Nuclear Fuel Performance

NE-533

Spring 2024

Housekeeping

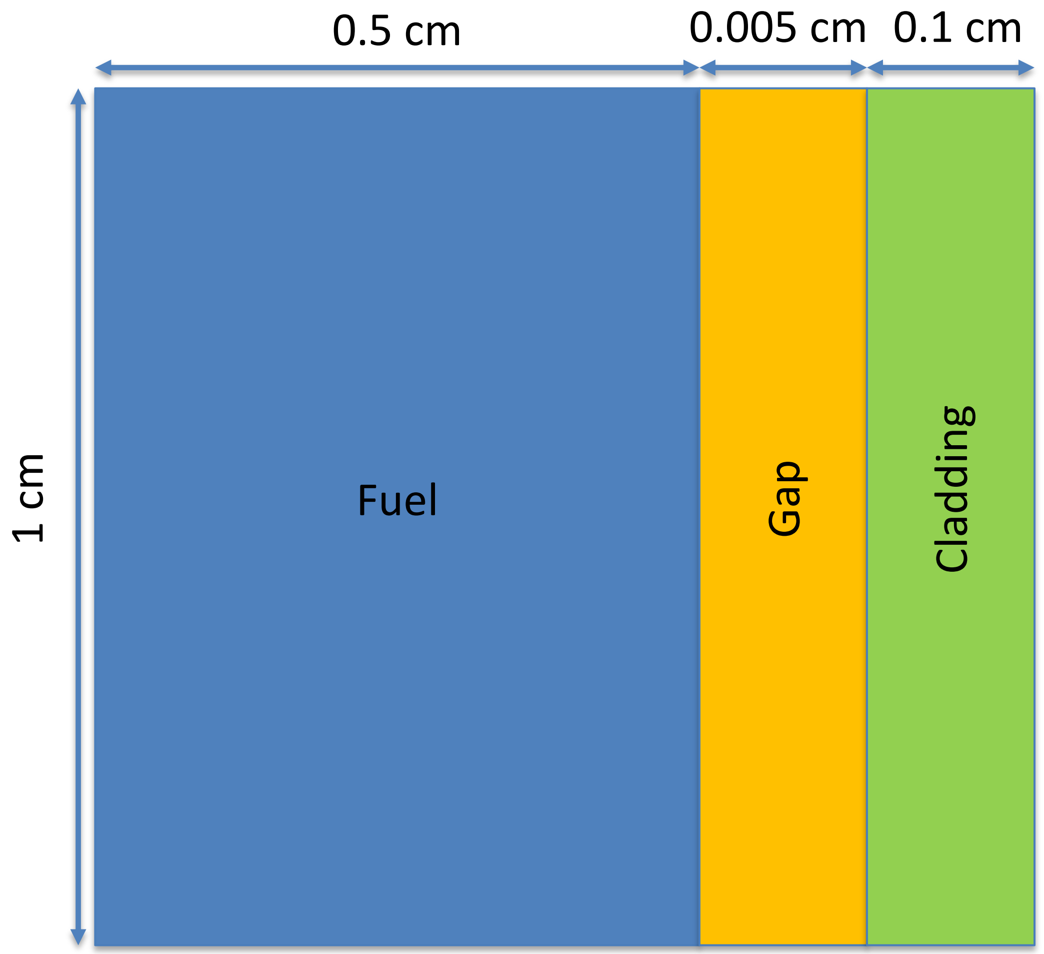
- Questions/comments on MOOSE?
- Exam grades:
  - Average: 84.7, Stdev: 10.4
  - Curve of 5 points applied to your scores
- Any questions/comments on grading, let me know and come to office hours
- Solutions posted on Moodle

MOOSE Project

- Three-part project
- Will upload input and output files to Moodle
- Will upload a final written report, max of 10 pages (including figures), times new roman, 12pt, 1.5 space, pdf
- Due April 23 – last day of classes
- This is an individual project, but some collaboration is encouraged

MOOSE Project Part 1

- Fuel pellet dimensions listed
- This is a 1-D problem, but I want your geometry to be set up in 2-D RZ
- Assume reasonable values for material properties
- Outer cladding temperature: 550 K
- Solve temperature profile for:
  - Steady-state: LHR = 350 W/cm^2
  - Compare against analytical solution
- Solve for centerline temperature vs time
  - Transient: LHR = 250*EXP(-((t-20)^2)/10)+150
  - for up to t=100
- Use both a constant k and a temperature-dependent k



Part 1 Writeup

- Will upload input and output files to Moodle
- Write up with deliverables from Part 1, choice of materials, mesh, details therein, etc.
- Part 1 writeup max of 5 pages

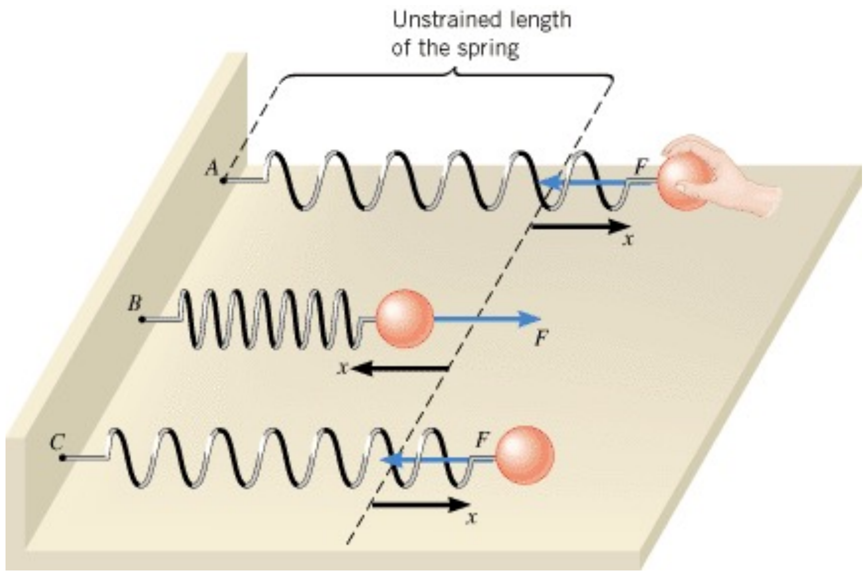
MECHANICS

Solid mechanics

- When a load is applied to a body, it changes shape and perhaps size
- Motions throughout a body are called **displacements**
  – $\mathbf{u}(\mathbf{r}, t)$
- Rigid body displacements do not change the shape and/or size
  – the rigid body is translated
- Changes in shape and/or size are call **deformations**
- The objective of **Solid Mechanics** is to relate loads (applied force) to deformation

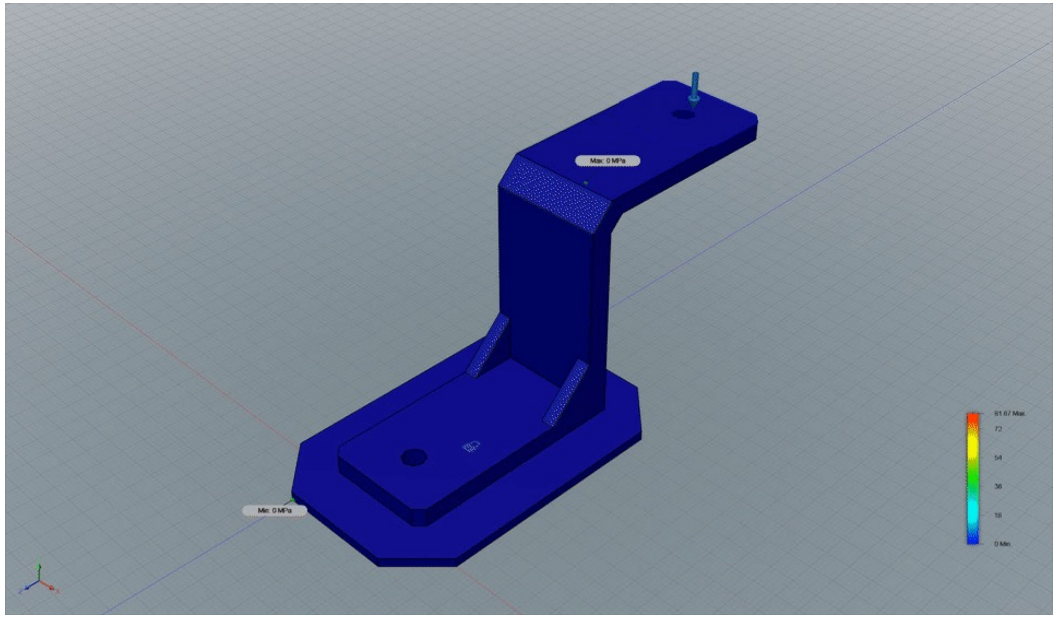
Ideal springs

- It can be instructive to view solids as a spring
- When we apply some force F, we get some displacement x
  - $F = k\,x$
- When the spring is displaced by x, there is force that responds in the opposite direction equal to kx
- Due to the displacement, there is a stored energy $E = \frac{1}{2}\,k\,x^2$



