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A Brief Introduction to Mechanical Responses of Materials

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My Thread This Week

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Mon
Intro to Mechanics of Materials

Tues
Intro to Molecular Dynamics

Wed
Plasticity in Amorphous Materials

Thurs
STZ Constitutive Theory

Mechanics of Materials

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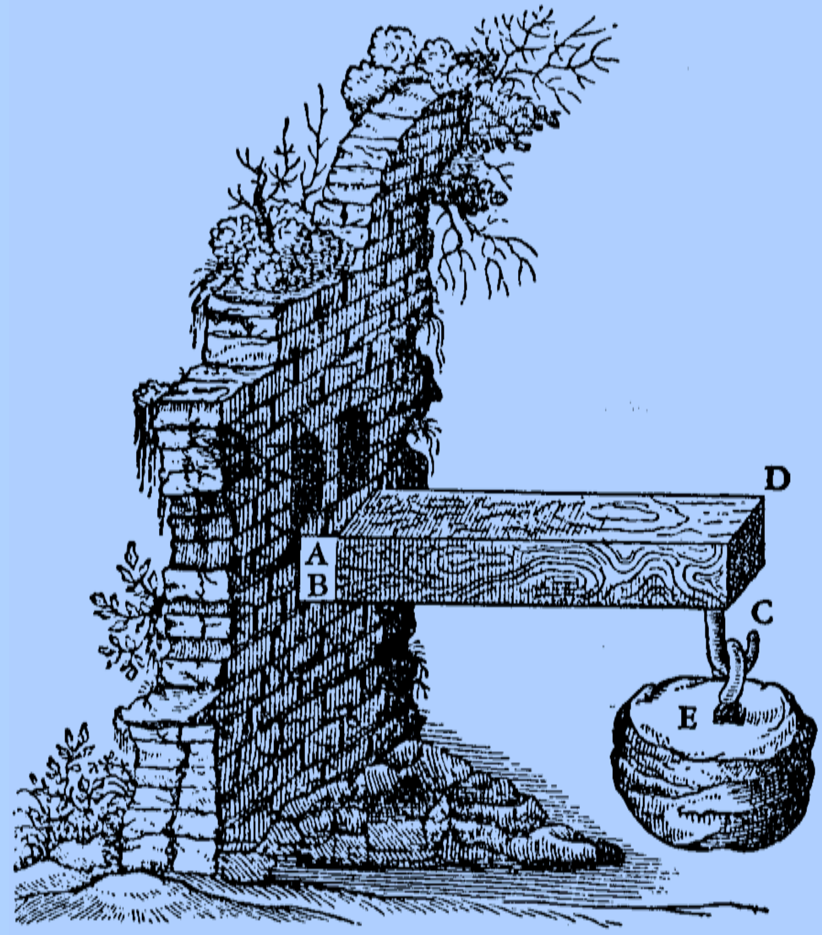
Yet I shall say it and will affirm that, even if the imperfections did not exist and matter were absolutely perfect, unalterable, and free from all accidental variations, still the mere fact that it is matter makes the larger machine, built of the same material and in the same proportion as the smaller, corresponding with exactness to the smaller in every respect except that it will not be so strong or so resistant against violent treatment; the larger the machine the greater the weakness.

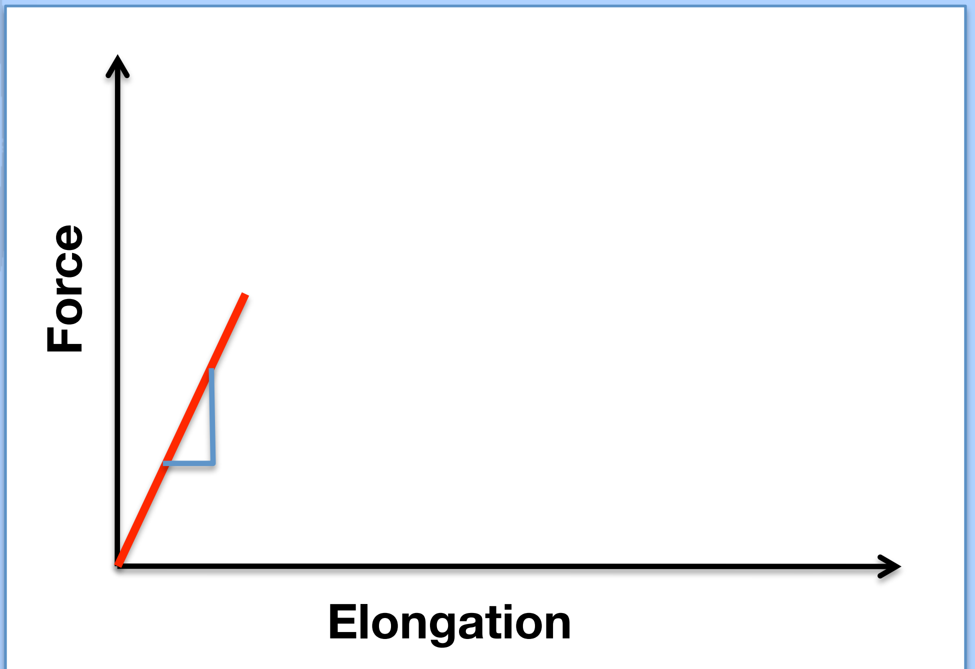
Galileo Galilei,

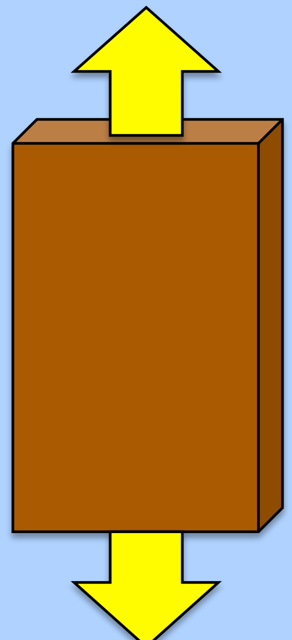
Dialogues Concerning the Two New Sciences, 1638



Typical Mechanical Behavior

- **What quantities can we measure that give measures of a material's response?**
  - Elastic modulus – stiffness





Typical Mechanical Behavior

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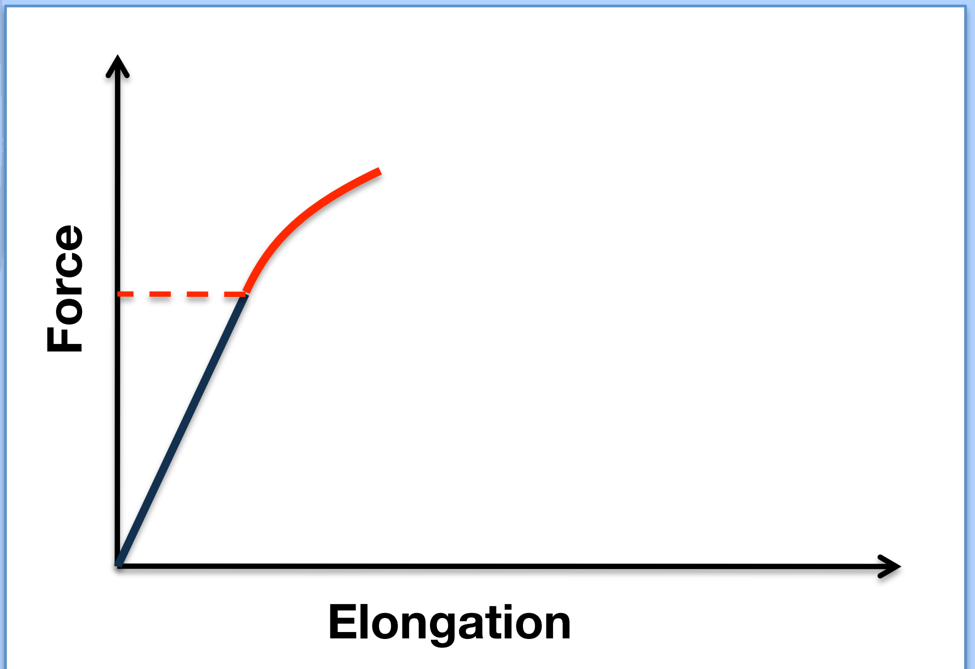
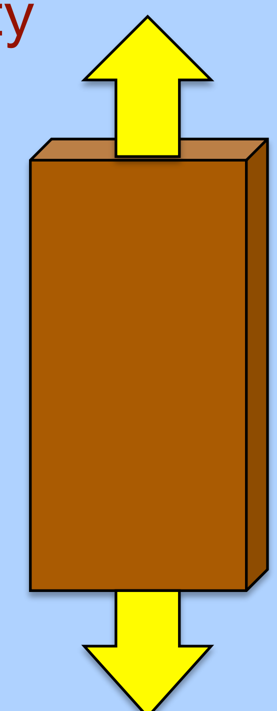
- What quantities can we measure that give measures of a material's response?
  - Yield Stress – Onset of Irreversibility





