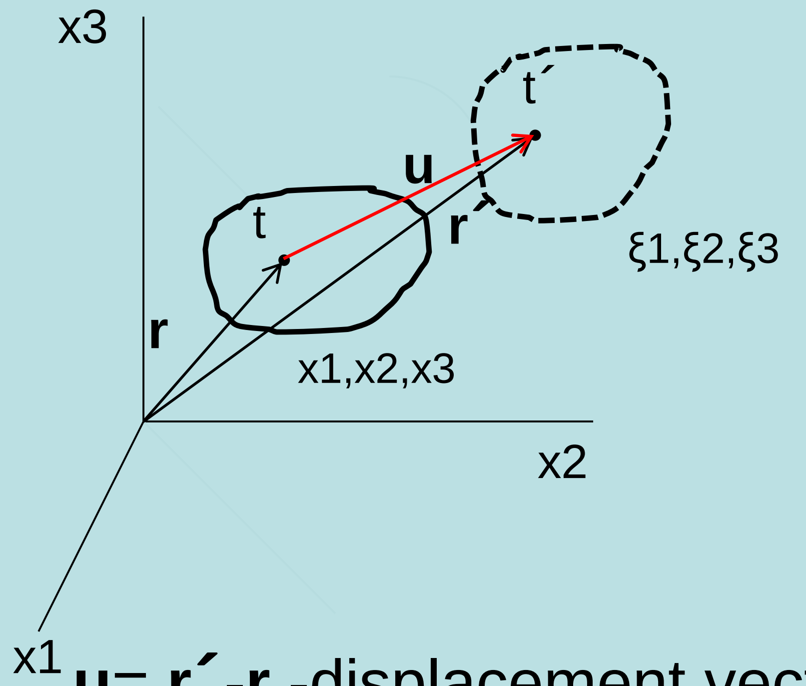
Lecture 1. How to model: physical grounds

Outline

- Physical grounds: parameters and basic laws
- Physical grounds: rheology

Physical grounds: displacement, strain and stress tensors

Strain



u= **r´**-**r** -displacement vector

Lagrangian

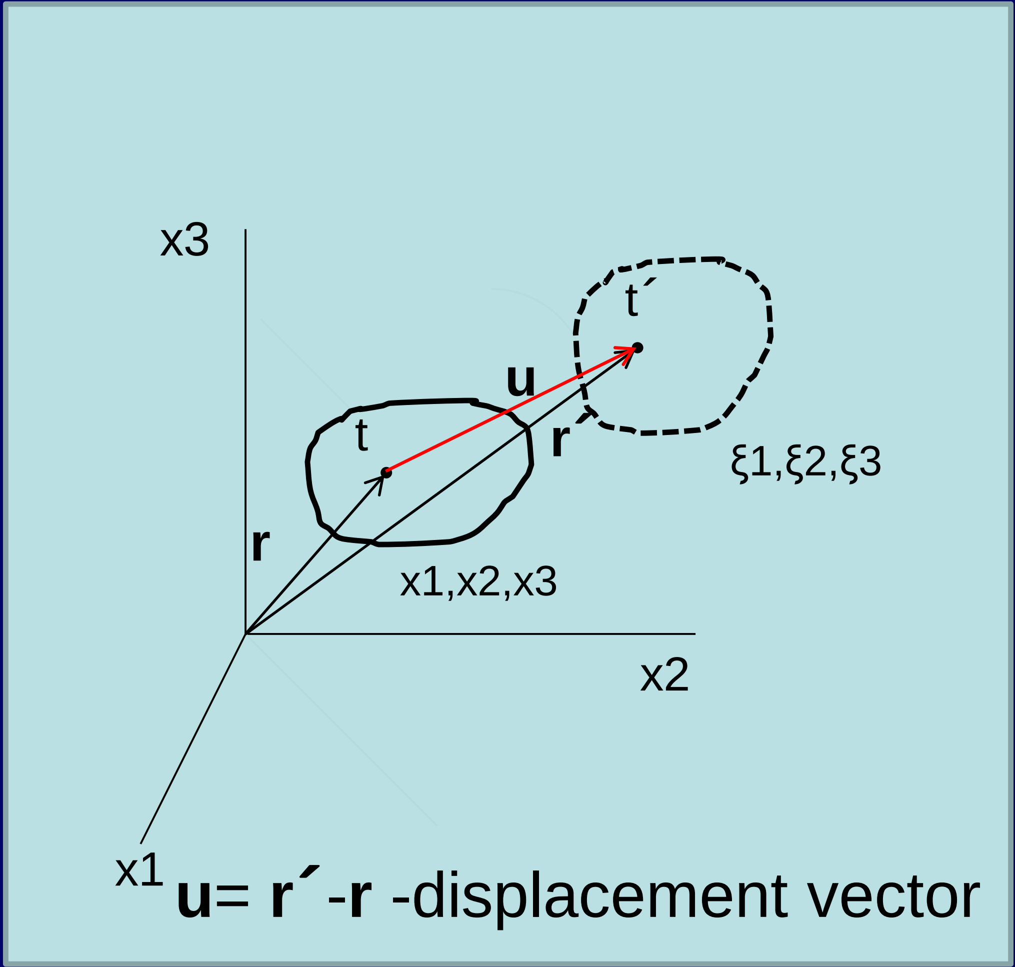
ξi= ξi (x1,x2,x3,t)
i=1,2,3

$$\det(\partial \xi i / \partial xj) \neq 0$$

xi= xi (ξ1,ξ2,ξ3,t)
i=1,2,3

ui= ξi -xi= ui (x1,x2,x3,t)
i=1,2,3

Strain



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i=1,2,3

Eulerian

Strain tensor

1

$$ds_0^2 = dx_1^2 + dx_2^2 + dx_3^2 = dx_i dx_i$$

$$ds^2 = d\xi_1^2 + d\xi_2^2 + d\xi_3^2 = d\xi_i d\xi_i$$

2

$$d\xi_i = \frac{\partial \xi_i}{\partial x_j} dx_j$$

$$ds^2 = d\xi_i d\xi_i = \frac{\partial \xi_i}{\partial x_j} \frac{\partial \xi_i}{\partial x_k} dx_j dx_k$$

$$ds^2 - ds_0^2 = \left(\frac{\partial \xi_i}{\partial x_j} \frac{\partial \xi_i}{\partial x_k} - \delta_{jk}\right) dx_j dx_k$$