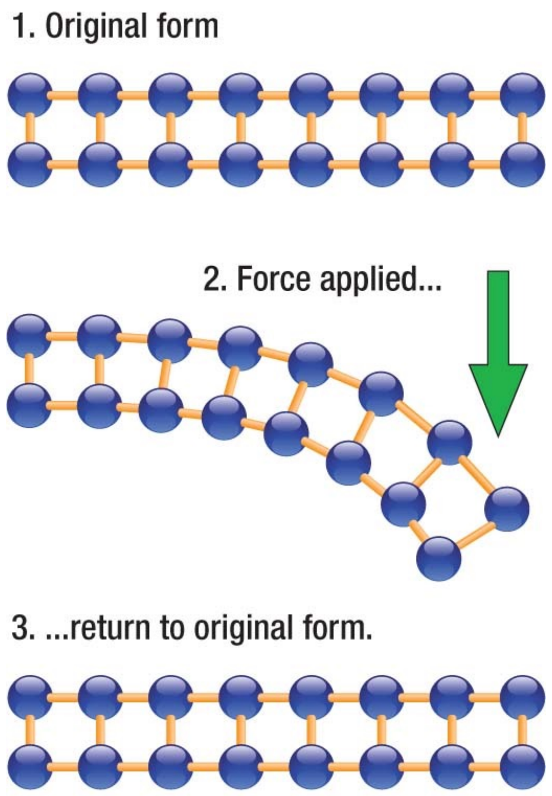
Observed deformation due to a force

- Solid mechanics is similar to the behavior of an ideal spring but throughout a body
- An applied load results results in deformation.
- The internal **strain** is like the displacements x
- The internal **stress** is like the internal force F



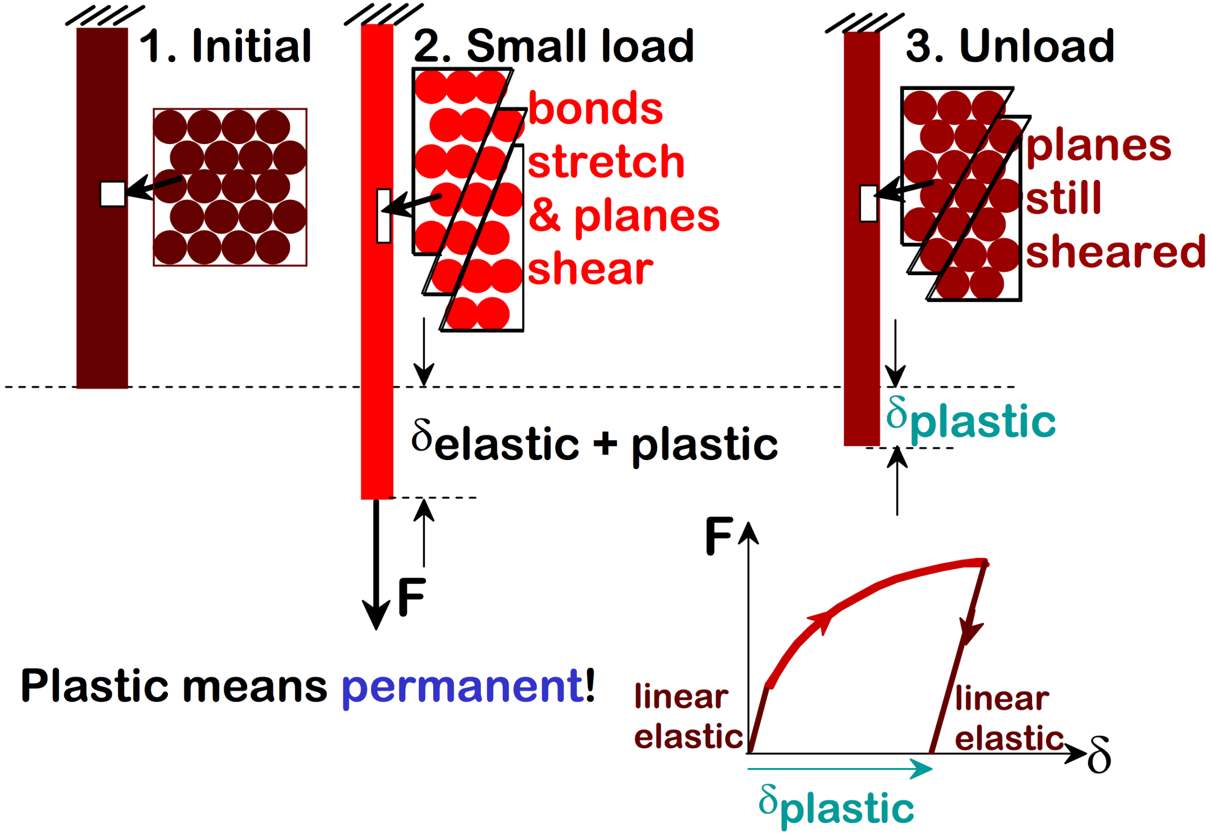
Elasticity

- 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



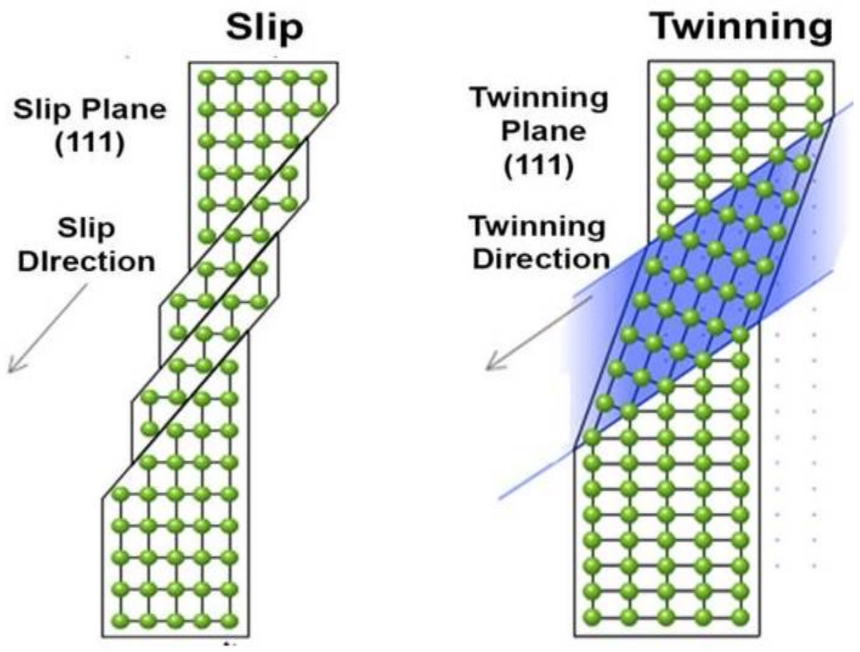
Plasticity

- 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

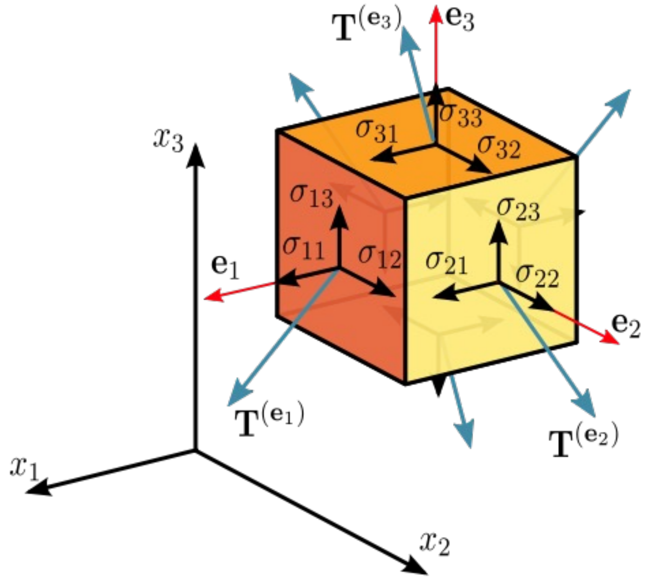
- Plasticity is typically caused by two modes of deformation in the crystal lattice: slip and twinning
  - Slip is a shear deformation which moves the atoms through many interatomic distances relative to their initial positions
  - Twinning is the plastic deformation which takes place along two planes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



