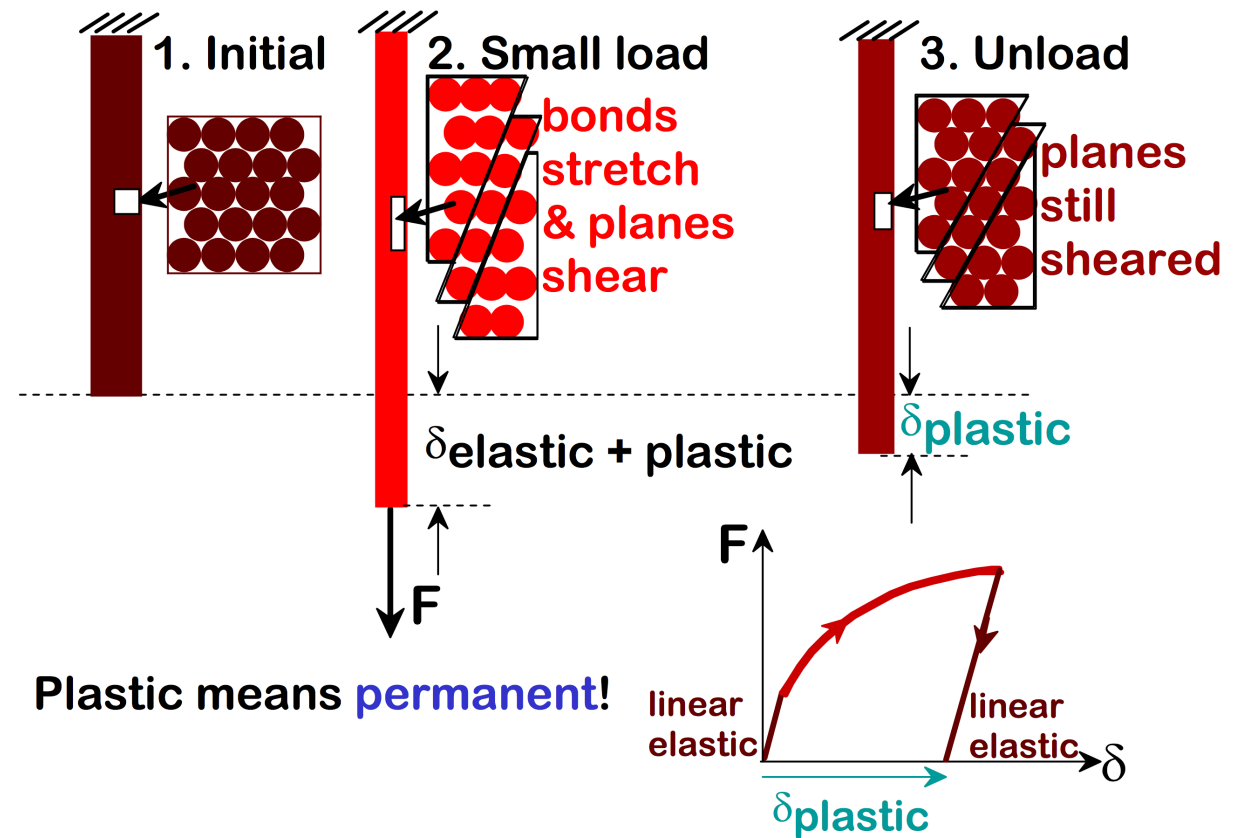


3. ...return to original form.



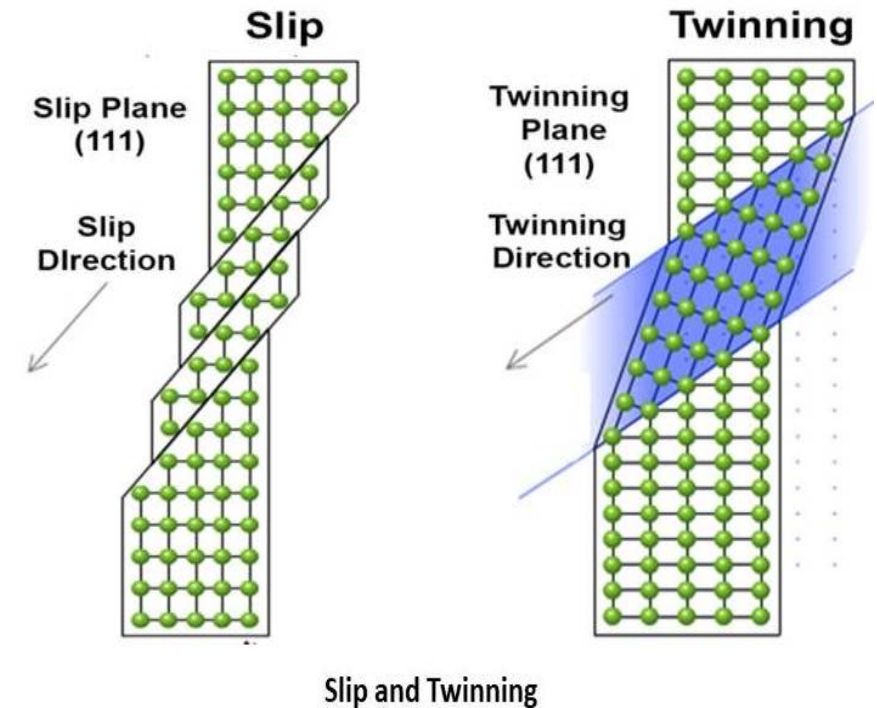
Plasticity

- Plasticity is the ability of a solid material to undergo permanent deformation, a non-reversible change of shape in response to applied forces
- Plastic deformation is observed in most materials
- The transition from elastic behavior to plastic behavior is known as yielding



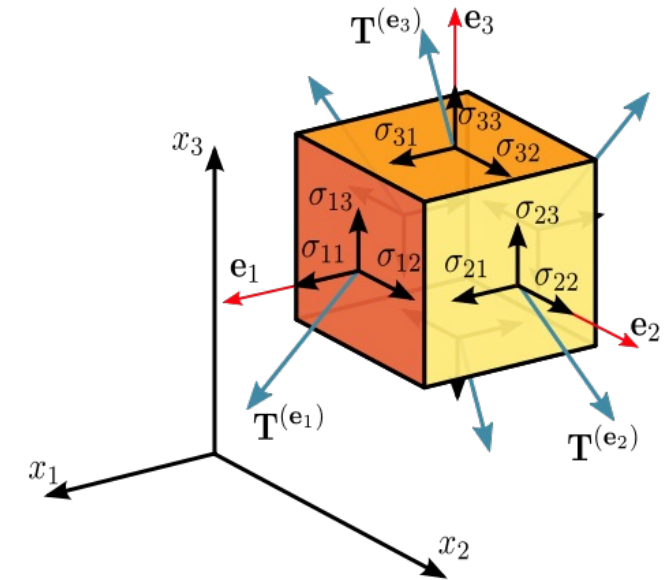
Plasticity

- Plasticity is typically caused by two modes of deformation in the crystal lattice: slip and twinning
 - Slip is a shear deformation which moves the atoms through many interatomic distances relative to their initial positions
 - Twinning is the plastic deformation which takes place along two planes due to a set of applied
- Ductility (total elongation), Yield Strength, etc. are dependent upon temperature and composition
- Plasticity typically increases at higher temperature