3

$$ds^2 - ds_0^2 = 2e_{jk} dx_j dx_k$$

$$2e_{jk} = \left(\frac{\partial \xi_i}{\partial x_j} \frac{\partial \xi_i}{\partial x_k} - \delta_{jk}\right)$$

Strain tensor

1

$$ds^2 - ds_0^2 = 2e_{jk}dx_jdx_k$$

$$2e_{jk} = \left(\frac{\partial \xi_i}{\partial x_j}\frac{\partial \xi_i}{\partial x_k} - \delta_{jk}\right)$$

2

$$u_i = \xi_i - x_i$$

$$\frac{\partial \xi_i}{\partial x_j} = \frac{\partial u_i}{\partial x_j} + \delta_{ij}$$

3

$$e_{jk} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k} + \frac{\partial u_l}{\partial x_j}\frac{\partial u_l}{\partial x_k}\right)$$

$$e_{jk} = e_{kj}$$

Strain tensor

1

$$ds^2 - ds_0^2 = 2e_{jk}\,dx_j\,dx_k$$

$$2e_{jk} = \left(\frac{\partial \xi_i}{\partial x_j}\frac{\partial \xi_i}{\partial x_k} - \delta_{jk}\right)$$

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3

$$e_{jk} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k} + \cancel{\frac{\partial u_l}{\partial x_j}\frac{\partial u_l}{\partial x_k}}\right)$$

$$e_{jk} = e_{kj}$$

Strain and strain rate tensors

$$\varepsilon_{jk} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k}\right)$$

$$u_k = v_k \, dt$$

$$\varepsilon_{jk} = \dot{\varepsilon}_{jk} \, dt$$

$$\dot{\varepsilon}_{jk} = \frac{1}{2}\left(\frac{\partial v_k}{\partial x_j} + \frac{\partial v_j}{\partial x_k}\right)$$

Geometric meaning of strain tensor

$$(ds - ds_0)/ds_0 = \varepsilon_{11}$$

Changing length

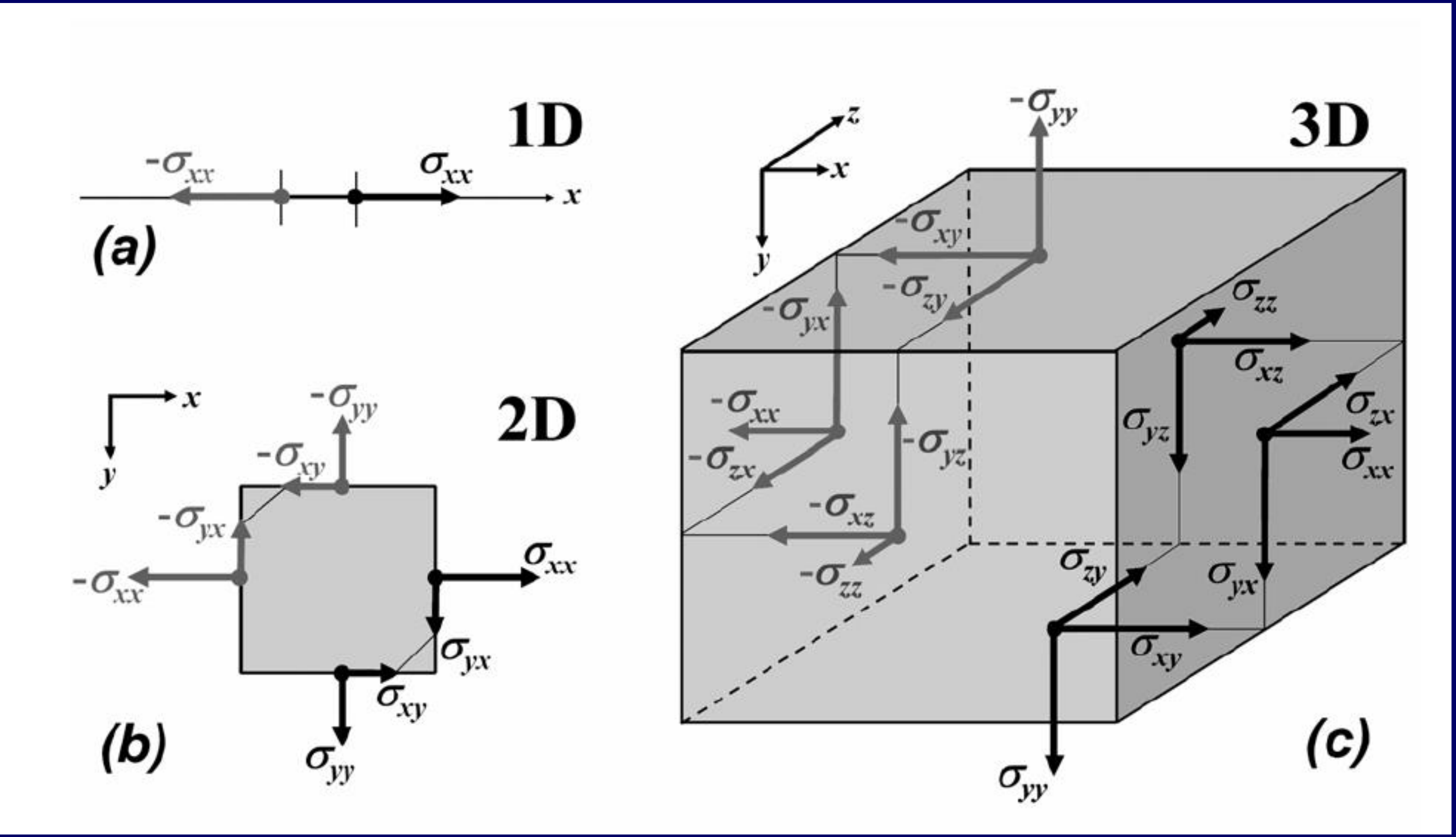
$$\cos\varphi_{12} = 0$$
$$\cos\varphi'_{12} = \varepsilon_{12}$$