Slip and Twinning

Stress

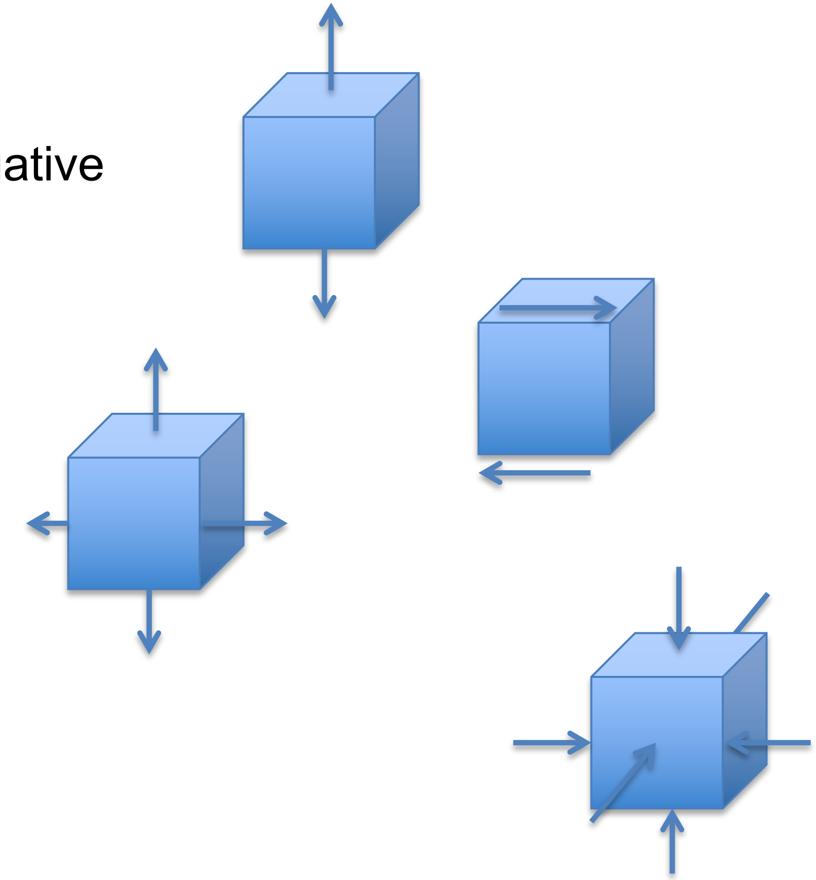
- Stress is a physical quantity that expresses the internal forces that neighboring particles of a continuous material exert on each other
- Stress is a force per unit area with SI units of Pa = N/m^2
- The stress is a 2nd order tensor (a 3 by 3 matrix): Cauchy stress tensor
- $\boldsymbol{\sigma}_{\mathbf{ij}} = \boldsymbol{F}_{\mathbf{ij}}/\boldsymbol{A}_{\mathbf{i}}$
  - 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



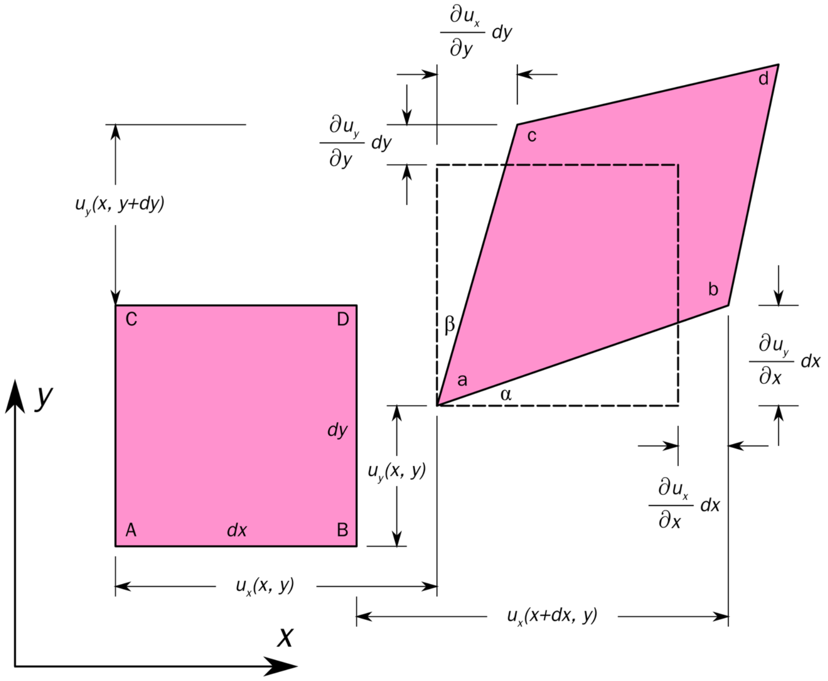
$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \equiv \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx}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

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

- Images shows strain as a second order tensor
  - Let **u** be a vector of the displacements
  - The small strain tensor is

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

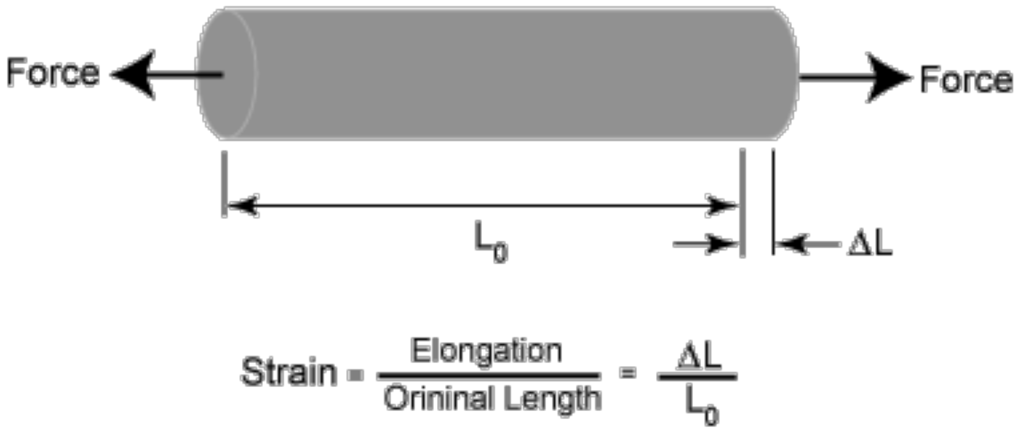
$$\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{1}{2}(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial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