Typical Mechanical Behavior

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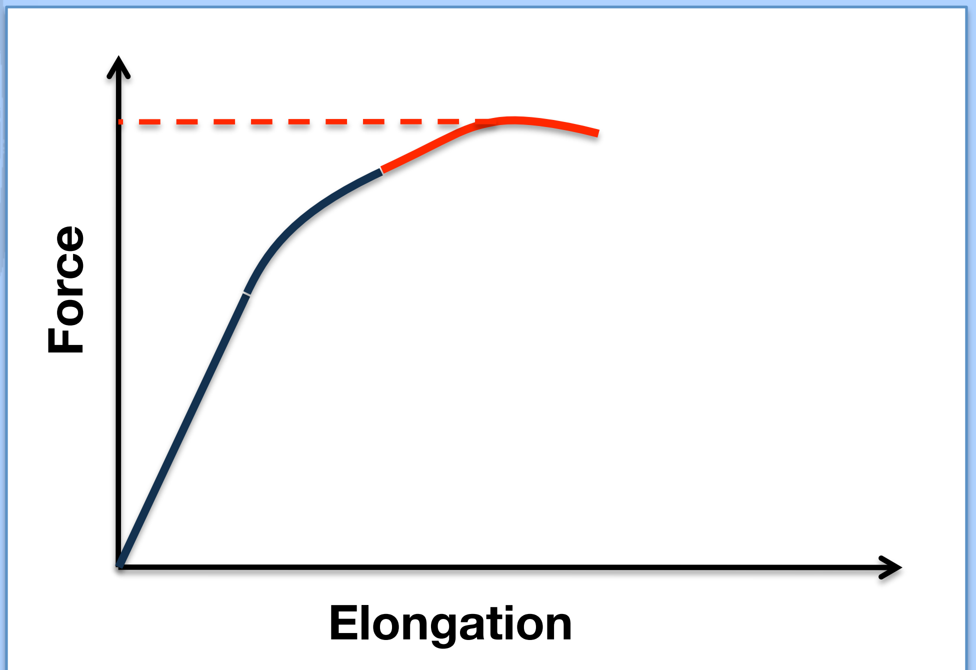
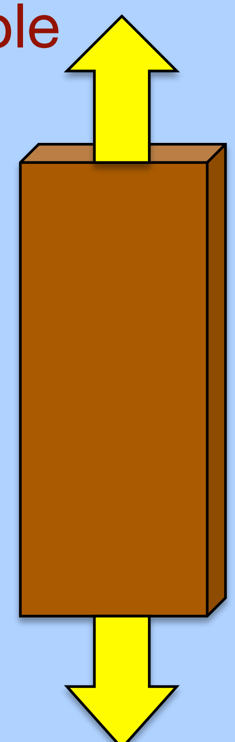
- **What quantities can we measure that give measures of a material's response?**
  - Strength – Maximum stress attainable





Typical Mechanical Behavior

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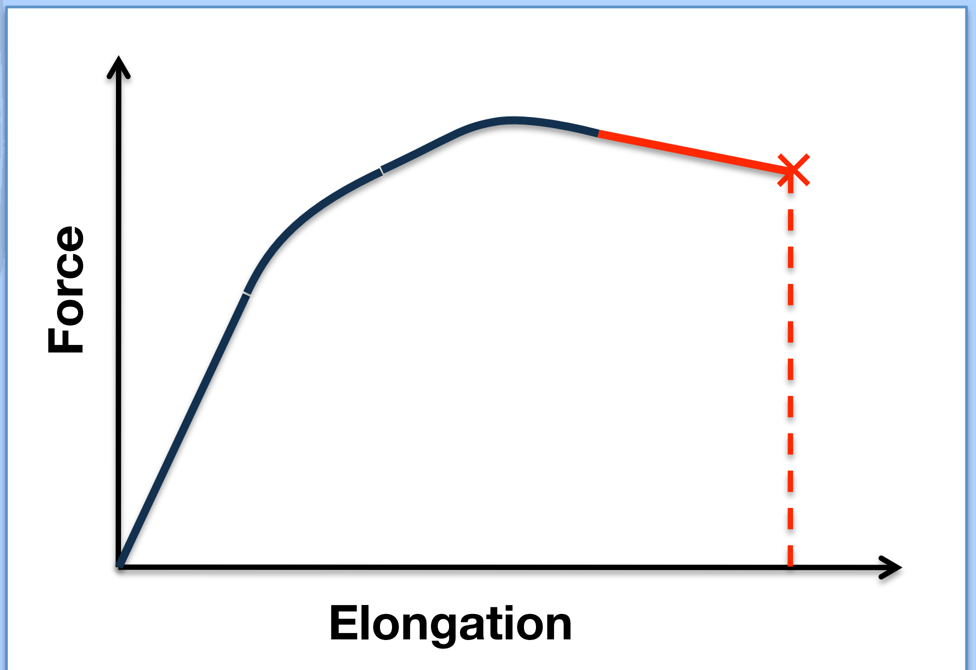
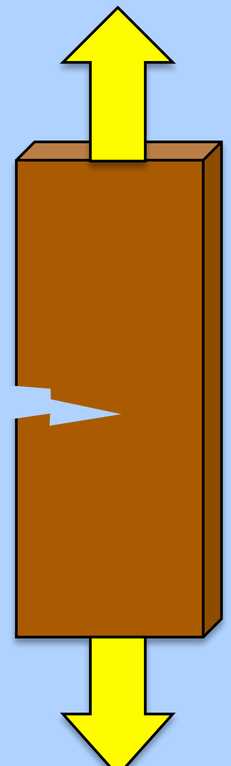
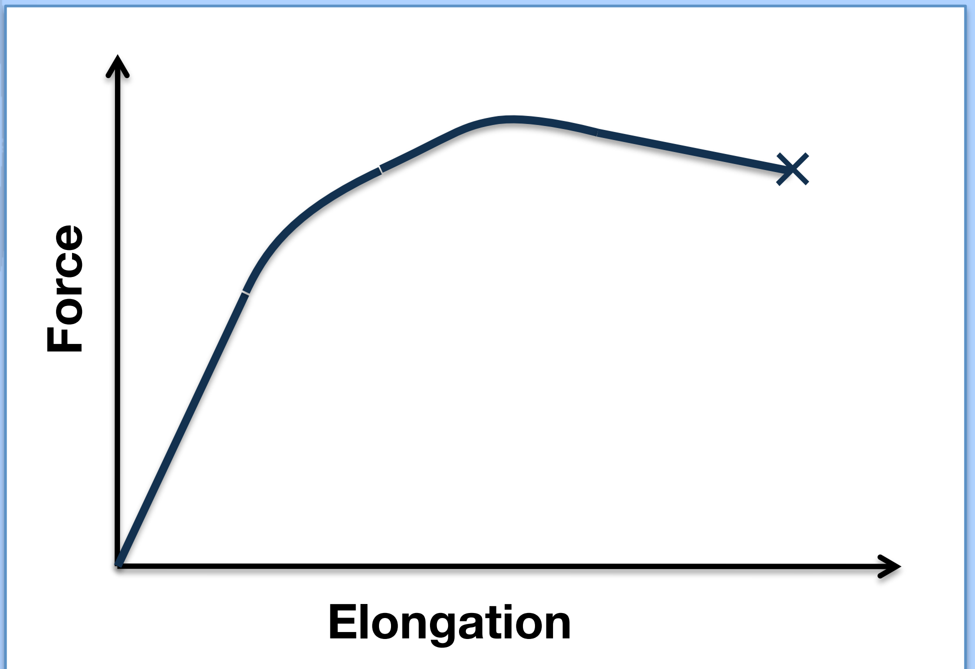
- **What quantities can we measure that give measures of a material's response?**
  - Ductility – Strain to failure