Changing angle

$$(\Delta V' - \Delta V)/\Delta V = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$$

Changing volume

Stress tensor



σ_{ij} is the ***i*** component of the force acting at the unit surface which is orthogonal to direction ***j***

$$\sigma_{ij} = \sigma_{ji}$$

Tensor invariants, deviators

$$I = \sigma_{kk} = \sigma_{11} + \sigma_{22} + \sigma_{33}$$

$$\tau_{ij} = \sigma_{ij} - \frac{1}{3} I \delta_{ij}, \tau_{kk} = 0$$

Stress deviator

$$\sigma_{ij} = -P\delta_{ij} + \tau_{ij}, P = -\frac{1}{3} I$$

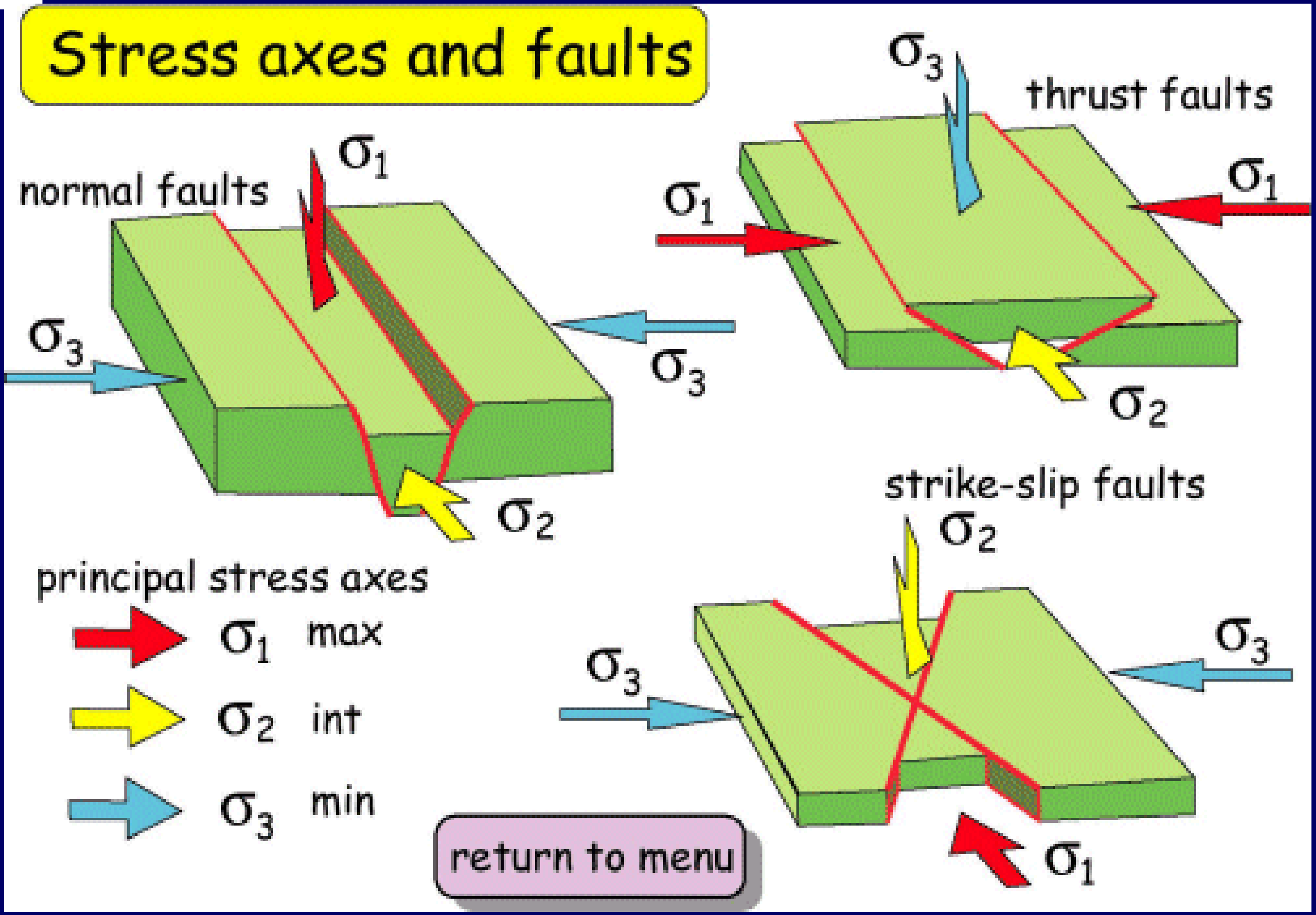
P is pressure

$$\sigma_{II} (or\ \tau_{II}) = \sqrt{\tau_{ij}\tau_{ij} / 2}$$

Stress norm

$$\begin{matrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{matrix}$$

Principal stress axes



Physical grounds: conservation laws

Mass conservation equation

$$\frac{\partial}{\partial t}\int_V \rho dV = -\int_S \rho v_i n_i dS$$

$$\frac{\partial}{\partial t}\int_V \rho dV = -\int_V \frac{\partial}{\partial x_i}(\rho v_i)dV$$

$$\int_V \left(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i)\right)dV = 0$$