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

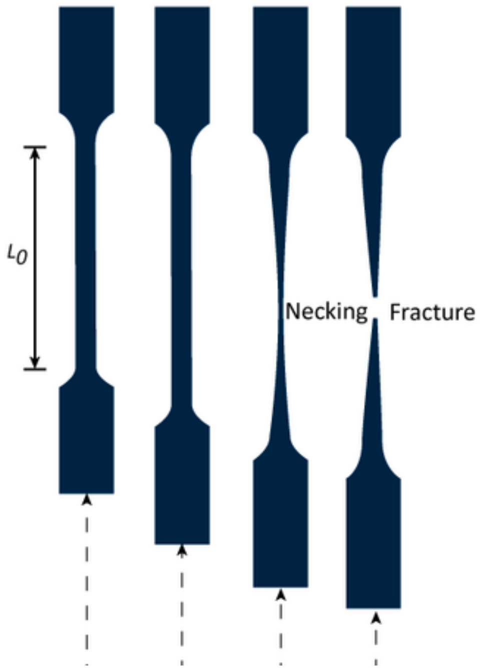
Strain produces stress

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

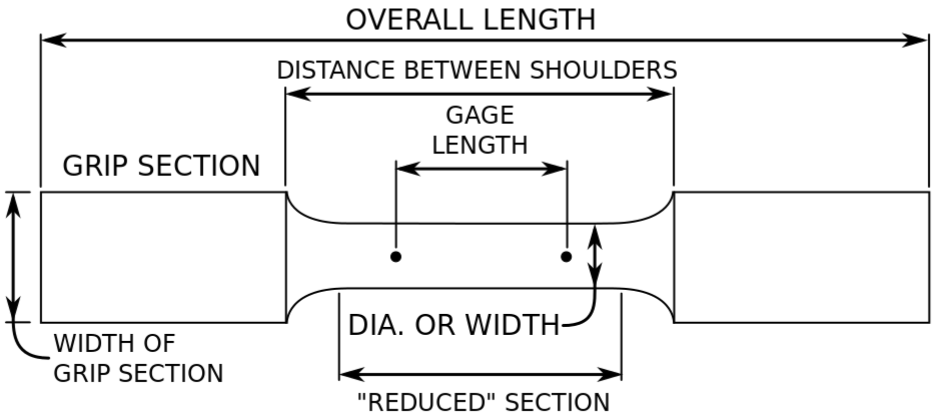
    $\boldsymbol{\sigma} = \mathcal{C}\boldsymbol{\epsilon}_e$
- The elastic energy density in a material is a scalar quantity equal to $E_{el} = \frac{1}{2}\boldsymbol{\epsilon}_e \cdot \boldsymbol{\sigma}$



Tensile testing



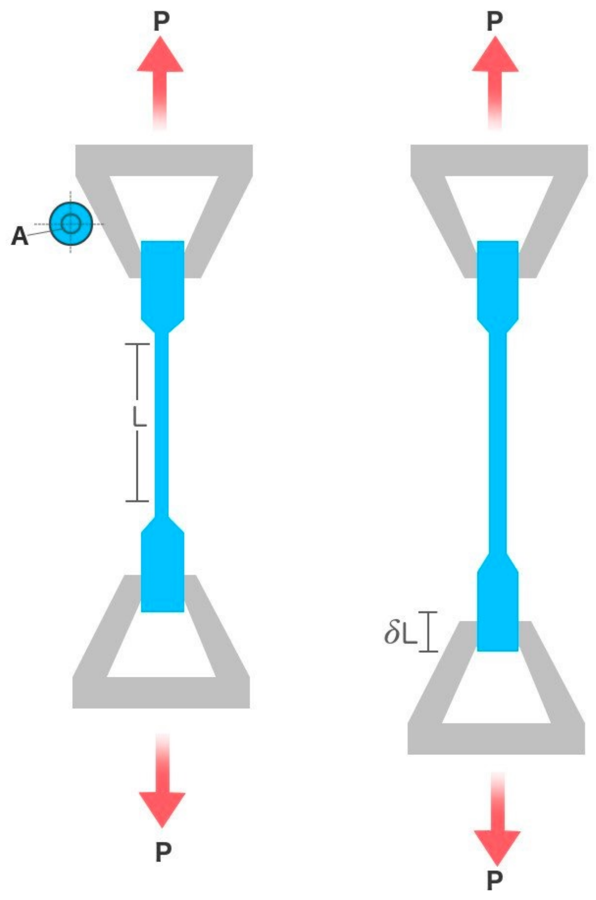
- The most common means of determining mechanical properties is a uniaxial tension test
- Apply a uniaxial load until failure
- Properties that are directly measured via a tensile test include ultimate tensile strength, maximum elongation, etc., which can be utilized to determine Young's modulus, Poisson's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



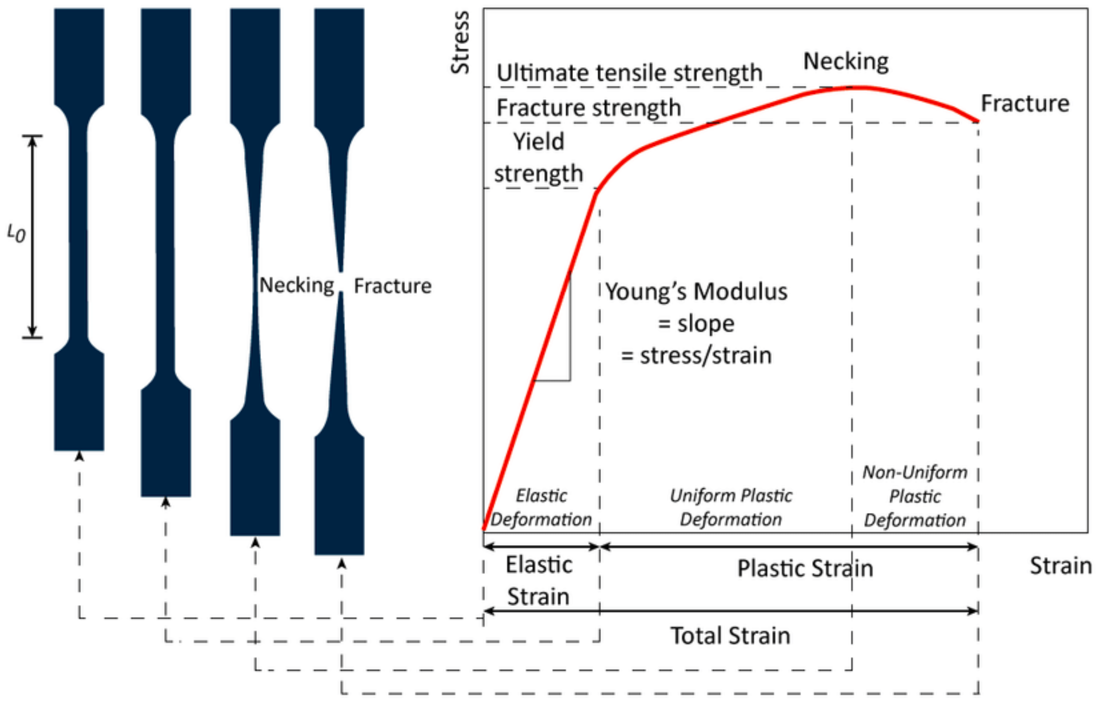
Stress/strain from a tensile test

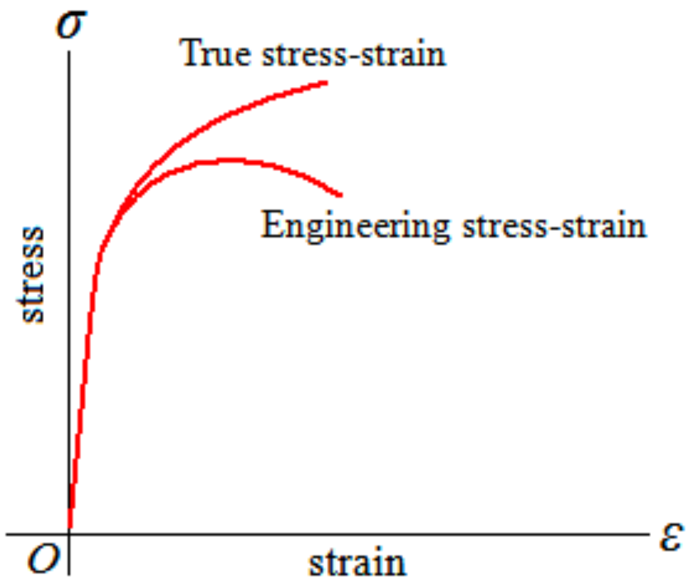
- A_0 = Initial cross section area
- A = deformed cross section area
- P or F applied load/force