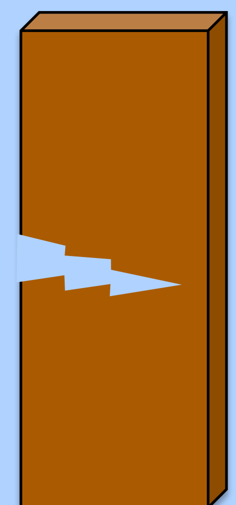




Typical Mechanical Behavior

- **What quantities can we measure that give measures of a material's response?**
  - Toughness – Energy expended per unit crack advance





Characterizing Materials

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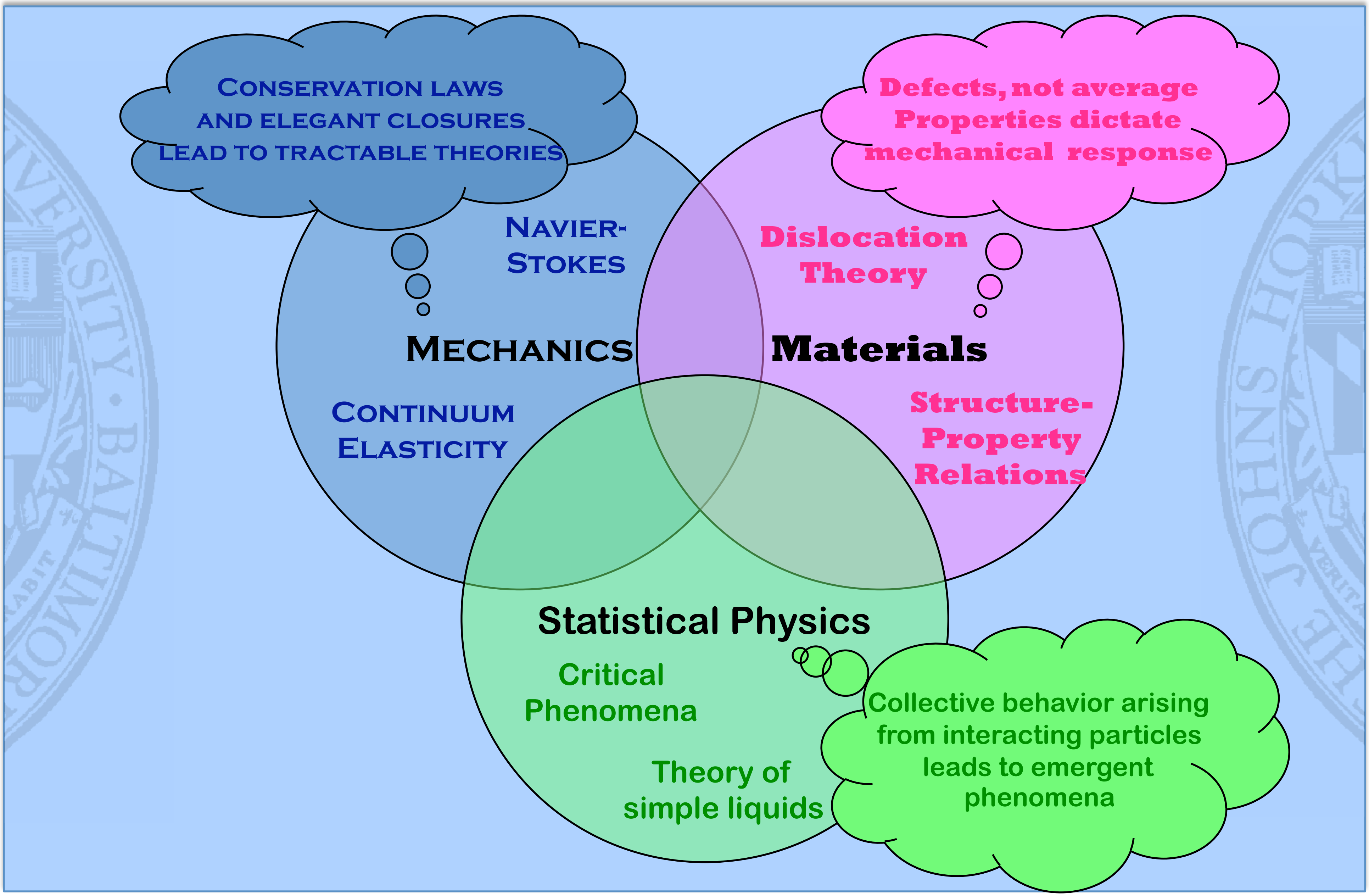
- **Different loadings can produce different values.**
- **What quantities can we measure that give invariant measures of a material's response?**
  - How do we define and quantify these?
  - What are the origins of these properties?
  - Can we predict these from first principles?
  - Fundamentally, how do we express material response?