Stress

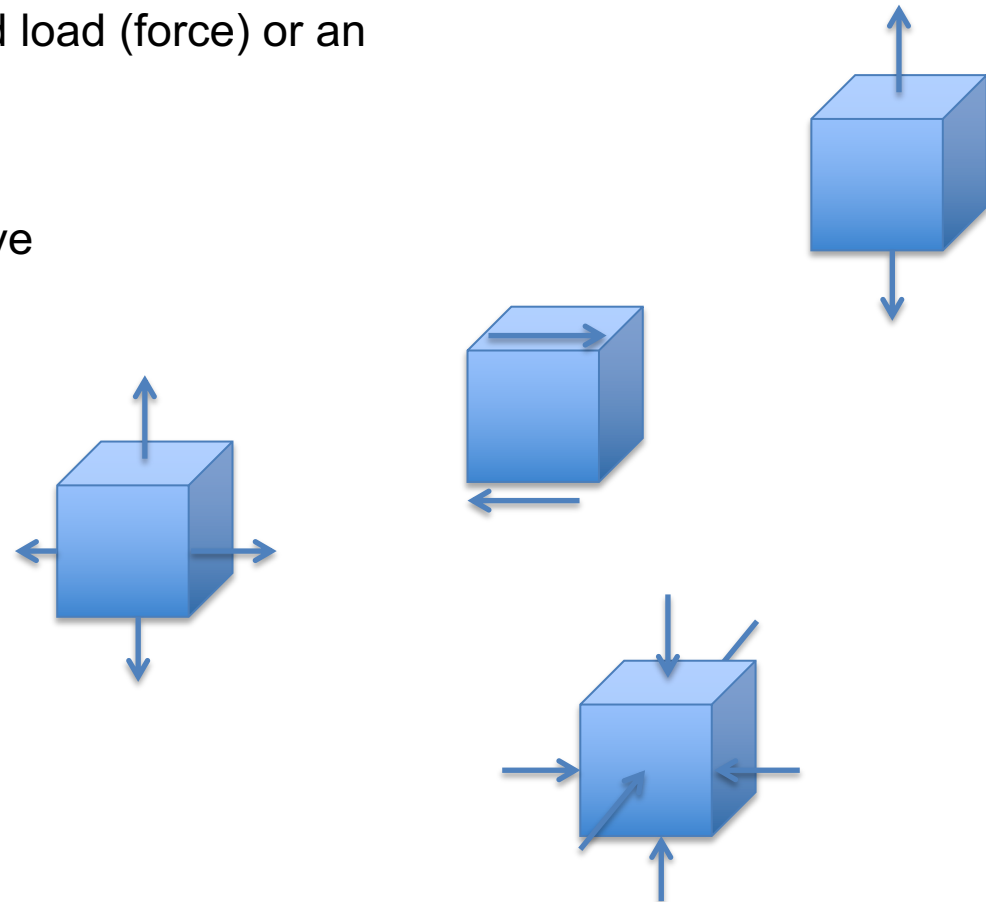
- Stress is a physical quantity that expresses the internal forces that neighboring particles of a continuous material exert on each other
- Stress is a force per unit area with SI units of Pa = N/m²
- The stress is a 2nd order tensor (a 3 by 3 matrix): Cauchy stress tensor
- $\sigma_{ij} = F_{ij}/A_i$
 - i is the face the force is applied and j is the direction it is applied
- Sigmas are normal stress components, taus are shear stress components



$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \equiv \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \equiv \begin{bmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z \end{bmatrix}$$

Stress as a response

- The stress in a material is the RESPONSE to an applied load (force) or an applied displacement
- Uniaxial tension or compression
 - Only one non-zero stress: σ_{ii} (σ_{11} , σ_{22} , σ_{33})
 - Tension means positive stress, compression negative
 - Examples: Cables, tension tests
- Pure shear
 - Only one non-zero stress: (σ_{12} , σ_{13} , σ_{23})
 - Examples: drive shaft
- Biaxial tension/compression
 - Two non-zero stress (e.g. $\sigma_{11} = 1$, $\sigma_{22} = 2$)
 - Examples: Pressure cylinder or vessel
- Hydrostatic compression (pressure)
 - $\sigma_{11} = \sigma_{22} = \sigma_{33} = -p$
 - Anything underwater

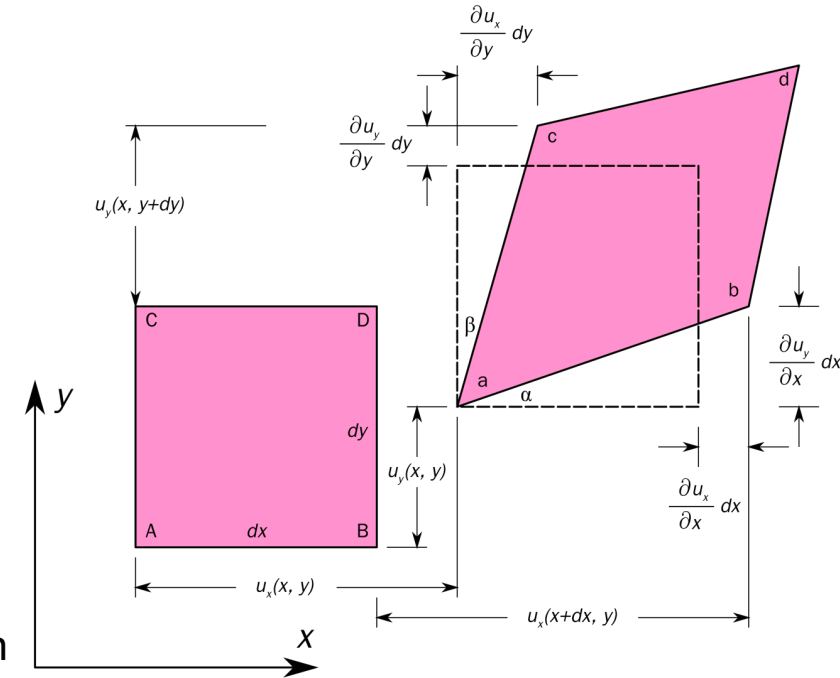


Strain

- Strain is a geometrical measure of deformation representing the relative displacement between particles in a material body
- The strain in a tensile test is the deformation divided by a representative length

$$e = \frac{\Delta L}{L} = \frac{\ell - L}{L}$$

- This is engineering strain, but strain can also be defined as “true strain,” accounts for shrinking of section area and the effect of developed elongation on further elongation



- Strain is a second order tensor, like the stress
 - Let \mathbf{u} be a vector of the displacements
 - The small strain tensor is

$$\epsilon_{ij} \equiv \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

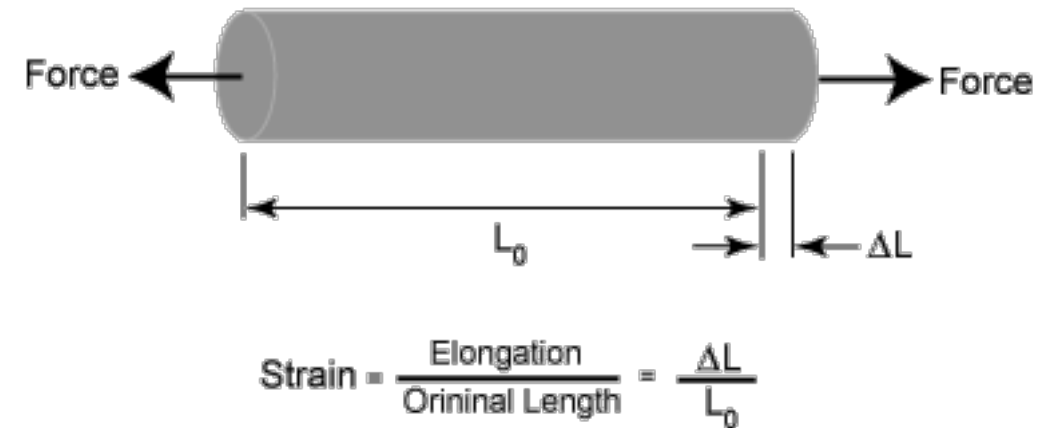
$$\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) & \frac{1}{2} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \\ \frac{1}{2} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \\ \frac{1}{2} \left(\frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) & \frac{1}{2} \left(\frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) & \frac{\partial u_3}{\partial x_3} \end{bmatrix}$$

- The common strain states are the same as the stress (uniaxial tension, etc.)