Mass conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_i)}{\partial x_i} = 0$$

Material flux

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_i}{\partial x_i} = 0 \qquad \frac{D\rho}{Dt} \equiv \frac{\partial \rho}{\partial t} + v_i \frac{\partial \rho}{\partial x_i}$$

Substantive time derivative

Mass conservation equation

$$\frac{D\rho}{Dt}=\frac{\partial\rho}{\partial P}\frac{DP}{Dt}+\frac{\partial\rho}{\partial T}\frac{DT}{Dt}=\frac{\rho}{K}\frac{DP}{Dt}-\rho\alpha\frac{DT}{Dt}$$

$$\frac{1}{K}\frac{DP}{Dt}-\alpha\frac{DT}{Dt}+\frac{\partial v_i}{\partial x_i}=0$$

Momentum conservation equation

Substantive time derivative

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = \rho \frac{Dv_i}{Dt}, \quad i = 1,..3$$

$$\frac{Dv_i}{Dt} \equiv \frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j}$$

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho \frac{Dv_i}{Dt}, \quad i = 1,..3$$

Energy conservation equation

Shear heating

$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \tau_{ij}\dot{\varepsilon}_{ij}^{ne} + \rho A + \Delta H_{chem}$$

Substantive time derivative

Heat flux

All conservation equations

$$\frac{1}{K}\frac{DP}{Dt} - \alpha\frac{DT}{Dt} + \frac{\partial v_i}{\partial x_i} = 0$$

mass

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho\frac{Dv_i}{Dt}$$

momentum

$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i}(\lambda\frac{\partial T}{\partial x_i}) + \frac{1}{\eta_{eff}}\tau_{ij}\tau_{ij} + \rho A + \Delta H_{chem}$$

energy

All conservation equations

$$\frac{1}{K}\frac{DP}{Dt} - \alpha\frac{DT}{Dt} + \frac{\partial v_i}{\partial x_i} = 0$$

mass

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho\frac{Dv_i}{Dt}$$

momentum

$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i}(\lambda\frac{\partial T}{\partial x_i}) + \frac{1}{\eta_{eff}}\tau_{ij}\tau_{ij} + \rho A + \Delta H_{chem}$$

energy

$$\dot{\varepsilon}_{ij}^{d} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}) - \frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k} = F(P, T, \tau_{ij}, v_j)$$

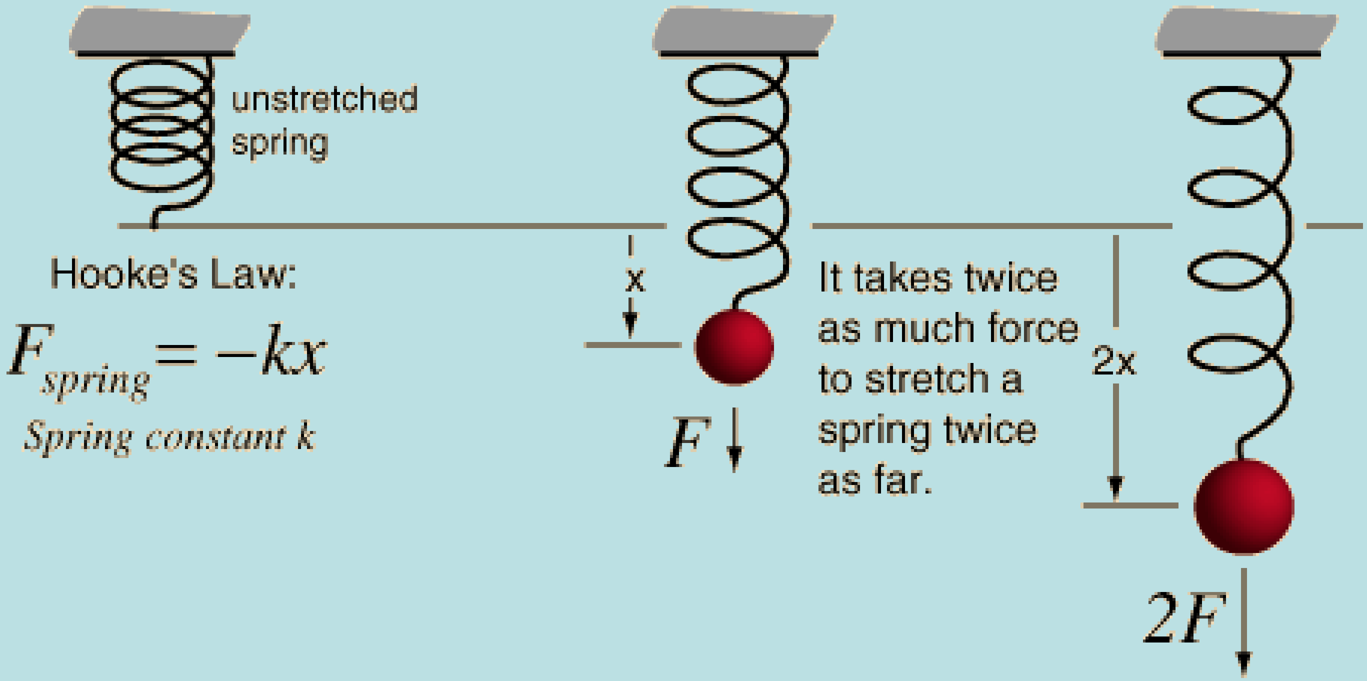
Physical grounds: constitutive laws

Rheology – the relationship between stress and strain

- Rheology for ideal bodies
  - Elastic
  - Viscous
  - Plastic

An isotropic, homogeneous elastic material follows **Hooke's Law**

Hooke's Law: $\sigma = E\varepsilon$



For an ideal Newtonian fluid:
differential stress = viscosity x strain rate
viscosity: measure of resistance to flow