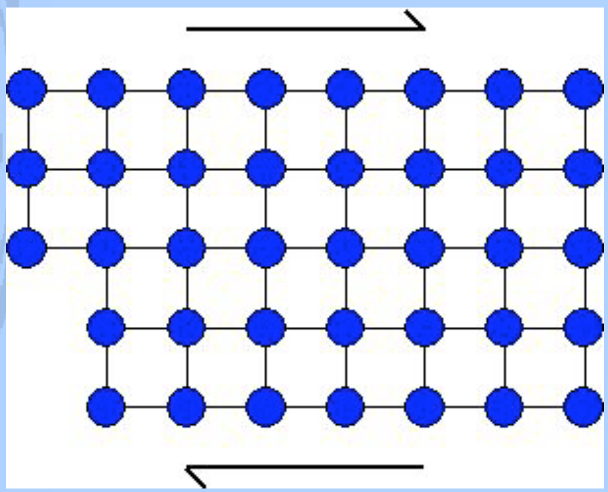
Schools of Thought

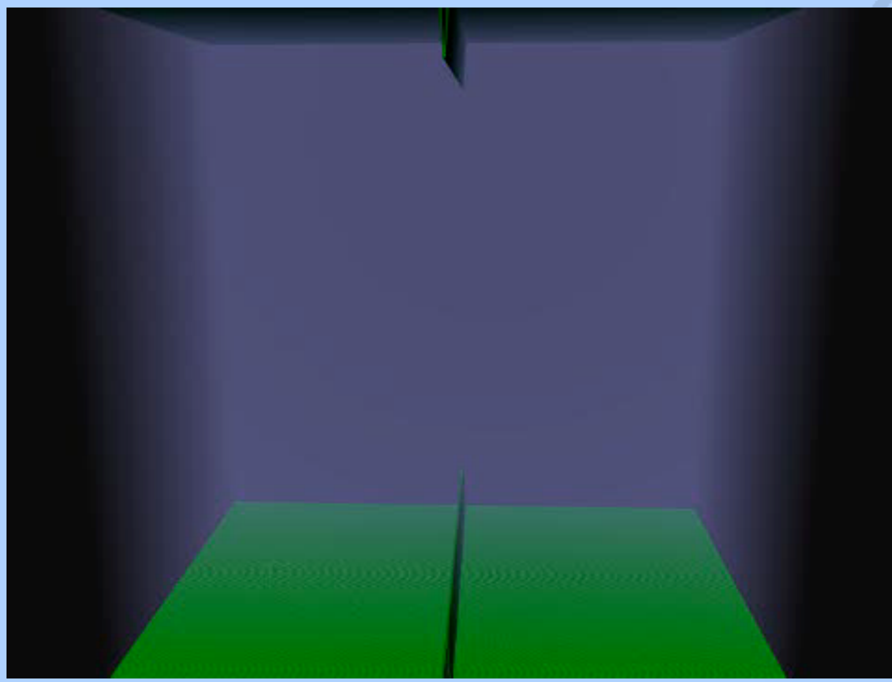


Challenge for Physicists

- How do we connect **macro-scale theory** to **micro-scale physics?**

Crystals



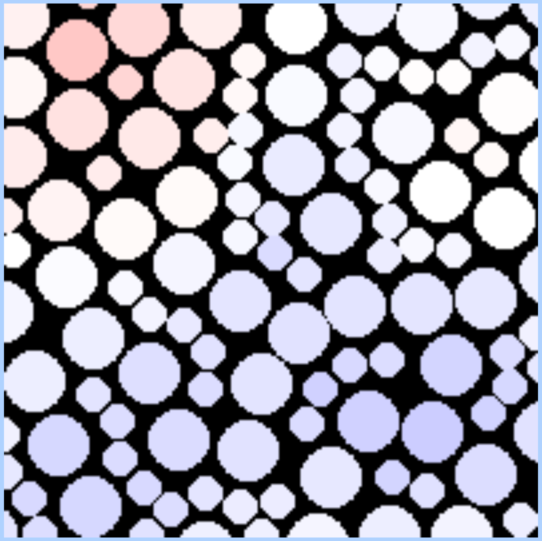


Farid Abraham (IBM), Mark Duchaineau and Tomas Diaz De La Rubia (LLNL)

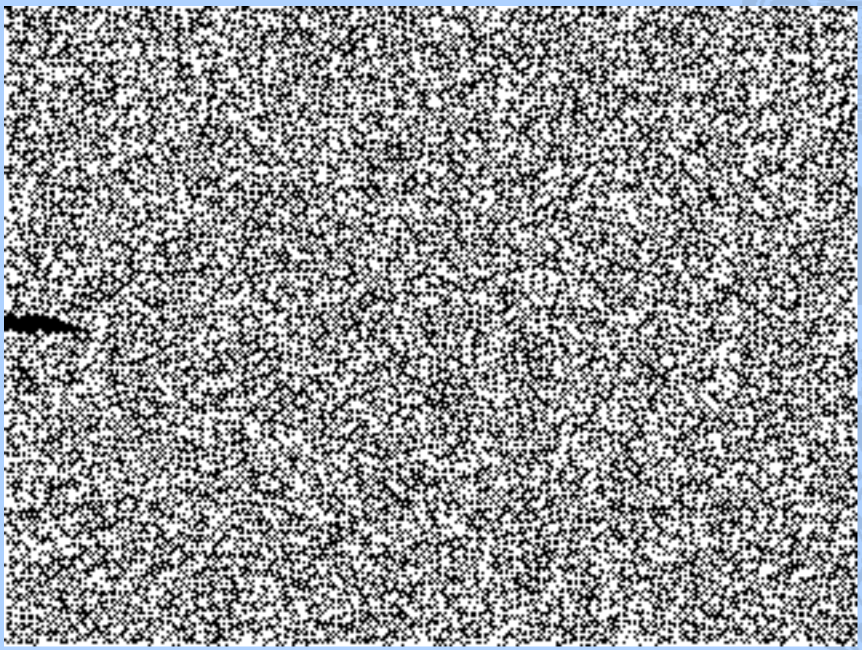
Challenge for Physicists

- How do we connect **macro-scale theory** to **micro-scale physics**?

Amorphous Solids



ML Falk, JS Langer, PRE 57, pp. 7192 (1998)



ML Falk, PRB 60, pp. 7062 (1999)

Fundamentals: Strain

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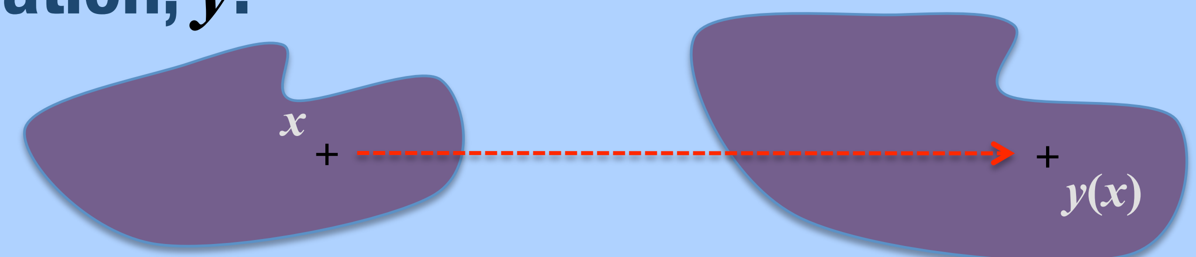
- Consider a body, where each material point is denoted in space by its initial location, $\boldsymbol{x}$.
- After deformation each material point is at a new location, $\boldsymbol{y}$.



- Define the **displacement** as $u(x)=y(x)-x$
- Define the **deformation gradient** at x as the 3x3 tensor $\mathbf{F} = \nabla y(x)$ or equivalently $F_{ij} = \partial y_i / \partial x_j$

Fundamentals: Strain

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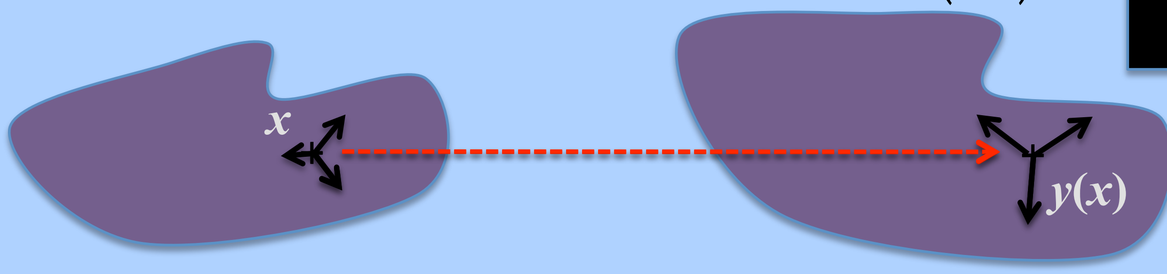
- The **deformation gradient**, **F**, can be used to map a small displacement on the original body to the deformed body as

$$y(x+\delta e) = y(x) + \nabla y \delta e + O\left(\delta^2\right)$$

e is a unit vector



- In other words $y(x+\Delta x) - y(x) \approx \mathbf{F}\Delta x$
- Any orthonormal frame (e_1, e_2, e_3) becomes a linearly independent triad $(\mathbf{F}e_1, \mathbf{F}e_2, \mathbf{F}e_3)$ in the deformed body
- The determinant of this new triad gives the local change in volume due to deformation.

$$det\,\mathbf{F} = \frac{V+\Delta V}{V}$$

Fundamentals: Strain

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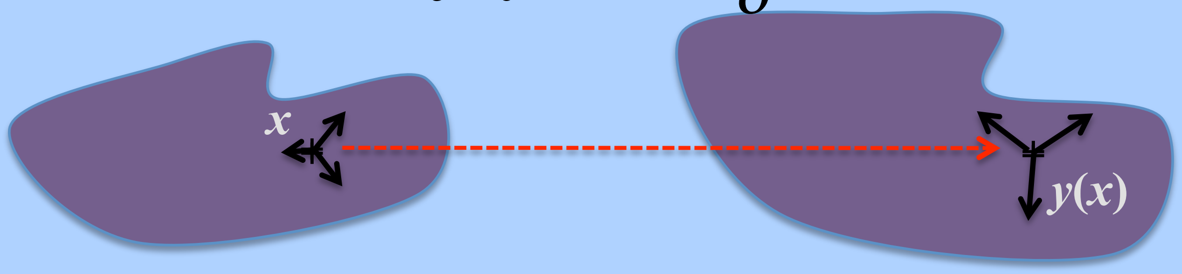
- We can also use this formalism to extract the changes in length to first order

$$\lim_{\delta \to 0} \frac{\left| y(x+\delta e) - y(x) \right|^2}{\delta^2} = \mathbf{F}e \cdot \mathbf{F}e = \mathbf{F}^T\mathbf{F}$$



- If the body is rigid then **F** must be a rotation and $\mathbf{F}^T\mathbf{F} = \mathbf{I}$
- Under more general conditions the on-diagonal terms in the matrix $\mathbf{F}^T\mathbf{F}$ are related to length changes of “fibers” along the principal axes, while the off-diagonal elements are related to changes in angles between these “fibers”.