Strain produces stress

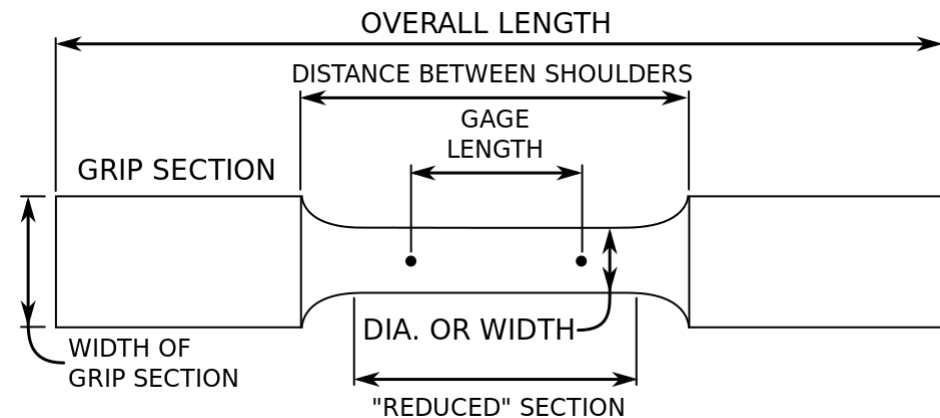
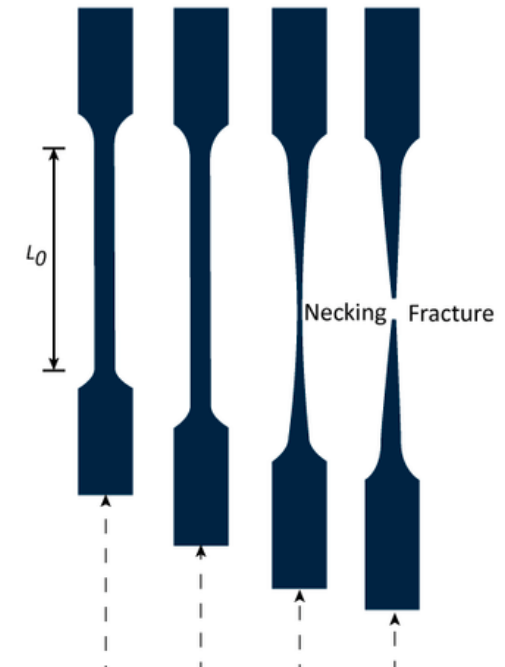
- A deformation (strain) results in stress within a material
- $\sigma = F(\epsilon)$
- For small strains, the stress is elastic and is a linear function of the strain
 - $\sigma = \mathcal{C}(\epsilon)$
- For larger deformation, some of the strain is elastic and increases the stress. The rest is plastic and does NOT contribute to the stress.
 - $\epsilon = \epsilon_e + \epsilon_p$
 - $\sigma = \mathcal{C}\epsilon_e$
- The elastic energy density in a material is a scalar quantity equal to

$$E_{el} = \frac{1}{2} \epsilon_e \cdot \sigma$$



Tensile testing

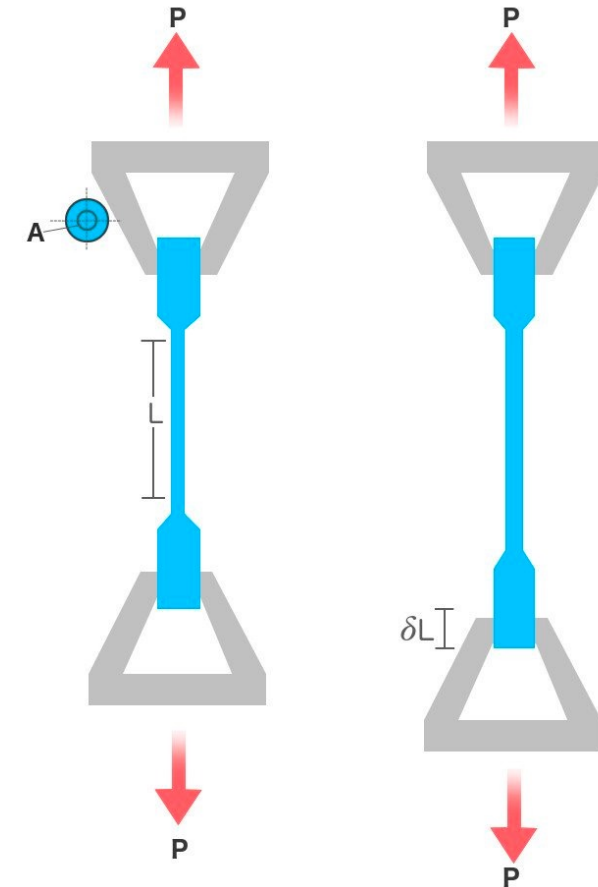
- The most common means of determining mechanical properties is a uniaxial tension test
- Apply a uniaxial load until failure
- Properties that are directly measured via a tensile test include ultimate tensile strength, maximum elongation, etc., which can be utilized to determine Young's modulus, Poisson's ratio, etc.



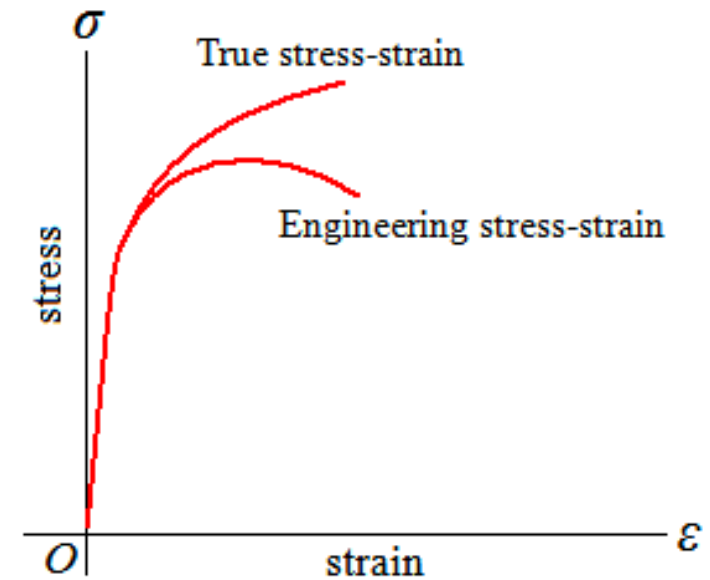
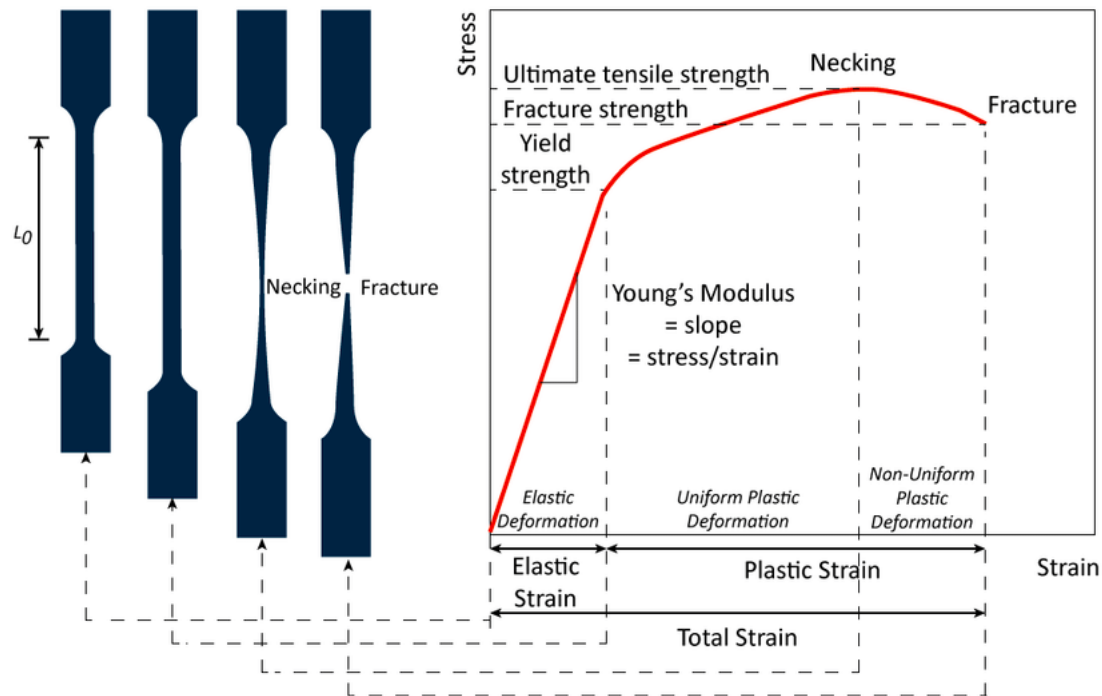
Stress/strain from a tensile test