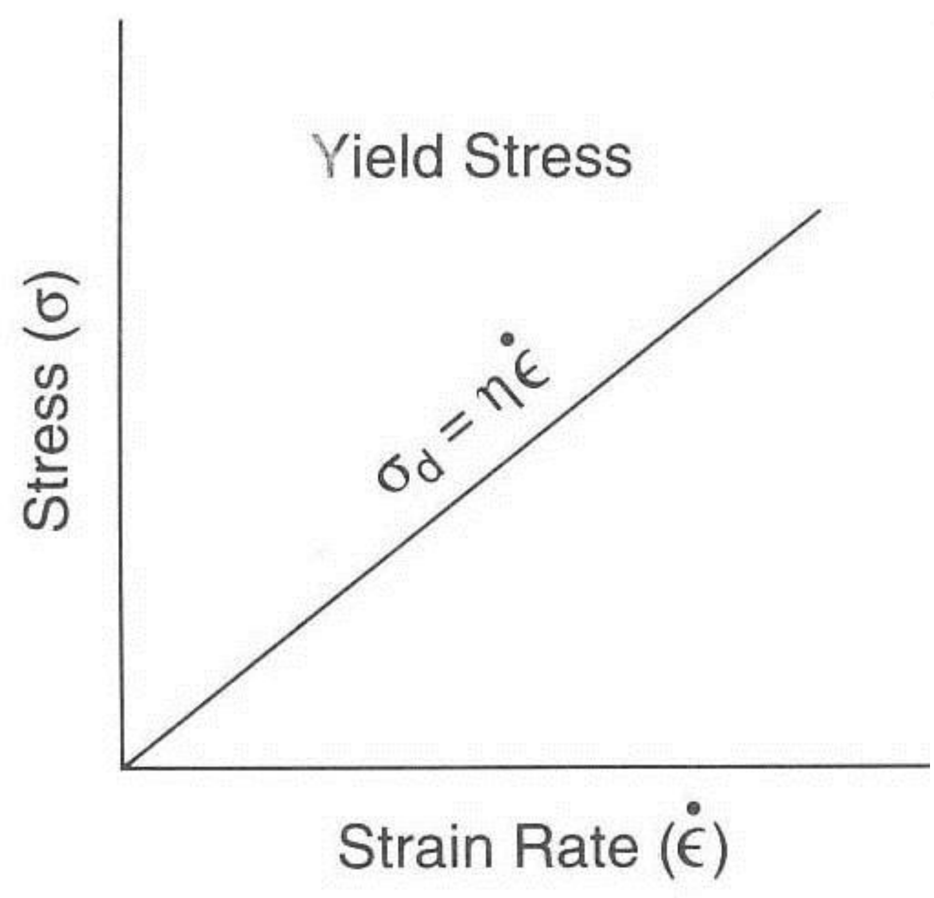
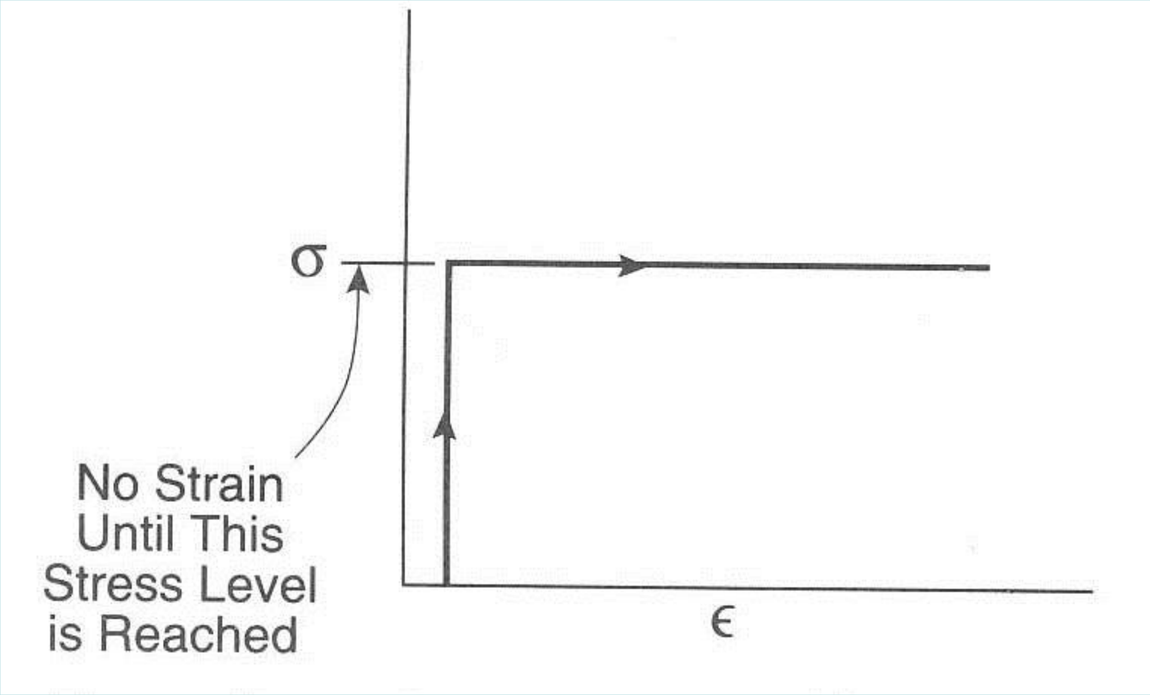


Table 5.5 Some Representative Viscosities (in Pa · s)

Air	10^{-5}
Water	10^{-3}
Olive oil	10^{-1}
Honey	4
Glycerin	83
Lava	$10–10^{4}$
Asphalt	10^{5}
Pitch	10^{9}
Ice	10^{12}
Rock salt	10^{17}
Sandstone slab	10^{18}
Asthenosphere (upper mantle)	10^{20}
Lower mantle	10^{21}

Sources: Several sources, including Turcotte and Schubert (1982).