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



Stress vs strain curves





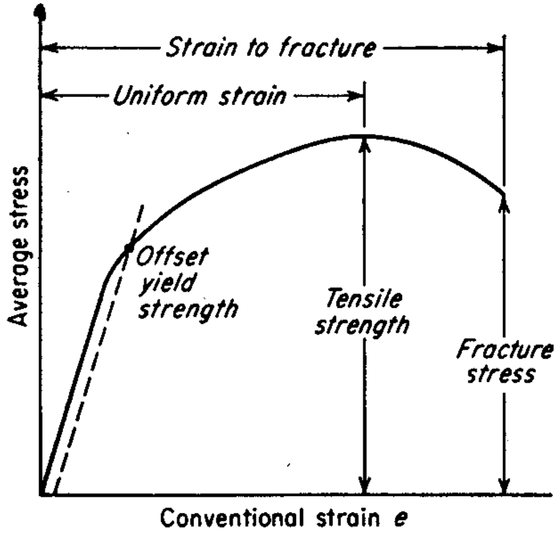
Using stress/strain curves

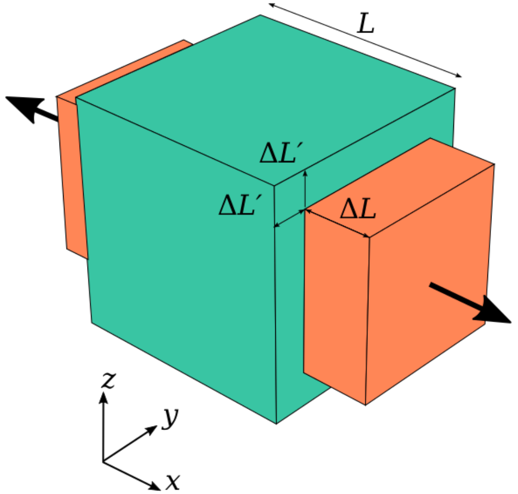
- In the elastic portion of the stress-strain curve, the stress varies linearly with strain
- The slope of the line is Young's Modulus, E: $\sigma = E\,\varepsilon$
- Poisson's ratio, ν, is the ratio of the shrinkage in cross section due to the extension in the pulling direction

$$\nu = -\frac{d\varepsilon_{\mathrm{trans}}}{d\varepsilon_{\mathrm{axial}}} = -\frac{d\varepsilon_{\mathrm{y}}}{d\varepsilon_{\mathrm{x}}} = -\frac{d\varepsilon_{\mathrm{z}}}{d\varepsilon_{\mathrm{x}}} \qquad \nu \approx \frac{\Delta L'}{\Delta L}.$$

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

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





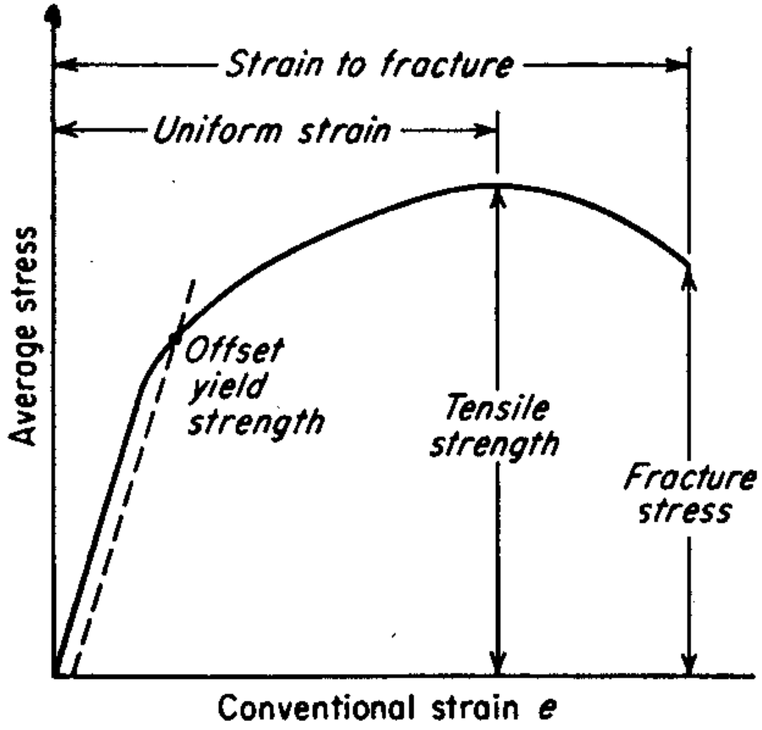
Using stress/strain curves

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

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

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

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



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

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

Isotropic and Anisotropic

- Being a linear mapping between the nine numbers σ_{ij} and the nine numbers ε_{kl}, the stiffness tensor **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

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

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

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

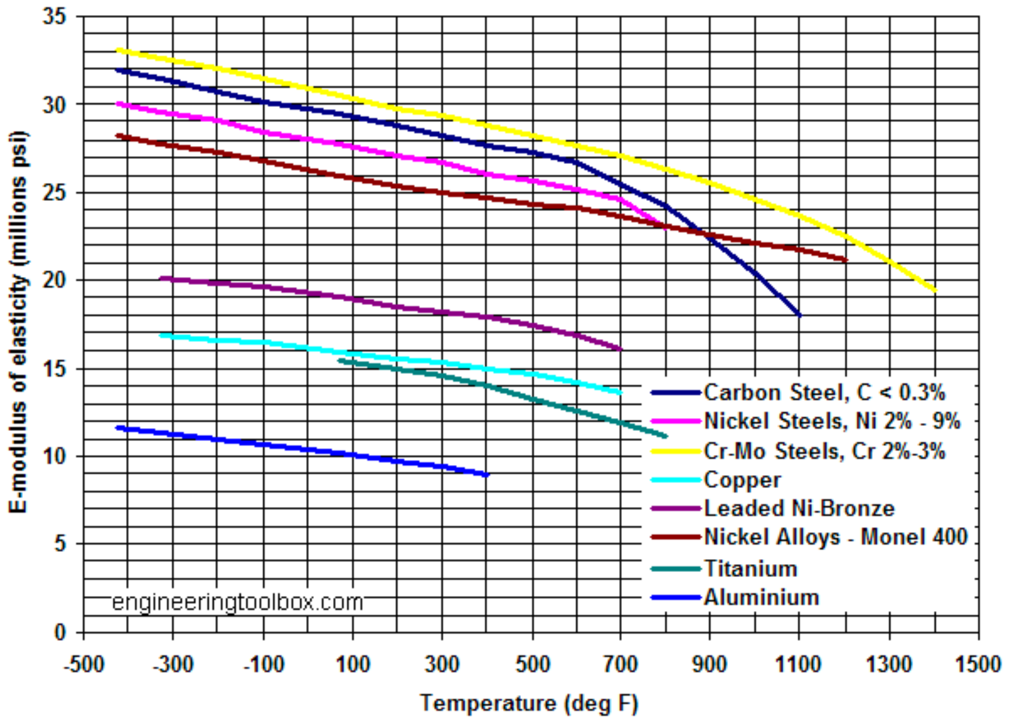
$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix}$$

Isotropic elastic properties for some materials

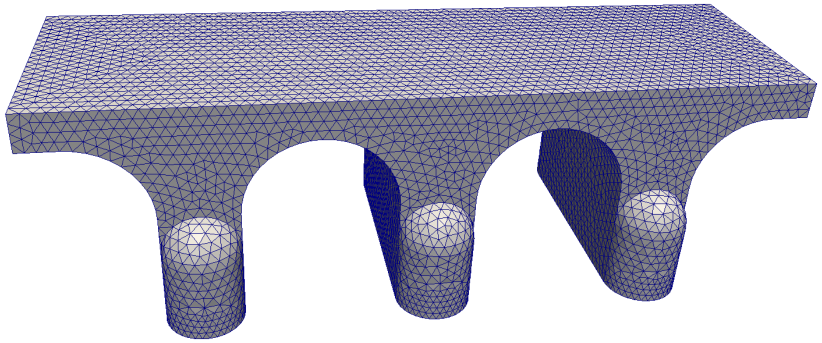
Material	E (GPa)	ν
Aluminum	70.3	0.345
Gold	78.0	0.44
Iron	211.4	0.293
Nickel	199.5	0.312
Tungsten	411.0	0.28
Zircaloy	80.0	0.41
UO_2	200.0	0.345