- A_0 = Initial cross section area
- A = deformed cross section area
- P or F applied load/force

	Engineering	True
stress σ	$\frac{F}{A_0}$	$\frac{F}{A}$
strain ϵ	$\frac{l - l_0}{l_0}$	$\int_{l_0}^l \frac{dl}{l} = \ln\left(\frac{l}{l_0}\right)$



Stress vs strain curves



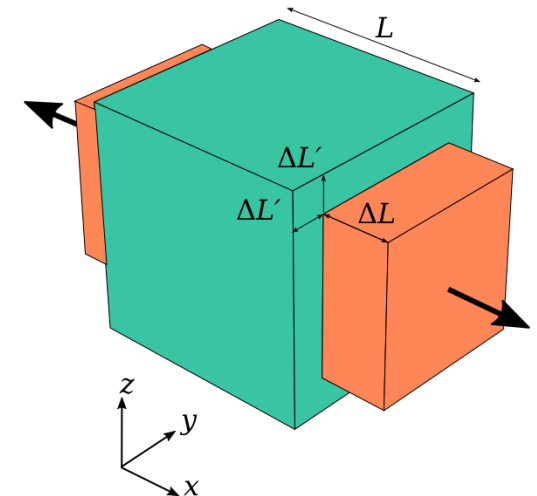
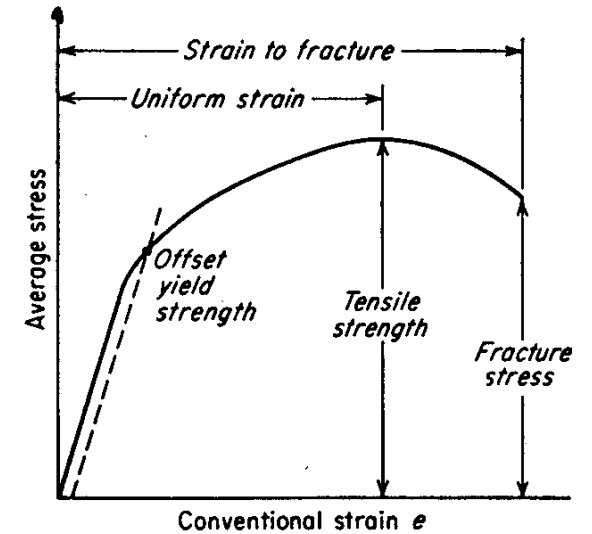
Using stress/strain curves

- In the elastic portion of the stress-strain curve, the stress varies linearly with strain
- The slope of the line is Young's Modulus, E : $\sigma = E \varepsilon$
- Poisson's ratio, ν , is the ratio of the shrinkage in cross section due to the extension in the pulling direction

$$\nu = -\frac{d\varepsilon_{\text{trans}}}{d\varepsilon_{\text{axial}}} = -\frac{d\varepsilon_y}{d\varepsilon_x} = -\frac{d\varepsilon_z}{d\varepsilon_x} \quad \nu \approx \frac{\Delta L'}{\Delta L}$$

- Can obtain the shear modulus from the elastic modulus and Poisson's ratio

$$G = \frac{E}{2(1 + \nu)}$$



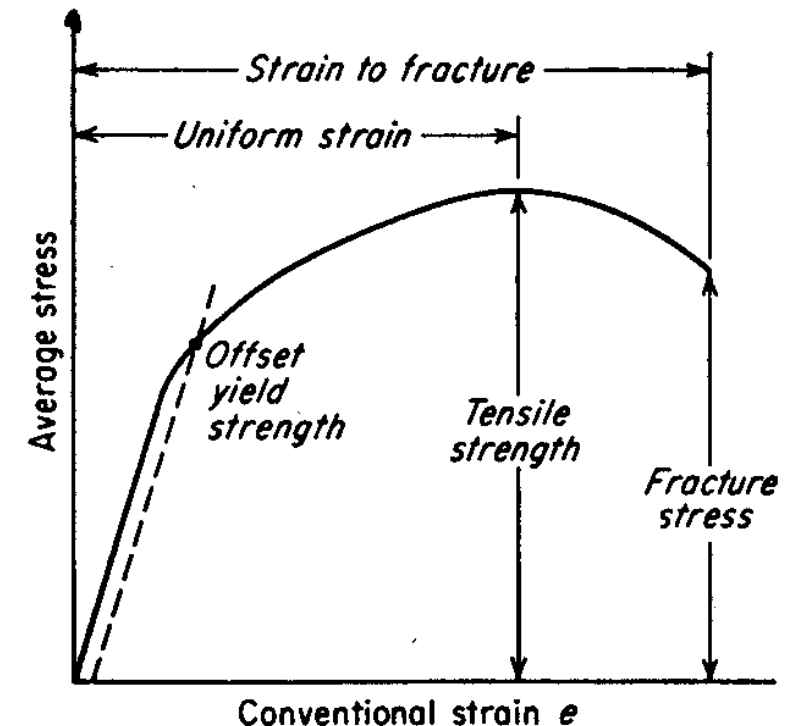
Using stress/strain curves

- The shear modulus, G , defines the stress to strain ratio in shear

$$\sigma_{12} = G\epsilon_{12}$$

- For isotropic materials, $G = E / (2(1 + \nu))$
- In matrix form, the elasticity/stiffness tensor from Hooke's law for isotropic materials can be written as

$$\begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{bmatrix} = \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{bmatrix} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2+2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2+2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2+2\nu \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$



$$\epsilon_{ij} = \frac{1}{E} (\sigma_{ij} - \nu(\sigma_{kk}\delta_{ij} - \sigma_{ij}))$$

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

Isotropic and Anisotropic

- Being a linear mapping between the nine numbers σ_{ij} and the nine numbers ε_{kl} , the stiffness tensor \mathbf{c} is represented by a matrix of $3 \times 3 \times 3 \times 3 = 81$ real numbers
- Given minor symmetries of the stiffness tensor, $c_{ijkl} = c_{jikl}$, this 81 elastic constants can be reduced to 36
- Major symmetries, $c_{ijkl} = c_{klij}$, reduce this number from 36 to 21
- Isotropic materials deform the same way no matter in what direction you deform them.
 - They have 2 unique elastic constants, C_{11} and C_{12}
- Anisotropic materials behave differently in different directions
 - The elasticity tensor can have 21 unique components defining anisotropy
 - Orthotropic materials have 9 unique elastic constants
 - Cubic structured materials have 3 unique elastic constants (UO_2)
 - Hexagonal structured materials have 5 unique elastic constants
- Polycrystalline anisotropic materials can behave as isotropic, because the various grains average out

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}; \quad \boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

$$\sigma_{ij} = - \sum_{k=1}^3 \sum_{l=1}^3 c_{ijkl} \varepsilon_{kl}$$

$$\begin{bmatrix} c_{1111} & c_{1122} & c_{1133} & c_{1123} & c_{1131} & c_{1112} \\ c_{2211} & c_{2222} & c_{2233} & c_{2223} & c_{2231} & c_{2212} \\ c_{3311} & c_{3322} & c_{3333} & c_{3323} & c_{3331} & c_{3312} \\ c_{2311} & c_{2322} & c_{2333} & c_{2323} & c_{2331} & c_{2312} \\ c_{3111} & c_{3122} & c_{3133} & c_{3123} & c_{3131} & c_{3112} \\ c_{1211} & c_{1222} & c_{1233} & c_{1223} & c_{1231} & c_{1212} \end{bmatrix}$$