Fundamentals: Strain

- The object **$C=F^TF$** is known as the **Green deformation tensor**
- We can define the **Lagrangian strain** **$E=\frac{1}{2}(C-I)$**
- Defined in the undeformed body's coordinates.

$$E_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right]$$

Lagrangian Strain

$$E^{*}_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial y_j} + \frac{\partial u_j}{\partial y_i} - \frac{\partial u_k}{\partial y_i}\frac{\partial u_k}{\partial y_j}\right]$$

Eulerian Strain

- Strain can be defined in the deformed body's coordinates. This is known as the **Eulerian strain**
- It is typical to consider deformation of solid bodies in a Lagrangian framework.
- Fluid mechanics is typically considered in an Eulerian framework.

Fundamentals: Strain

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- For applications in which the deformation is small, the third term on the RHS is negligible and the deformation can be expressed in terms of an **"infinitesimal strain"**

$$E_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right]$$

Lagrangian Strain

$$E^{*}_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial y_j} + \frac{\partial u_j}{\partial y_i} - \frac{\partial u_k}{\partial y_i}\frac{\partial u_k}{\partial y_j}\right]$$

Eulerian Strain

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

Infinitesimal Strain

Fundamentals: Strain

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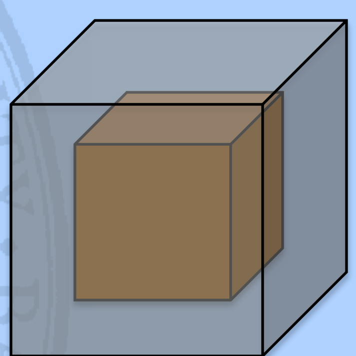
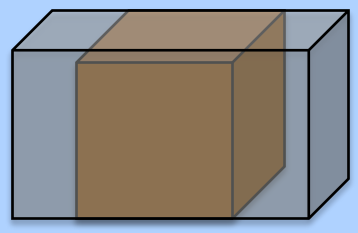
Uniform Dilation



$$u(x) = \alpha(x - x_0)$$

$$\varepsilon_{ij} = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}$$

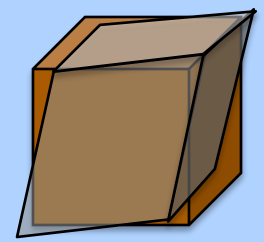
Simple Extension



$$u(x) = \lambda[e_1 \cdot (x - x_0)]e_1$$

$$\varepsilon_{ij} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Pure Shear



$$u(x) = \begin{matrix} \gamma\{[e_1 \cdot (x - x_0)]e_2 \\ +[e_2 \cdot (x - x_0)]e_1\} \end{matrix}$$

$$\varepsilon_{ij} = \begin{bmatrix} 0 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Fundamentals: Stress

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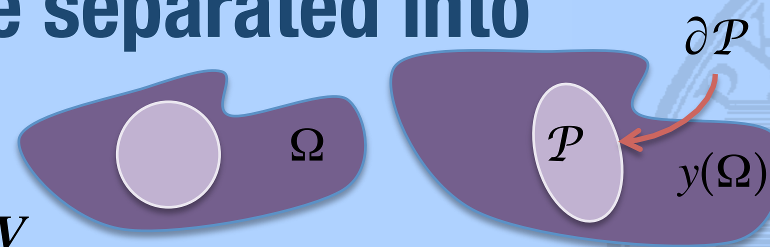
- The forces on a body can be separated into body and surface forces



$$F(\mathcal{P}) = \int_{\mathcal{P}} \boldsymbol{b}(\boldsymbol{y})\,d\boldsymbol{V}_y + \int_{\partial\mathcal{P}} \boldsymbol{s}(\boldsymbol{y},\boldsymbol{n}(\boldsymbol{y}))\,d\boldsymbol{A}_y = \int_{\mathcal{P}} \rho(\boldsymbol{y})\ddot{\boldsymbol{u}}(\boldsymbol{y})\,d\boldsymbol{V}_y$$

- Cauchy's Theorem: ∃ a sym. tensor σ_{ij} such that $\boldsymbol{s}(\boldsymbol{y},\boldsymbol{n}(\boldsymbol{y})) = \sigma(\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})$
- Which, by the divergence theorem implies that

$$0 = \int_{\mathcal{P}} \left[\rho(\boldsymbol{y})\ddot{\boldsymbol{u}}(\boldsymbol{y}) - \boldsymbol{b}(\boldsymbol{y}) - \nabla\cdot\sigma\right]d\boldsymbol{V}_y \qquad \rho\ddot{u}_i = b_i + \frac{\partial\sigma_{ij}}{\partial x_j}$$

- In equilibrium this reduces to $\boxed{b_i + \frac{\partial\sigma_{ij}}{\partial x_j} = 0}$

Fundamentals: Thermodynamics

- Work done (integrate force x velocity)

$$\mathcal{W} = \int_{\mathcal{P}} \left[b_i \dot{u}_i + \frac{\partial \sigma_{ij}}{\partial x_j} \dot{u}_i \right] dV = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \frac{\partial \dot{u}_i}{\partial x_j} \right] dV = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \dot{\varepsilon}_{ij} \right] dV$$

- If energy stored in the material per unit volume is denoted ψ then the energy dissipated is

$$\mathcal{D} = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \dot{\varepsilon}_{ij} - \dot{\psi} \right] dV \geq 0$$

The Missing Ingredients

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- At this point, assuming 3D, we have a **displacement field** from which we can derive the strain (3 unknowns
- We have a **stress** (6 unknowns)
- We also have **equilibrium** (3 equations)
- Since the problem remains **underdetermined** we need a set of equations that will relate the stresses to the strains, and thereby to the displacement field.
- These equations are known as **constitutive equations**.

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

$$\sigma_{ij}$$

$$b_i + \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

Linear Elasticity

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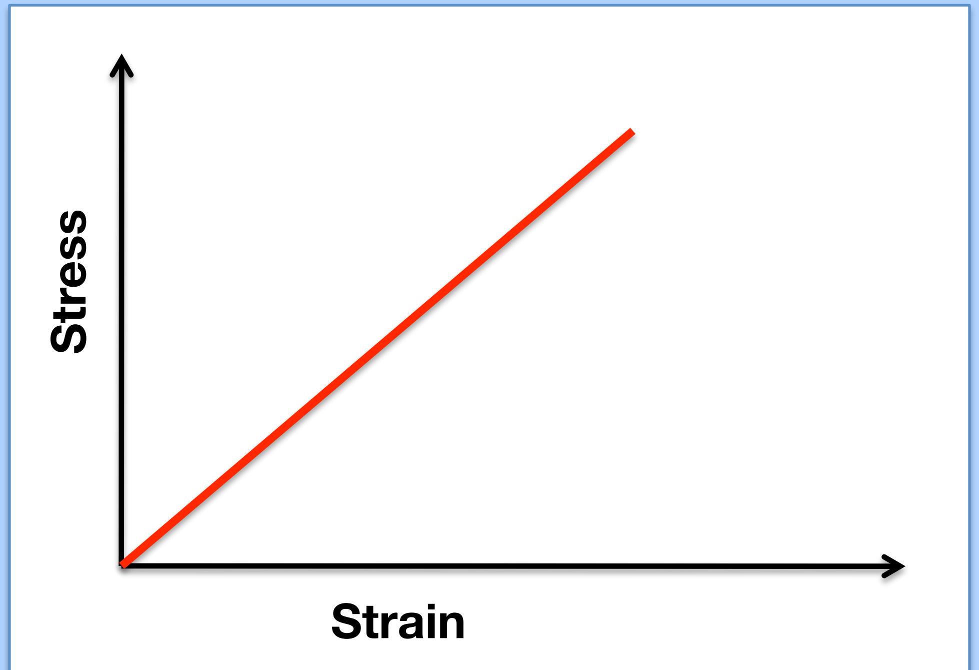
- **Linear elasticity is the simplest constitutive equation and assumes proportionality between stress and strain**