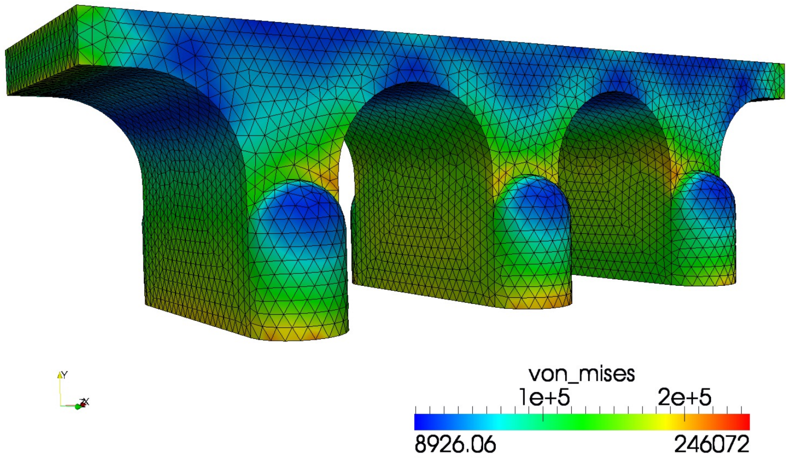
Elastic constants are not "constant"

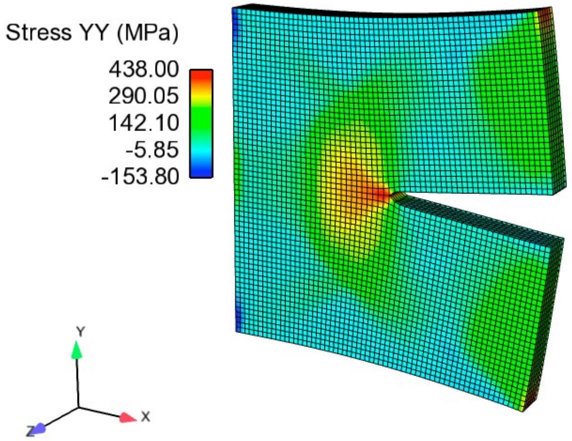
- Properties change with temperature
- Softening can be referred to as the decrease in elastic constants with temperature
- Young's modulus is typically a function of temperature, decreasing with increasing temperature
- Shear Modulus and Poisson's ratio can also change with T

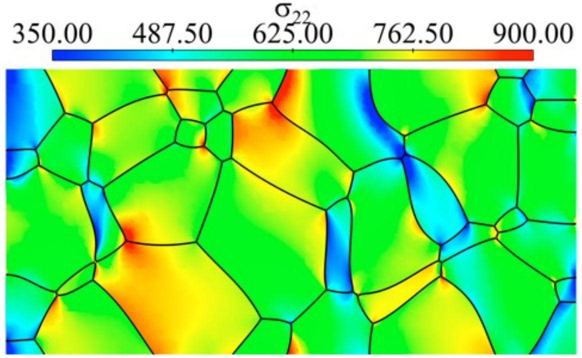


In actual materials, the stress and the strain change throughout the material





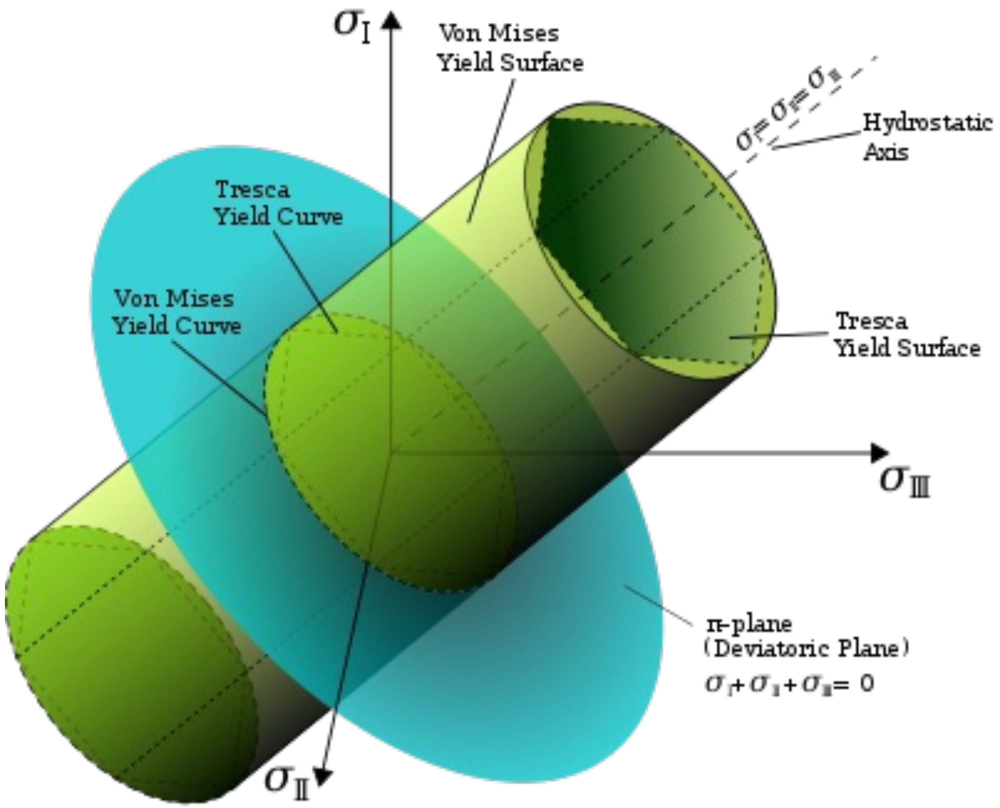




von Mises yield criterion

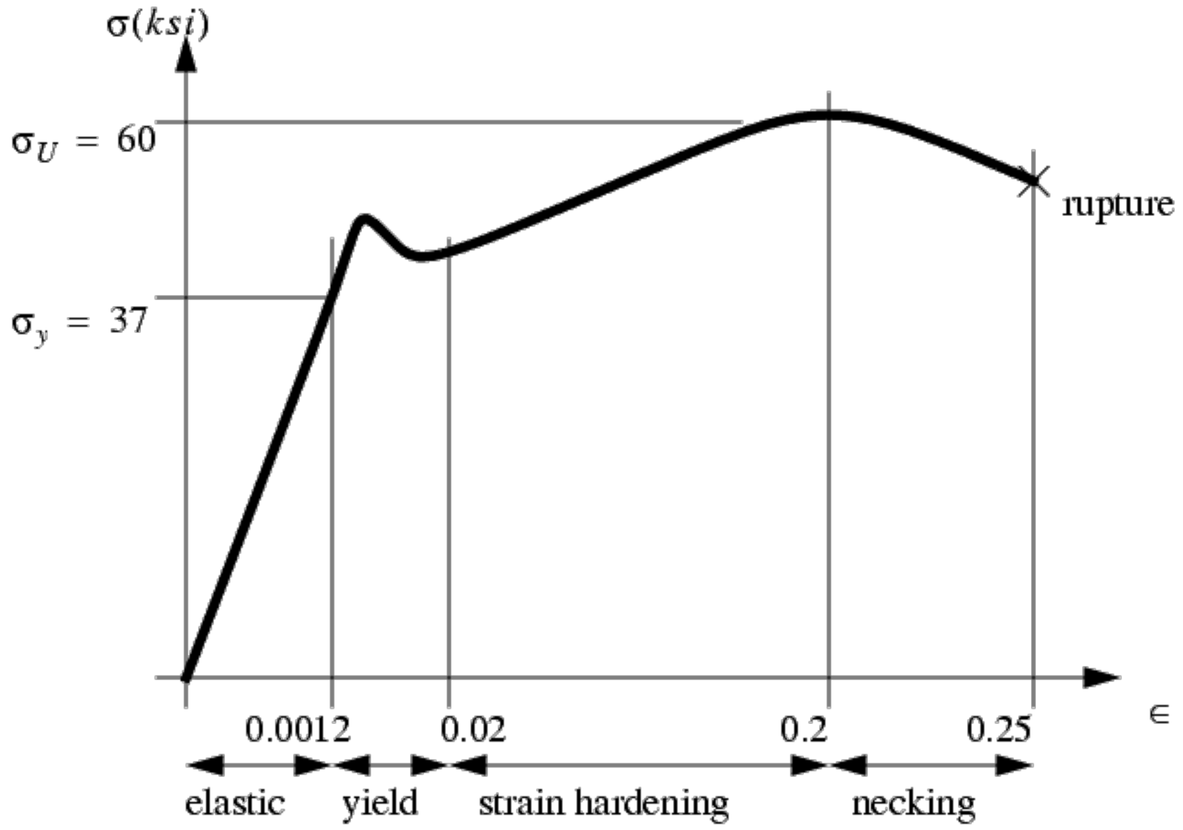
- The maximum distortion criterion (also von Mises yield criterion) states that yielding of a ductile material begins when the second invariant of deviatoric stress (J2) reaches a critical value
- A material is said to start yielding when the von Mises stress reaches the yield strength
- The von Mises 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