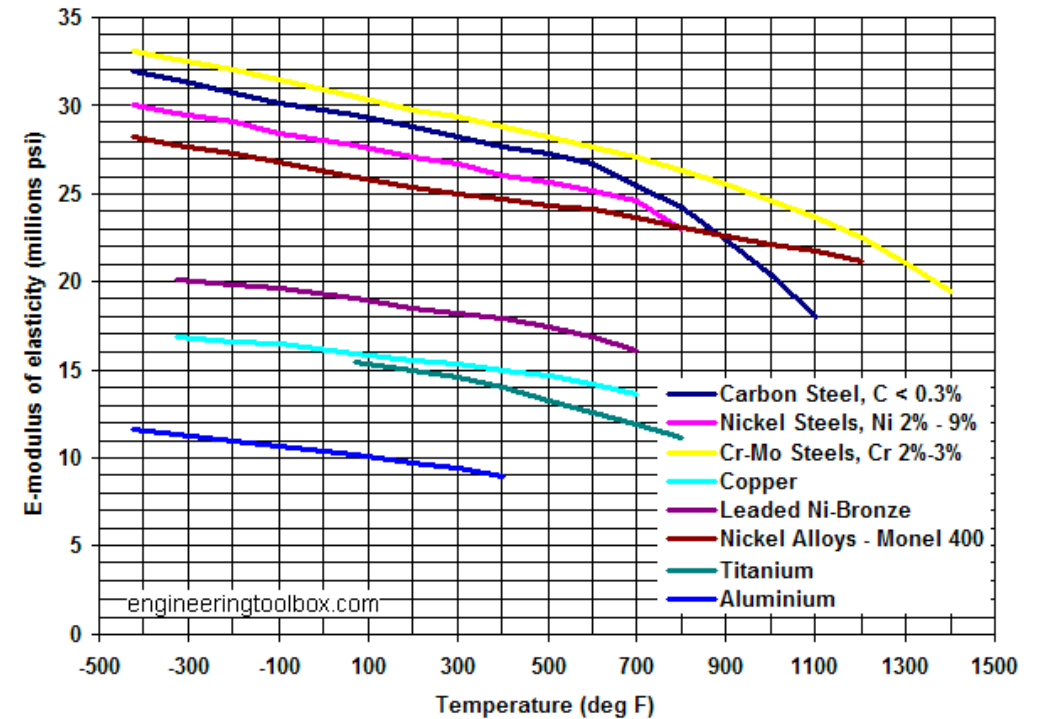
$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix}$$

Isotropic elastic constants for some materials

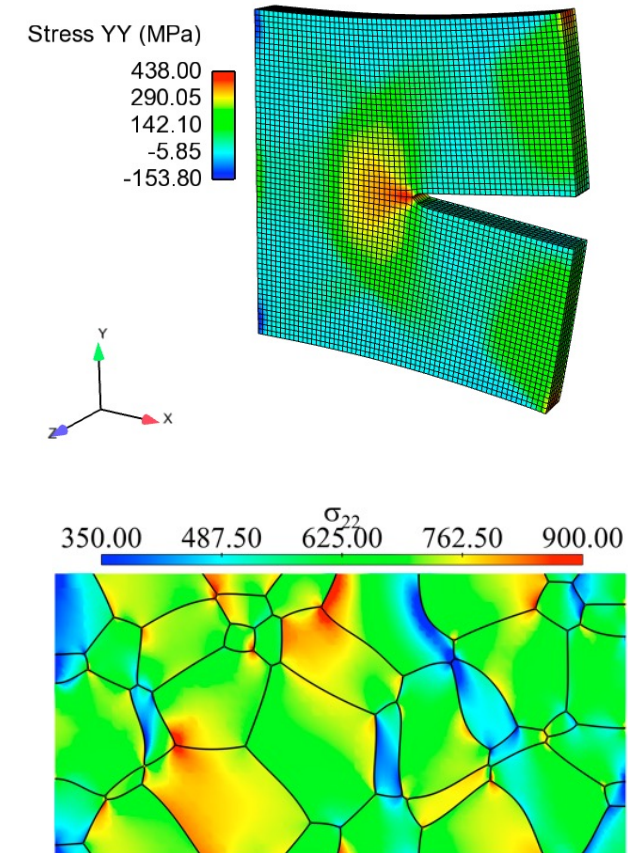
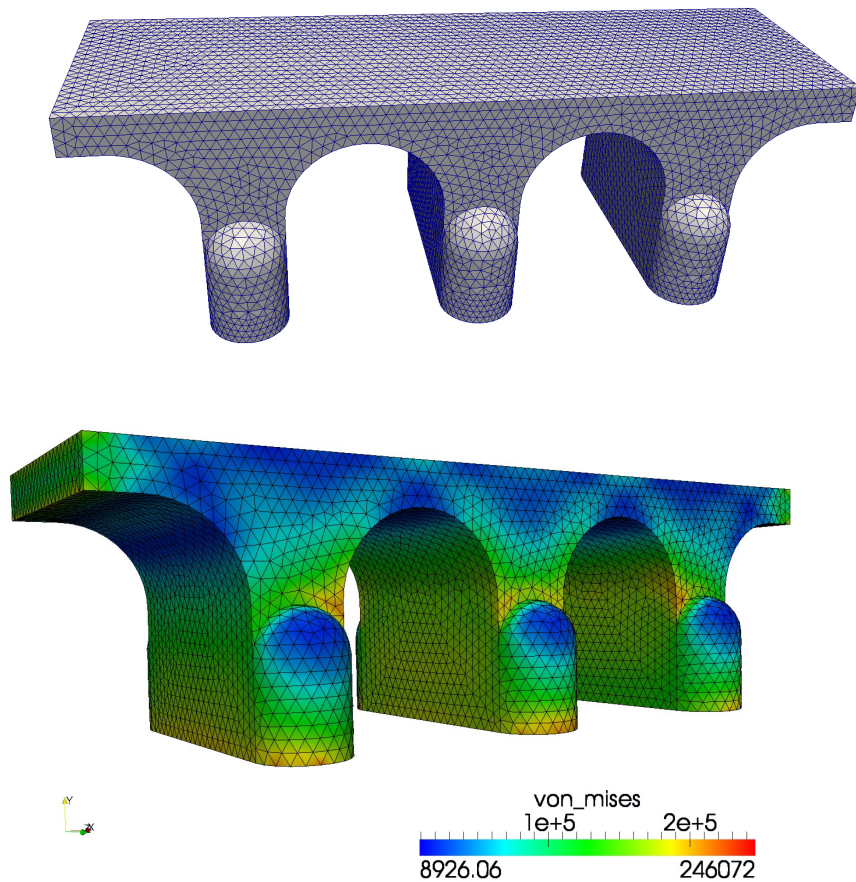
Material	E (GPa)	ν
Aluminum	70.3	0.345
Gold	78.0	0.44
Iron	211.4	0.293
Nickel	199.5	0.312
Tungsten	411.0	0.28
Zircaloy	80.0	0.41
UO ₂	200.0	0.345

Elastic constants are not “constant”

- Properties change with temperature
- Softening can be referred to as the decrease in elastic constants with temperature
- Young's modulus is typically a function of temperature, decreasing with increasing temperature
- Shear Modulus and Poisson's ratio can also change with T