Ideal plastic behavior



Constitutive laws

$$\dot{\varepsilon}_{ij\,elastic} = \frac{1}{2G}\frac{D\tau_{ij}}{Dt}$$

Elastic strain rate

$$\dot{\varepsilon}_{ij\,visc} = \frac{1}{2\eta}\tau_{ij}$$

Viscous flow strain rate

$$\dot{\varepsilon}_{ij\,plastic} = \frac{\dot{\gamma}}{\tau_{II}}\tau_{ij}$$

Plastic flow strain rate

$$\tau_{II} = \sqrt{\tau_{ij}\tau_{ij}}$$

Superposition of constitutive laws

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij\,elastic} + \dot{\varepsilon}_{ij\,visc} + \dot{\varepsilon}_{ij\,plastic}$$

$$\dot{\varepsilon}_{ij} = \frac{1}{2G}\frac{D\tau_{ij}}{Dt} + \left(\frac{1}{2\eta} + \frac{\dot{\gamma}}{\tau_{II}}\right)\tau_{ij} \quad ; \quad \tau_{II} = \sqrt{\tau_{ij}\tau_{ij}}$$

$$\dot{\varepsilon}_{ij} = \frac{1}{2G}\frac{D\tau_{ij}}{Dt} + \frac{1}{2\eta_{eff}(P,T,\tau_{II})}\tau_{ij}$$

Full set of equations

$$\frac{1}{K}\frac{DP}{Dt} - \alpha\frac{DT}{Dt} + \frac{\partial v_i}{\partial x_i} = 0$$

mass

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho\frac{Dv_i}{Dt}$$

momentum

$$\rho C_p\frac{DT}{Dt} = \frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i}\right) + \frac{1}{\eta_{eff}}\tau_{ij}\tau_{ij} + \rho A + \Delta H_{chem}$$

energy

$$\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k} = \frac{1}{2G}\frac{D\tau_{ij}}{Dt} + \frac{1}{2\eta_{eff}(P, T, \tau_{II})}\tau_{ij}$$

↑

$$\dot{\varepsilon}^{d}_{ij}$$

Full set of equations

$$\cancel{\frac{1}{K}\frac{DP}{Dt}} - \alpha \cancel{\frac{DT}{Dt}} + \frac{\partial v_i}{\partial x_i} = 0$$

mass

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i = \rho \frac{D v_i}{Dt}$$

momentum

$$\dot{\varepsilon}_{ij}^{d} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k} = \cancel{\frac{1}{2G}\frac{D\tau_{ij}}{Dt}} + \frac{1}{2\eta_{eff}(P,T,\tau_{II})}\tau_{ij}$$

$$t_{ij} = h\left(\frac{¶ v_i}{¶ x_j} + \frac{¶ v_j}{¶ x_i}\right) - \frac{2}{3} h d_{ij} \cancel{\frac{¶ v_k}{¶ x_k}}$$

Navier -Stokes equations

Continuity equation → $$\frac{\partial v_i}{\partial x_i} = 0$$ mass

$$-\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right) + \rho g_i = \rho \frac{Dv_i}{Dt}$$ momentum

(the term $\rho \frac{Dv_i}{Dt}$ is struck through)

Navier- Stokes equations

Stokes equations

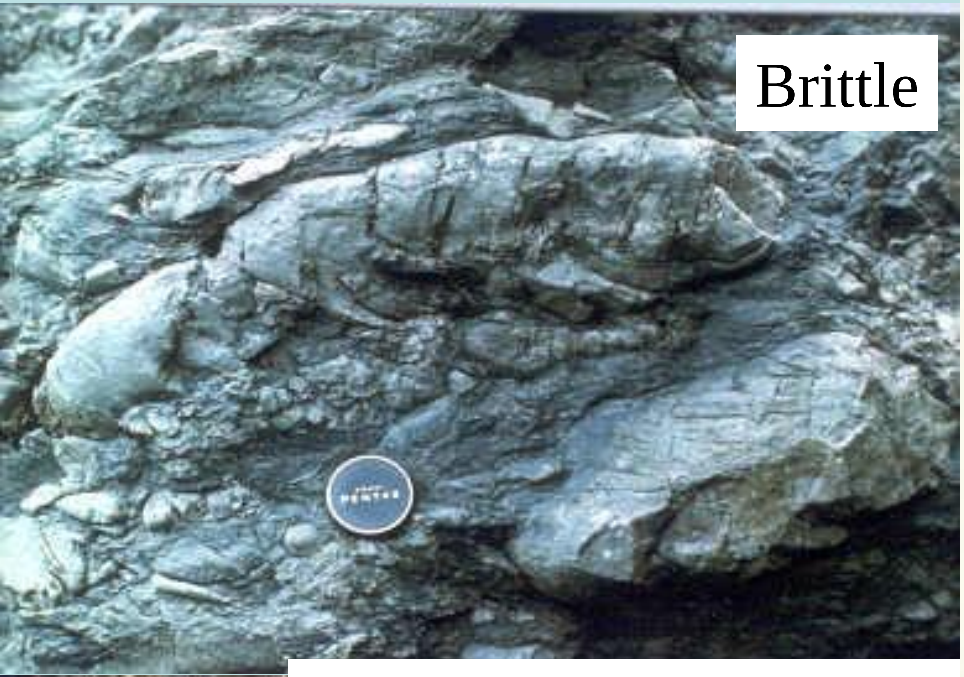
Continuity equation → $$\frac{\partial v_i}{\partial x_i} = 0$$ mass