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



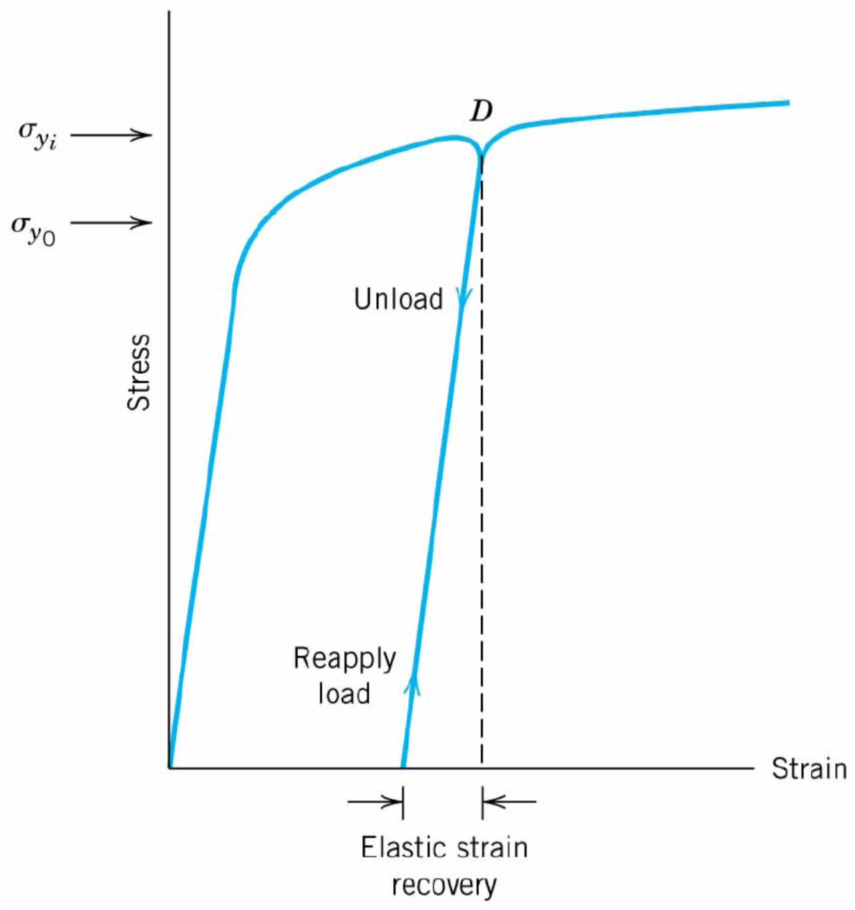
Stress/Strain Regions

- 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

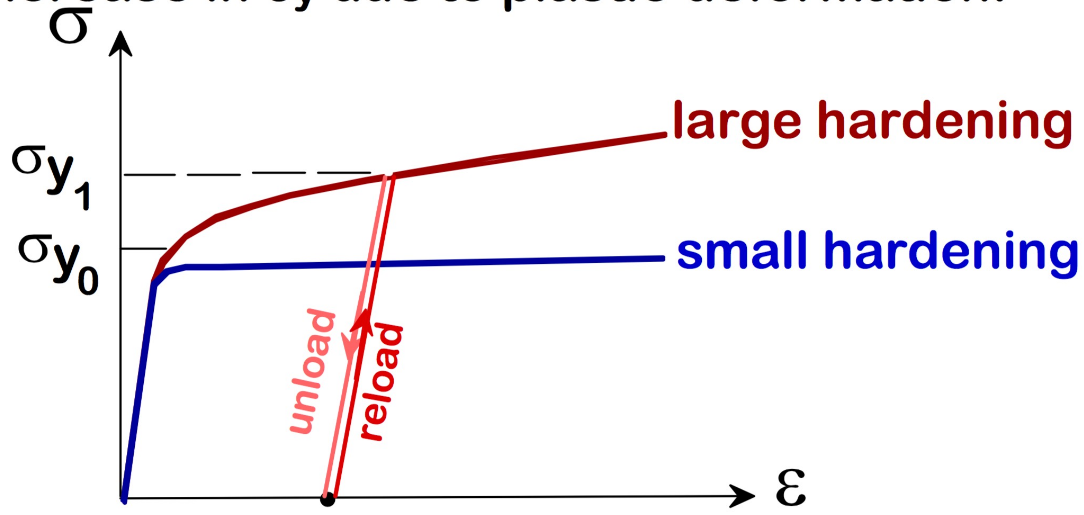


The hardening behavior changes for different materials

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

- 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:**

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

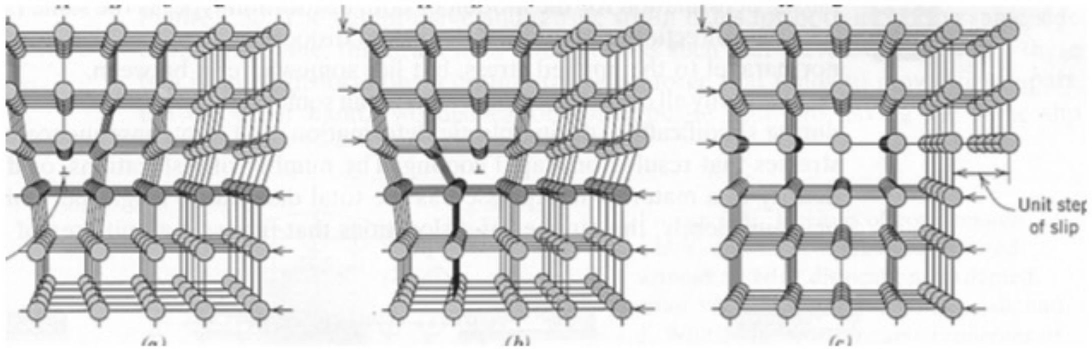
hardening exponent:
n=0.15 (some steels)
to n=0.5 (some copper)

"true" stress (F/A)

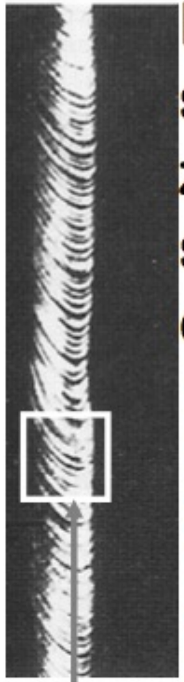
"true" strain: $\ln(L/L_o)$

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

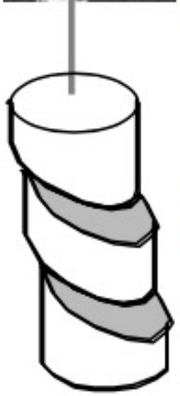


Adapted from Fig. 7.1, *Callister 6e.* (Fig. 7.1 is adapted from A.G. Guy, *Essentials of Materials Science*, McGraw-Hill Book Company, New York, 1976. p. 153.)



Plastically stretched zinc single crystal.