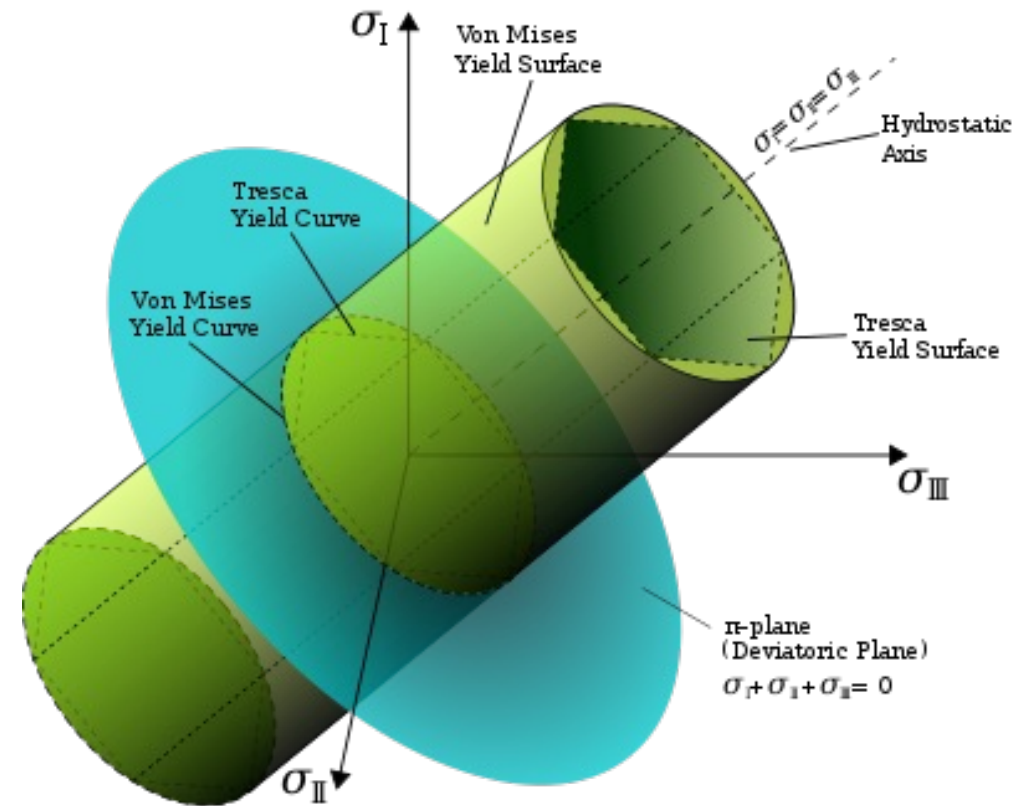
In actual materials, the stress and the strain change throughout the material



von Mises yield criterion

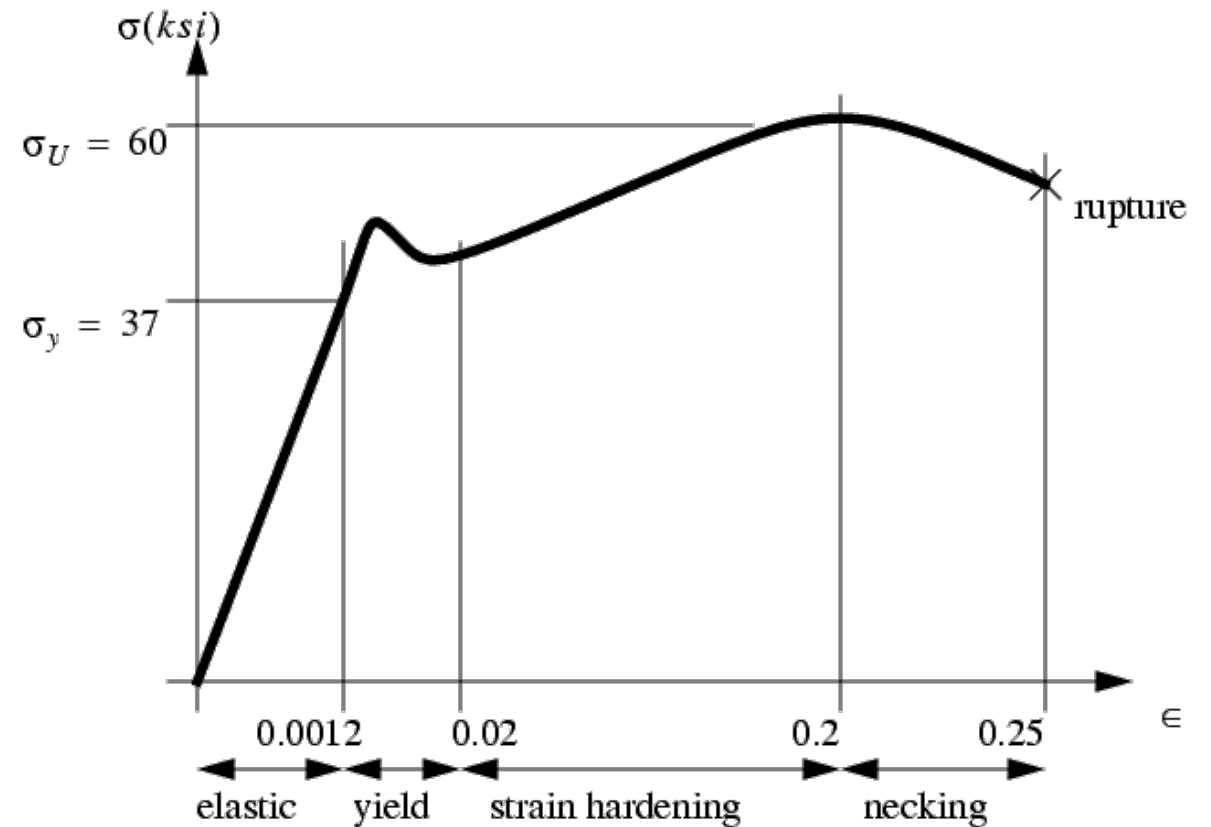
- The maximum distortion criterion (also von Mises yield criterion) states that yielding of a ductile material begins when the second invariant of deviatoric stress (J_2) reaches a critical value
- A material is said to start yielding when the von Mises stress reaches the yield strength
- The von Mises stress satisfies the property where two stress states with equal distortion energy have an equal von Mises stress
- The von Mises stress is used to predict yielding of materials under complex loading from the results of uniaxial tensile tests

$$\sigma_v^2 = \frac{1}{2} [(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6(\sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2)]$$



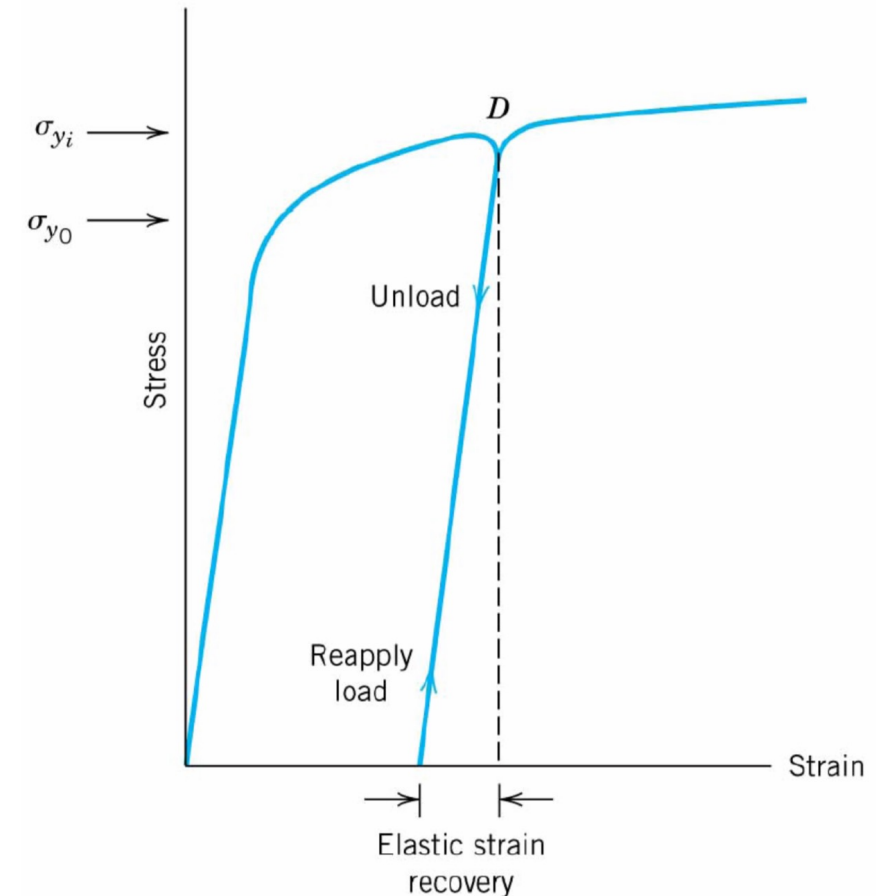
Stress/Strain Regions

- Once the stress reaches the yield stress, it plastically deforms
- σ_y is the yield stress
- σ_U is the ultimate tensile stress
- The final stress before rupture is called the fracture stress