Linear Elasticity

- Linear elasticity is the simplest constitutive equation and assumes proportionality between stress and strain

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}\,, \qquad \sigma_{ij} = \frac{\partial\psi}{\partial\varepsilon_{ij}}$$

- If the material is isotropic this reduces to a simpler equation

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij}$$

- Here μ is the shear modulus and the bulk modulus K is related to μ and λ by

$$\tfrac{1}{3}\sigma_{ii} = \left(\tfrac{2}{3}\mu + \lambda\right)\varepsilon_{ii} = K\varepsilon_{ii}$$

- Since the energy per unit volume is given by $\psi = \frac{1}{2}\varepsilon_{ij}C_{ijkl}\varepsilon_{kl}$ assuming no body forces

$$d = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{\psi} = 0$$

Viscoelasticity

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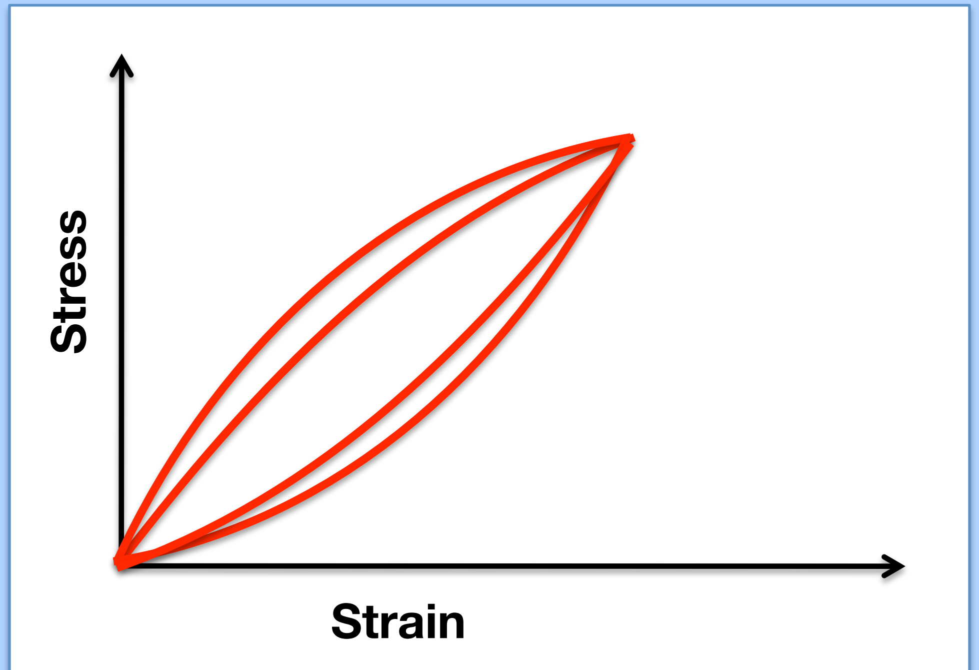
- Viscoelasticity introduces dissipation by allowing the stress to be strain rate dependent



Viscoelasticity

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- Viscoelasticity introduces dissipation by allowing the stress to be strain rate dependent

$$\sigma_{ij} = \frac{\partial \psi}{\partial \varepsilon_{ij}} + \sigma_{ij}^{diss}$$

- To assure compliance with 2nd law of thermodynamics

$$d = \left(\frac{\partial \psi}{\partial \varepsilon_{ij}} + \sigma_{ij}^{diss} \right) \dot{\varepsilon}_{ij} - \dot{\psi} = \frac{\partial \psi}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} + \sigma_{ij}^{diss} \dot{\varepsilon}_{ij} - \dot{\psi} = \sigma_{ij}^{diss} \dot{\varepsilon}_{ij} \geq 0$$

- One reasonable choice would be

$$\sigma_{ij}^{diss} = \eta \dot{\varepsilon}_{ij}$$

- Which we could cast as a "dissipative potential"

$$\phi = \tfrac{1}{2} \eta \dot{\varepsilon}^2, \quad \sigma^{diss} = \frac{\partial \phi}{\partial \dot{\varepsilon}}$$

- Any choice of ϕ that is convex and minimized at 0 will satisfy thermodynamics

Plasticity

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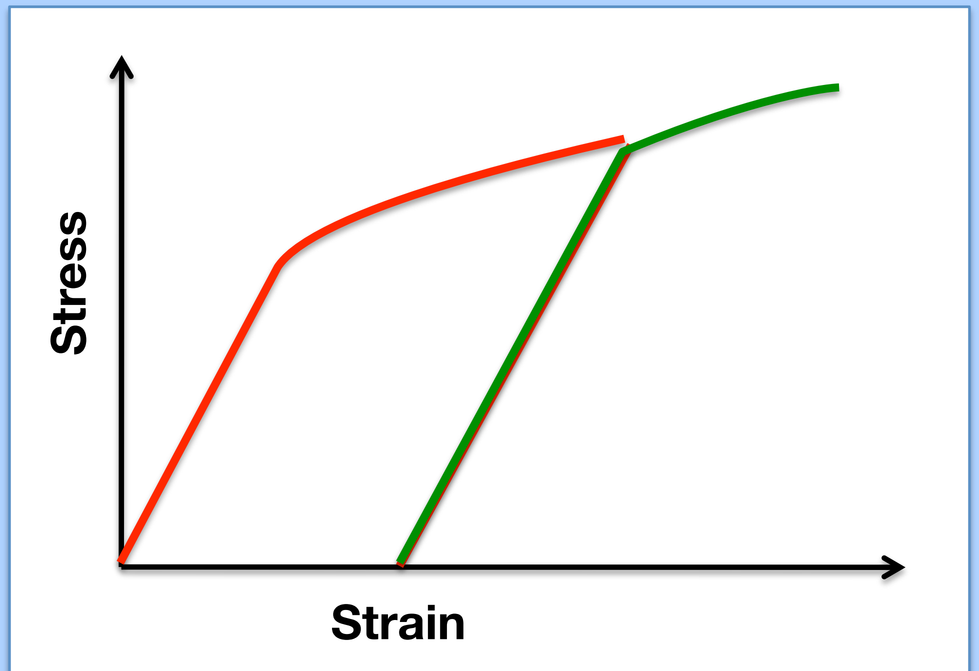
- In plasticity (as opposed to elasticity) the material deforms irreversibly.