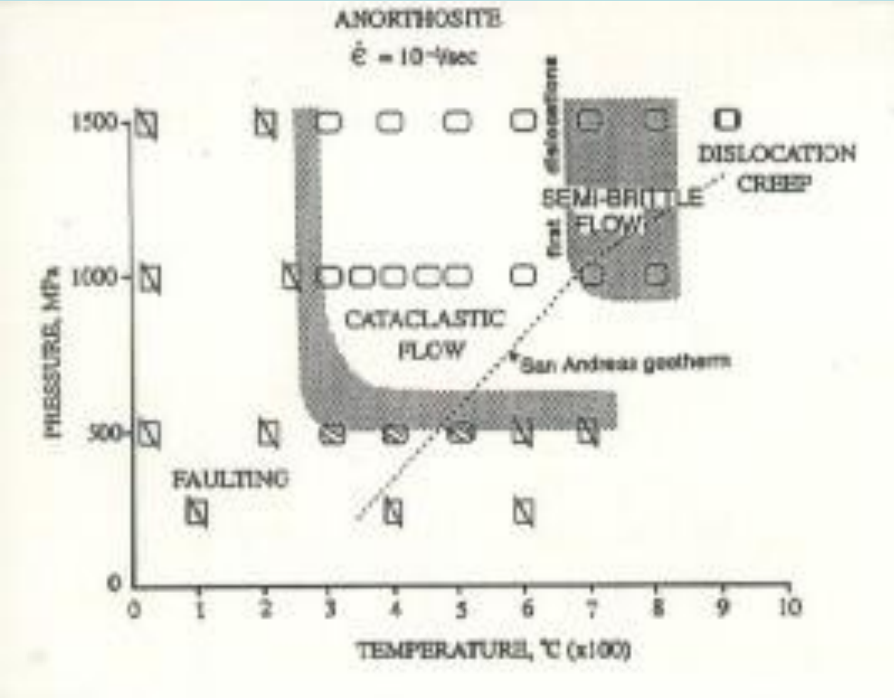
$$-\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right) + \rho g_i = 0$$ momentum

Stokes equations

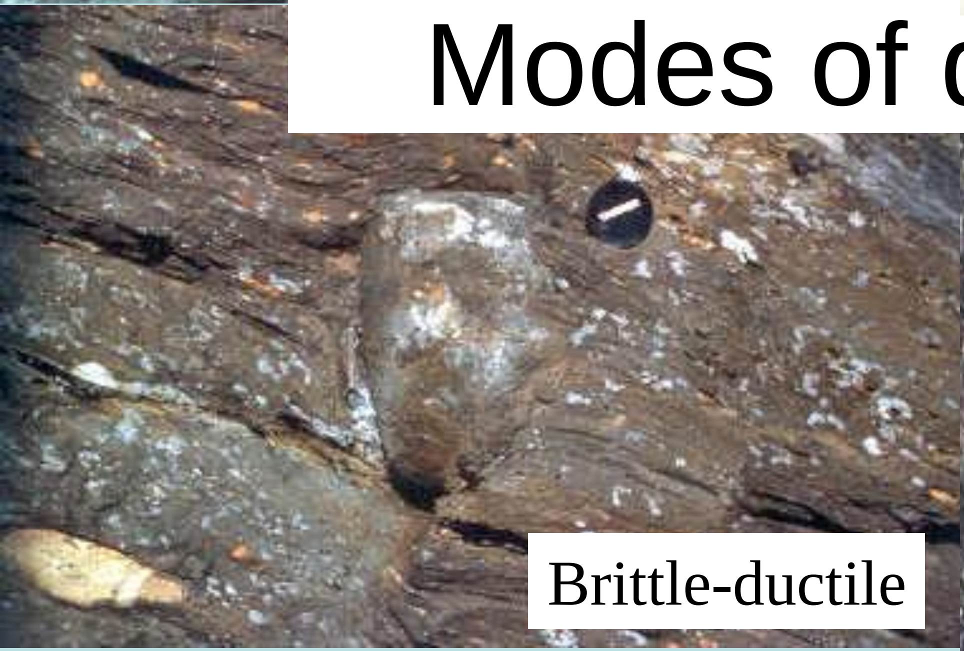
How Does Rock Flow?

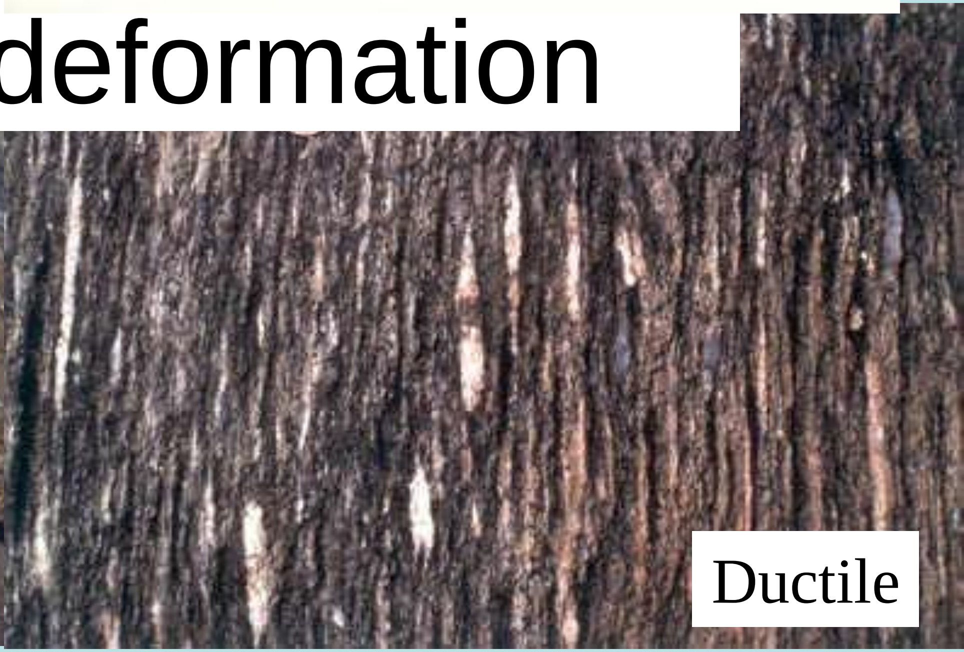
- Brittle – Low T, low P
- Ductile – as P, T increase