Permanent Strain

- After plastic deformation, if you unload the sample, it still has the permanent strain
- The plastic behavior has modified the microstructure, and has increases the yield point
- After unloading, the strain hardening has changed the material
- Thus, if you reload, the yield strain is often higher than it was previously

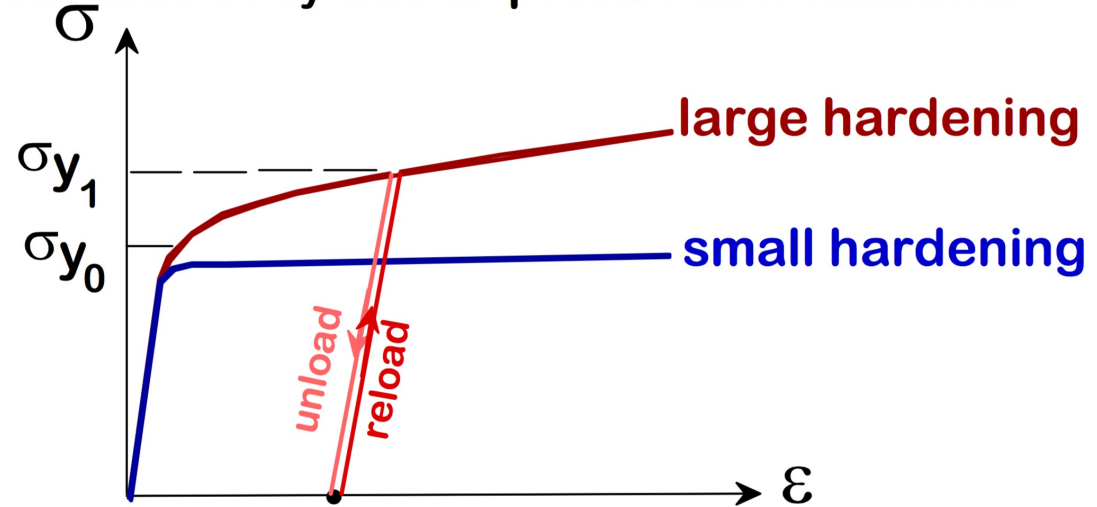


The hardening behavior changes for different materials

$$\sigma = \sigma_y + K(\epsilon_0 + \epsilon_p)^n$$

- K is a strength coefficient, n is the strain hardening exponent, ϵ_0 is the prior plastic strain, ϵ_p is the plastic strain, and σ_y is the yield strength
- The strain hardening exponent is a material property, with a value between 0 and 1
- A value of 0 means that a material is a perfectly plastic solid, while a value of 1 represents a 100% elastic solid.

- An increase in σ_y due to plastic deformation.



- Curve fit to the stress-strain response:

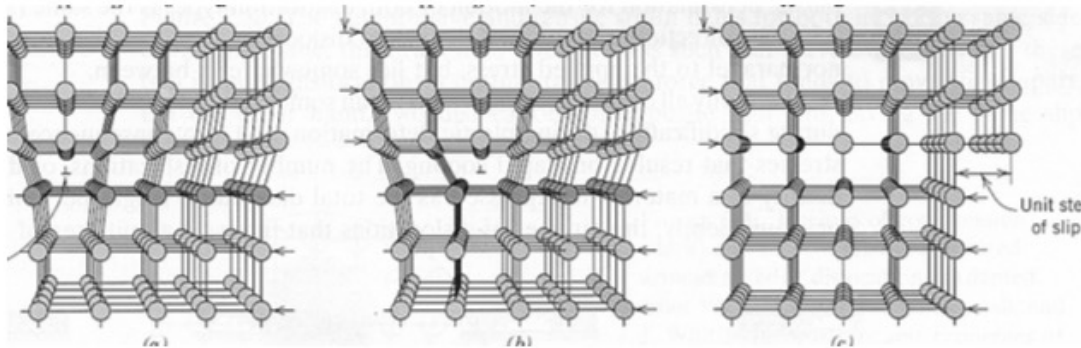
$$\sigma_T = C(\epsilon_T)^n$$

“true” stress (F/A) “true” strain: $\ln(L/L_0)$

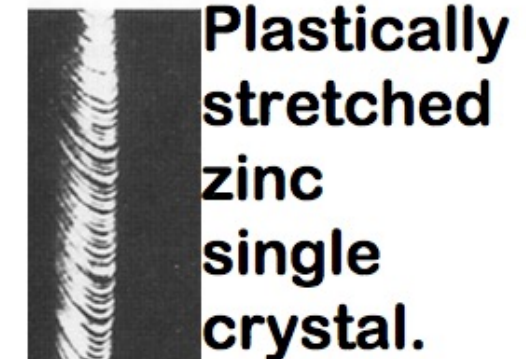
hardening exponent:
 $n=0.15$ (some steels)
 to $n=0.5$ (some copper)

Dislocation motion

- Plastic deformation occurs due to dislocation motion
- A dislocation is a line defect
 - Edge and screw type
- When it moves, only a small number of bonds are broken at a time



Adapted from Fig. 7.1, *Callister 6e*. (Fig. 7.1 is adapted from A.G. Guy, *Essentials of Materials Science*, McGraw-Hill Book Company, New York, 1976. p. 153.)



Adapted from Fig. 7.9, *Callister 6e*. (Fig. 7.9 is from C.F. Elam, *The Distortion of Metal Crystals*, Oxford University Press, London, 1935.)



Adapted from Fig. 7.8, *Callister 6e*.