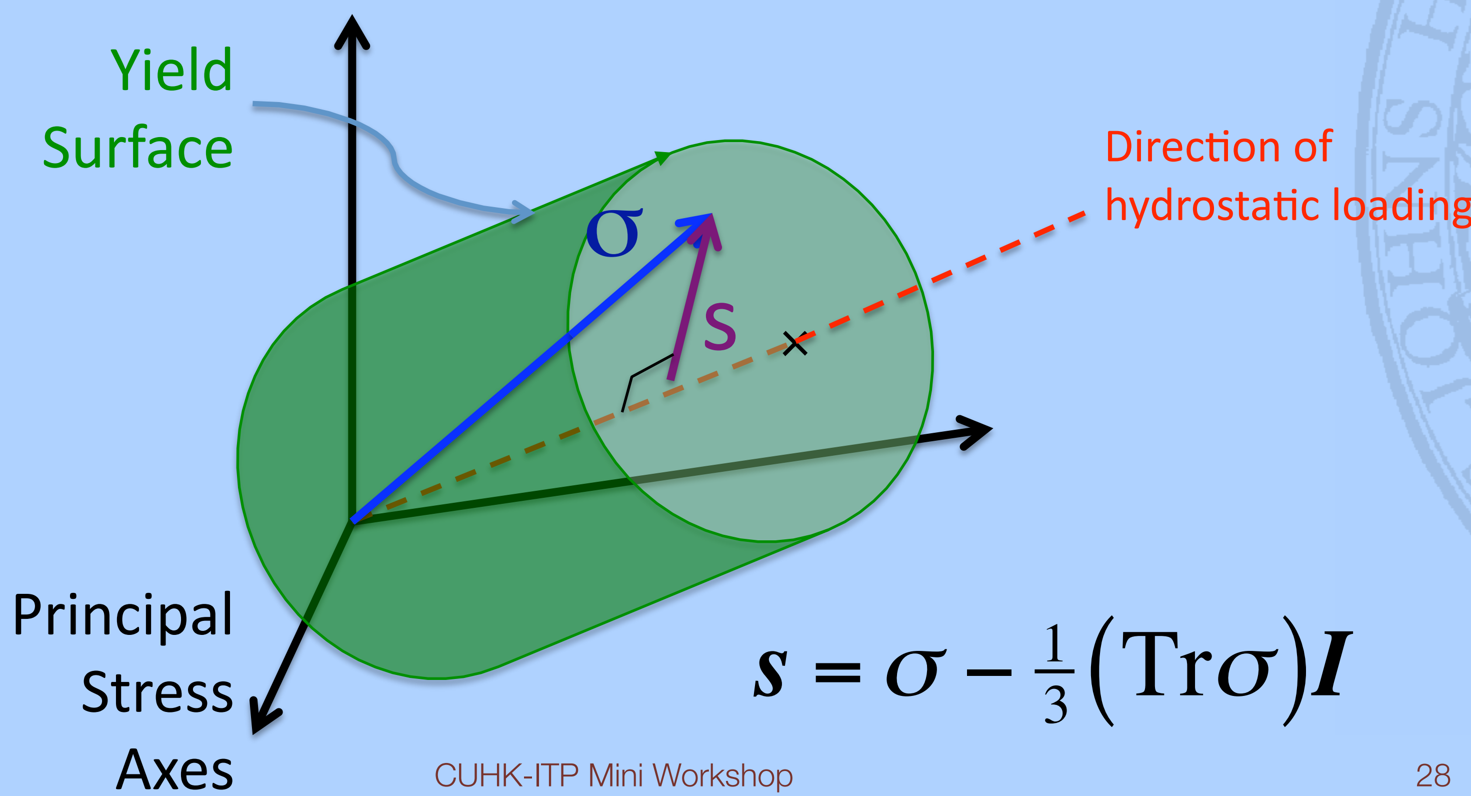


Plasticity

- In plasticity (as opposed to elasticity) the material deforms irreversibly.
- This implies that the material does not retain memory of the initial state.
- This argues for models in which the change in the internal state of the material is an intrinsic feature of the theory.

The Yield Surface

- Deformation takes place in shear, not dilation, so the operative stress is the deviatoric stress, s



$$s = \sigma - \tfrac{1}{3}\left(\mathrm{Tr}\,\sigma\right)I$$

Plasticity

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- Traditional plasticity theories consider the yield stress to be such an intrinsic property

$$\varepsilon[\boldsymbol{u}] = \varepsilon^{el} + \varepsilon^{pl}$$

$$\sigma = \boldsymbol{C}\varepsilon^{el} = \boldsymbol{C}\left(\varepsilon[\boldsymbol{u}] - \varepsilon^{pl}\right)$$

- To determine how the plastic strain evolves it is postulated that there exists a yield criterion $f(\sigma,\zeta)$ such that

$$f(\sigma,\zeta) = |\boldsymbol{s}| - \zeta$$

$$f(\sigma,\zeta) < 0: \quad \text{purely elastic response}$$

$$f(\sigma,\zeta) = 0: \quad \zeta \text{ evolves to remain on yield surface}$$

Plasticity

- **Two functions describe how the yield surface will evolve**

$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial \boldsymbol{f}(\sigma,\zeta)}{\partial\sigma} = \dot{\gamma}\boldsymbol{N}(\sigma,\zeta),\ \dot{\gamma} \geq 0$$

$$\dot{\zeta} = \dot{\gamma}\boldsymbol{h}(\sigma,\zeta)$$

- **Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface**

$$0 = \dot{\boldsymbol{f}} = \frac{\partial \boldsymbol{f}}{\partial\sigma}\cdot\dot{\sigma} + \frac{\partial \boldsymbol{f}}{\partial\zeta}\dot{\zeta} = \frac{\partial \boldsymbol{f}}{\partial\sigma}\cdot\boldsymbol{C}\left(\dot{\varepsilon} - \dot{\varepsilon}^{pl}\right) + \frac{\partial \boldsymbol{f}}{\partial\zeta}\dot{\zeta}$$

$$0 = \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} - \dot{\gamma}\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} + \dot{\gamma}\frac{\partial \boldsymbol{f}}{\partial\zeta}\boldsymbol{h}$$

$$\dot{\gamma} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} - \frac{\partial \boldsymbol{f}}{\partial\zeta}\boldsymbol{h}} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} + \boldsymbol{H}(\sigma,\zeta)},\ when\ \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0$$

Perfect Plasticity

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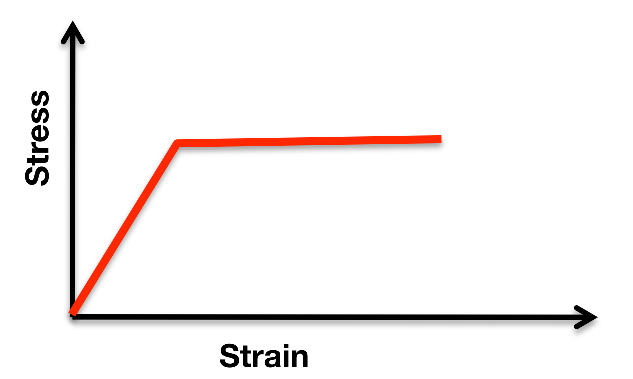
- Consider one particular case where H=0

$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial f(\sigma,\zeta)}{\partial\sigma} = \dot{\gamma}N(\sigma,\zeta),\ \dot{\gamma} \geq 0$$

$$\dot{\zeta} = 0$$



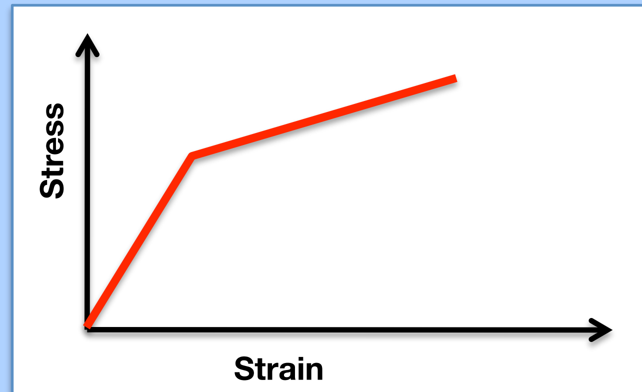
- Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface

$$\dot{\gamma} = \frac{N \cdot C\dot{\varepsilon}}{N \cdot CN},\ \text{when}\ N \cdot C\dot{\varepsilon} > 0$$

$$\dot{\sigma} = C\left(\dot{\varepsilon} - \dot{\varepsilon}^{pl}\right) = \begin{cases} 0, & N \cdot C\dot{\varepsilon} > 0 \\ C\dot{\varepsilon}, & N \cdot C\dot{\varepsilon} \leq 0 \end{cases}$$