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 and move during deformation

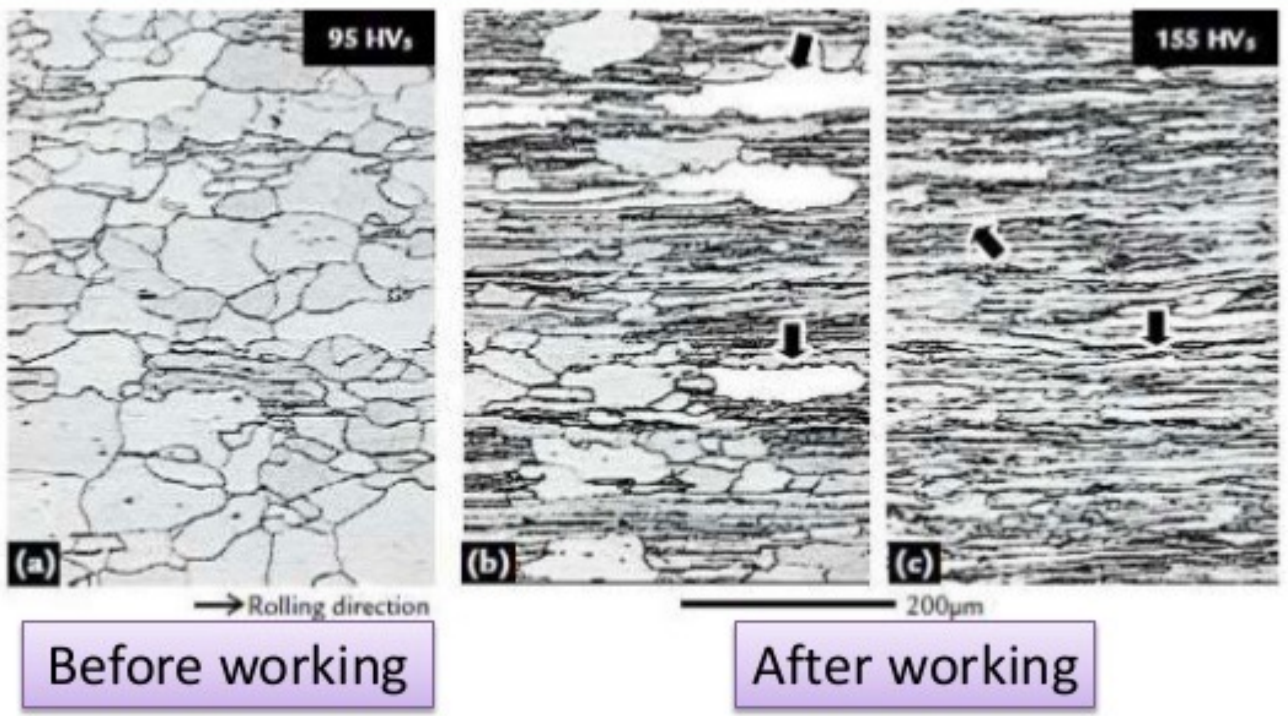
https://www.youtube.com/watch?v=EXbiEopDJ_g

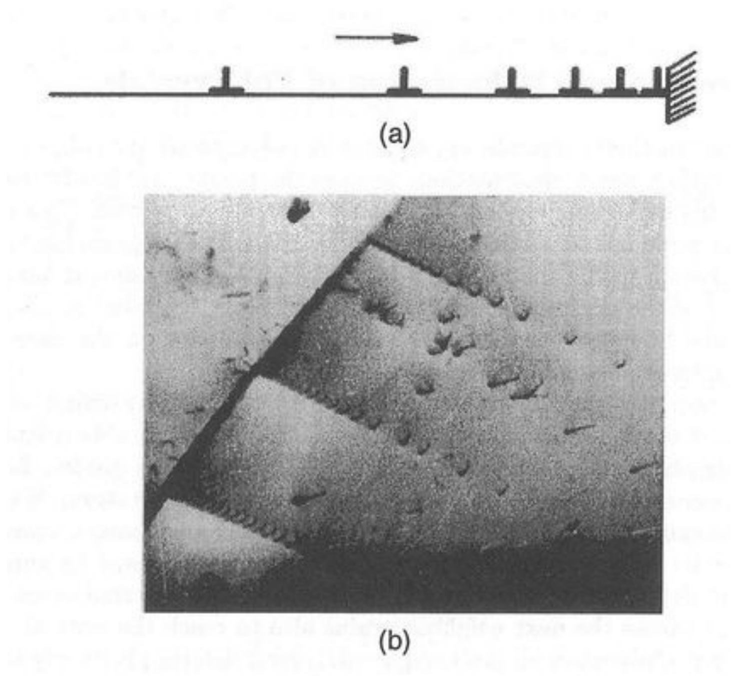
Dislocation motion causes plastic deformation, dislocation pileup causes hardening

https://www.youtube.com/watch?v=JjWdEj_LjZo

Dislocation Pile Up

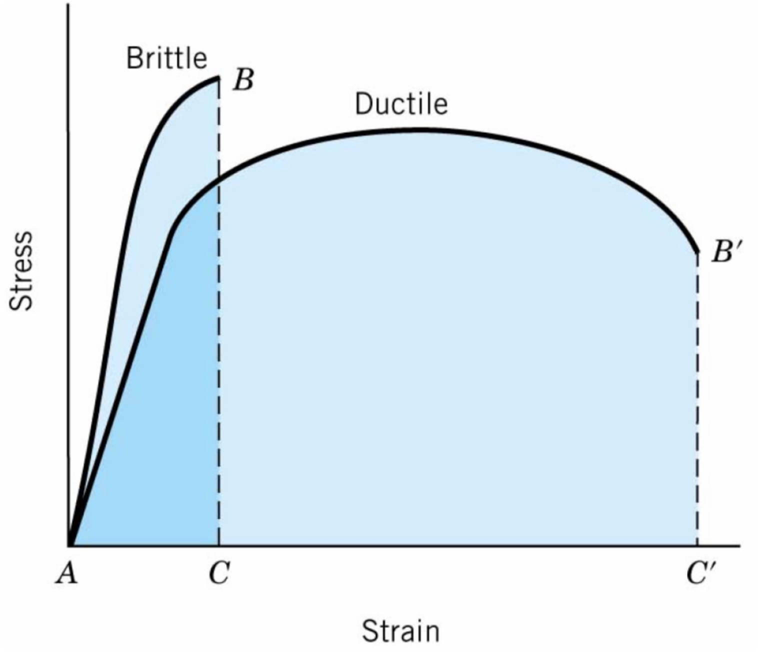
- Dislocation motion can be inhibited by barriers, including grain boundaries, precipitates, voids, bubbles, etc.





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



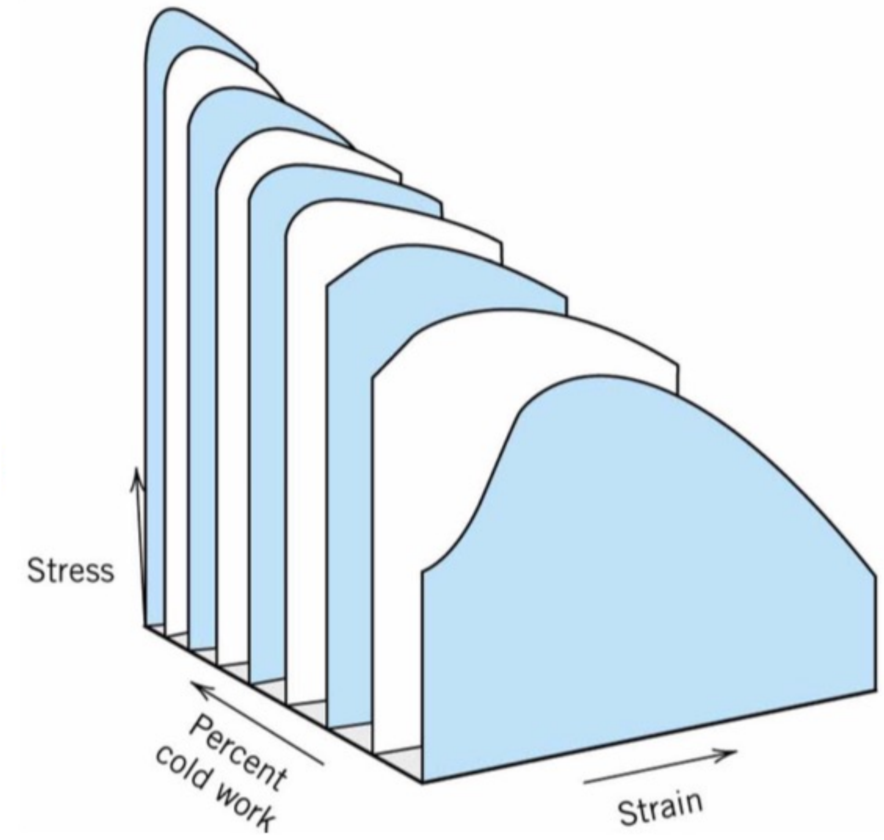
$$\%EL = \frac{(l_f - l_0)}{l_0} \times 100$$

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

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 form the breaking of bonds
- Elastic moduli and Elastic constants