Dislocation are produced during deformation

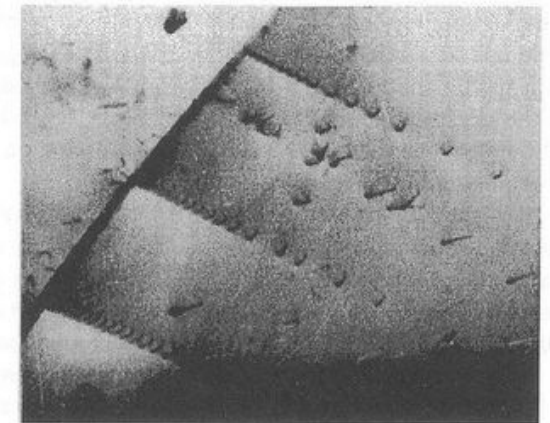
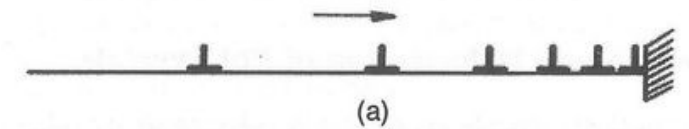
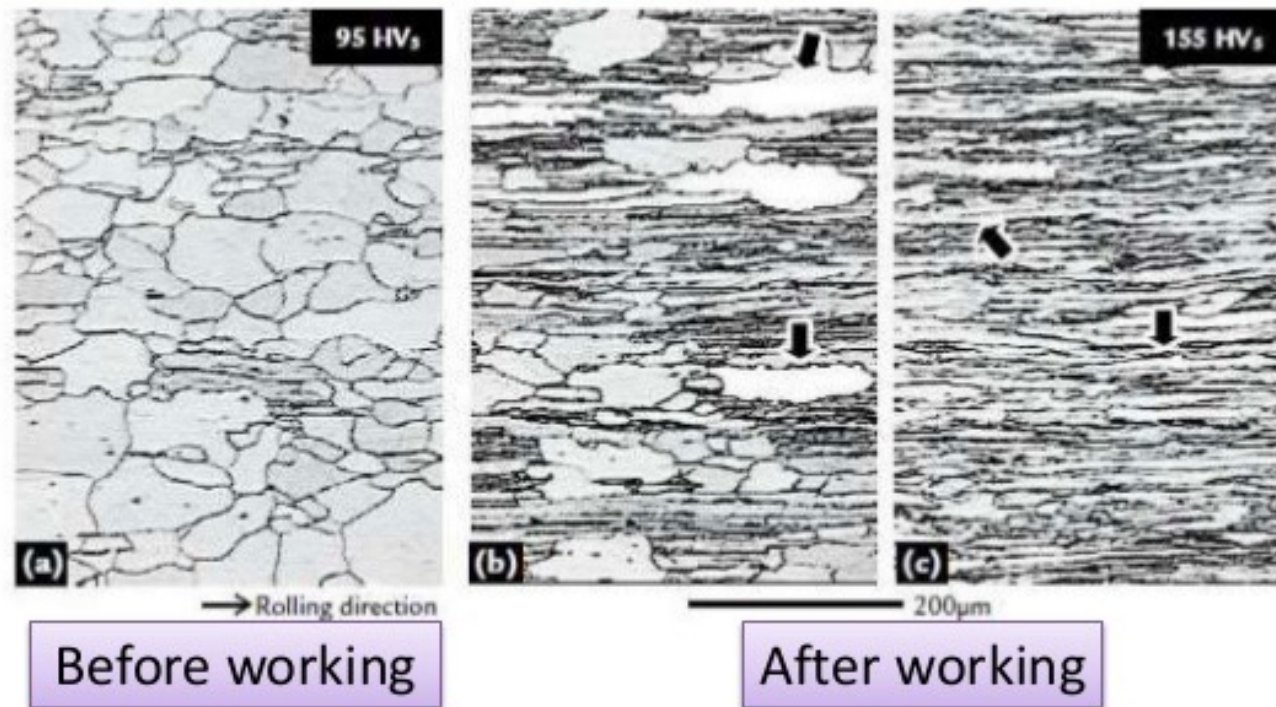


**Dislocation motion causes plastic deformation,
dislocation pileup causes hardening**



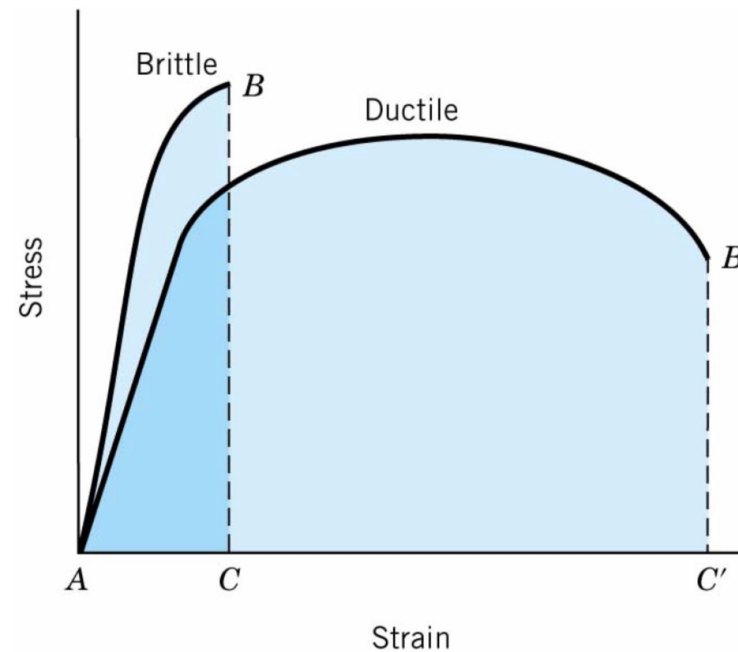
Dislocation Pile Up

- Dislocation motion can be inhibited by barriers, including grain boundaries, precipitates, voids, bubbles, etc.



Ductility

- Ductile materials plastically deform significantly, brittle materials do not
- Quantities defining ductility are total percent elongation at fracture (%EL) and the percent reduction in area (%RA)
- The ductile–brittle transition temperature (DBTT) of a metal is the temperature at which the fracture energy passes below a predetermined value
- Below the DBTT, failure is brittle
- Cold working and neutron irradiation can increase the DBTT, potentially reducing ductility of reactor components



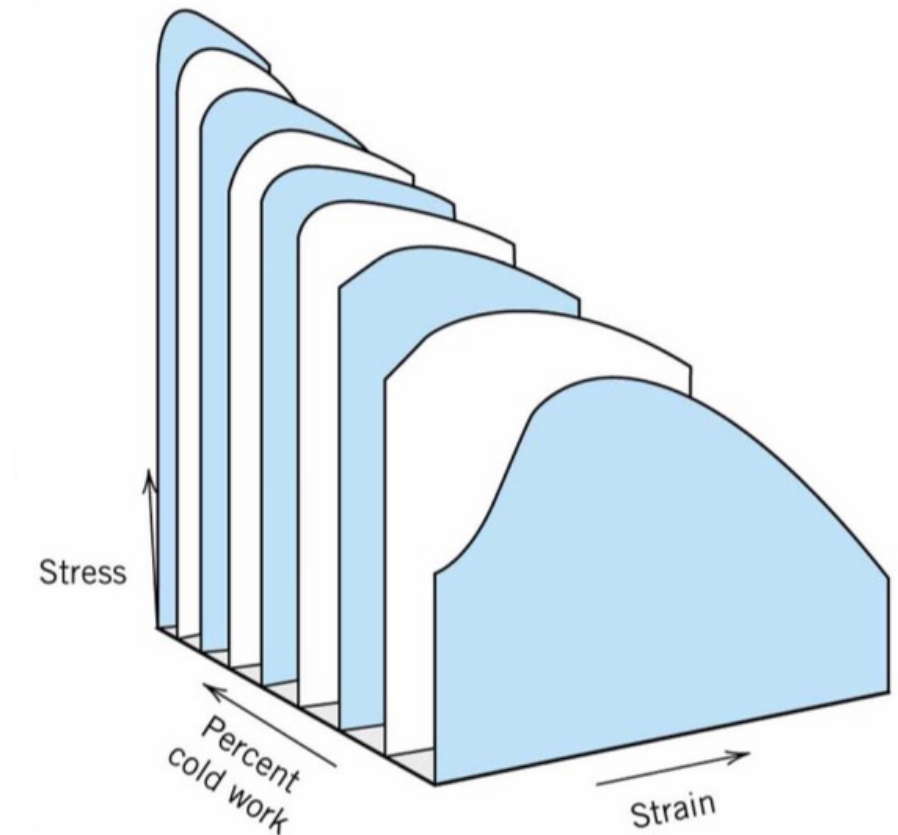
$$\%EL = \frac{(l_f - l_0)}{l_0} \times 100$$

$$\%RA = \frac{(A_0 - A_f)}{A_0} \times 100$$

l_f = length at fracture
 A_f = section area at fracture

As the strength increases due to dislocation pile-up, the ductility decreases

- Toughness is the ability of a material to absorb energy and plastically deform without fracturing
- Toughness is related to the area under the stress–strain curve
- In order to be tough, a material must be both strong and ductile
- Materials are often work hardened prior to utilization to modify mechanical properties



Summary

- Solid mechanics predicts the deformation of a body from its applied load
- The strain defines the deformation
- The stress defines the material's response to the strain
- Materials can have recoverable and permanent deformation
 - Elastic deformation is recoverable and occurs due to the stretching of the atomic lattice
 - Plastic deformation is permanent and results from the breaking of bonds
- Elastic moduli and Elastic constants