Isotropic Hardening

- Consider one particular case where H=h=const



$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial f(\sigma,\zeta)}{\partial\sigma} = \dot{\gamma}N(\sigma,\zeta),\ \dot{\gamma}\geq 0$$

$$\dot{\zeta} = \dot{\gamma}\mathrm{h}$$

- Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface

$$\dot{\gamma} = \frac{N\cdot C\dot{\varepsilon}}{N\cdot CN+\mathrm{h}},\ \text{when } N\cdot C\dot{\varepsilon}>0$$

$$\dot{\sigma} = C\left(\dot{\varepsilon}-\dot{\varepsilon}^{pl}\right) = \begin{cases}\left(\dfrac{\mathrm{h}C\dot{\varepsilon}}{N\cdot CN+\mathrm{h}}\right), & N\cdot C\dot{\varepsilon}>0\\ C\dot{\varepsilon}, & N\cdot C\dot{\varepsilon}\leq 0\end{cases}$$

A Critical Assessment

- **What is missing from this picture of plasticity?**
  - Rate dependence
  - A relation between the internal variables (in this case the yield stress ζ) and microscopic physics of deformation and microstructural evolution
  - As such the theory remains entirely empirical

- **The reason this is a suitable problem for physicists, is that we don't yet have tools suitable for abstracting our understanding of material microstructure to inform continuum theory.**

Material Failure

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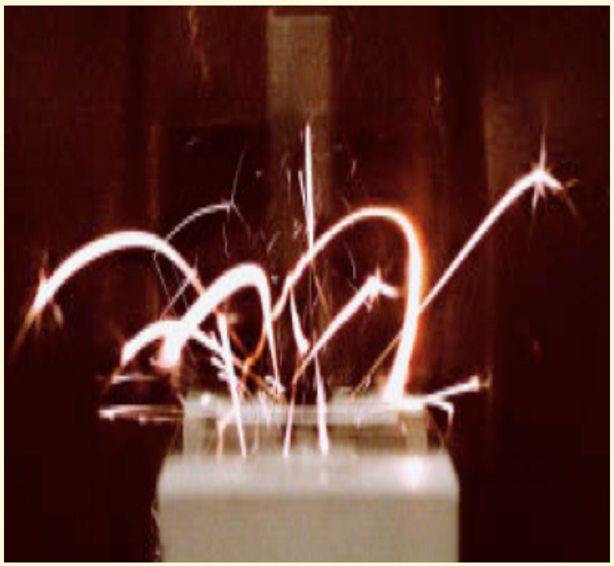
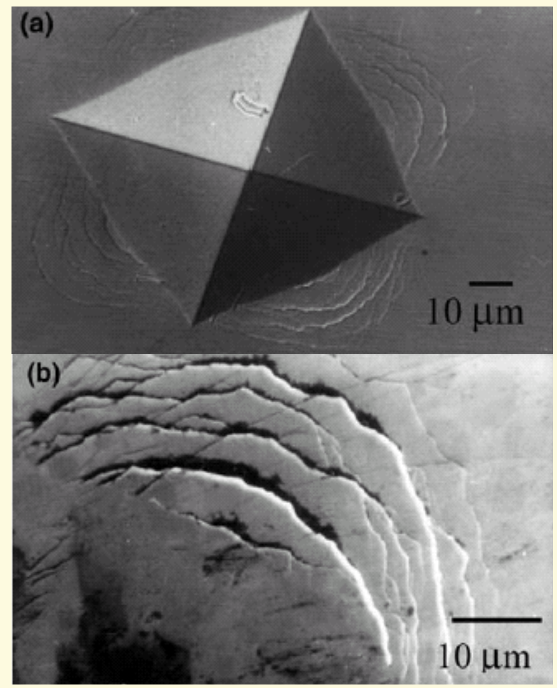
Fracture



Sparks during fracture of Zr based bulk metallic glass

From C.J. Gilbert, APL 74, 3809 (1999).

Shear Banding



"Hardness and plastic deformation in a bulk metallic glass"
Ramamurty, Jana, Kawamura, Chattopadhyay, Acta Materialia (2005)

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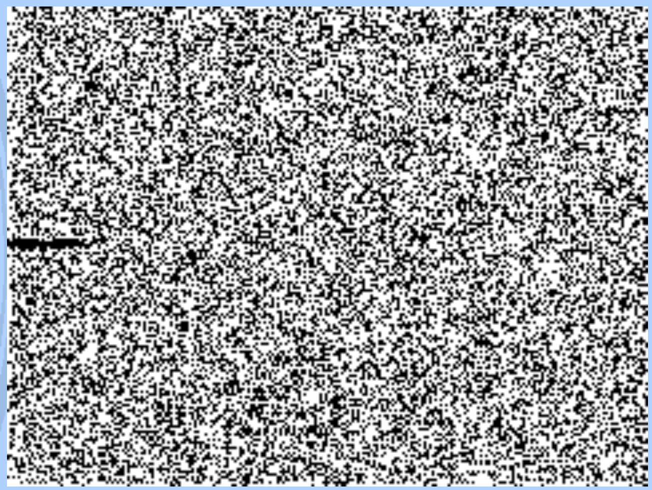
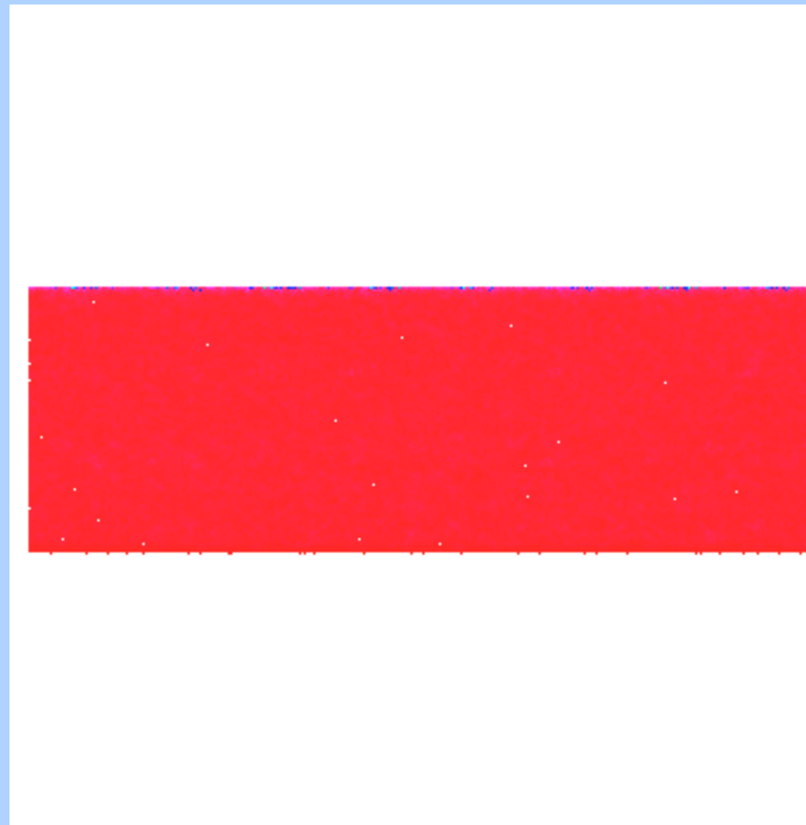
Fracture



ML Falk, PRB 60, pp. 7062 (1999)

Shear Banding



Y Shi, ML Falk, Acta Mat 55, pp. 4317 (2007)

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- Understanding material failure, including fracture and shear banding, involves additional analysis
- Fracture – Energy input and instabilities associated with surface creation during growth of existing flaws
- Shear Bands – Plastic instabilities associated with material softening