Modes of deformation



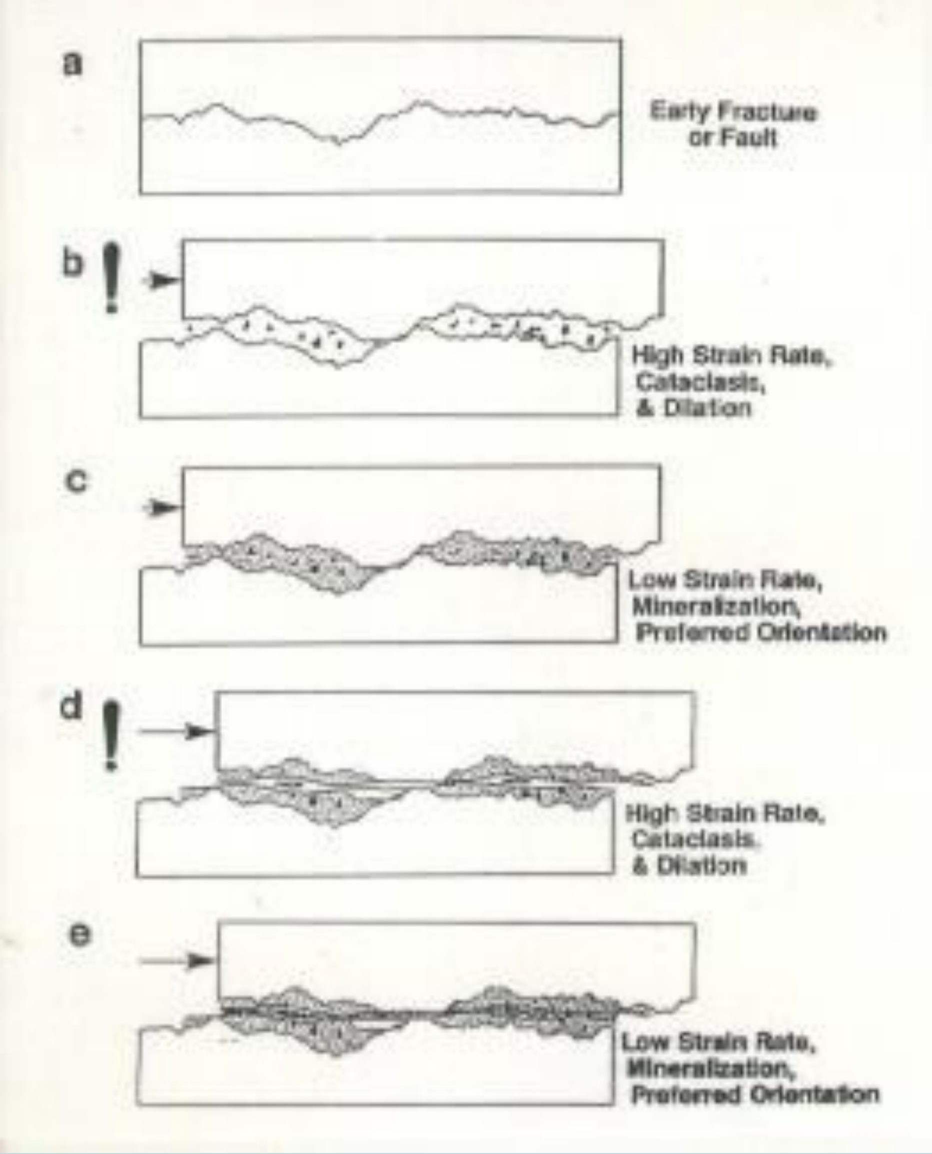


Deformation Mechanisms

- Brittle
  - Cataclasis
  - Frictional grain-boundary sliding
- Ductile
  - Diffusion creep
  - Power-law creep
  - Peierls creep

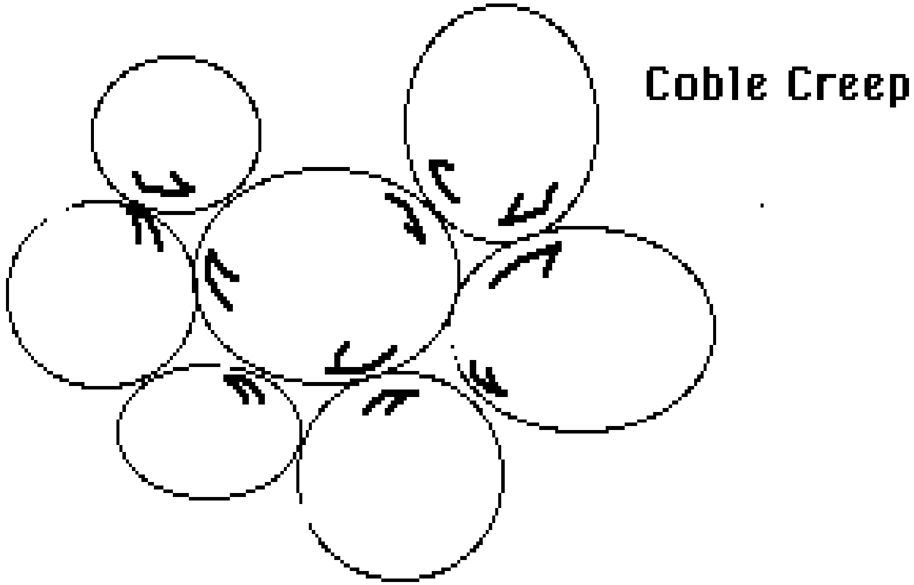
Cataclasis

- Fine-scale fracturing and movement along fractures.
- Favoured by low-confining pressures



Frictional grain-boundary sliding

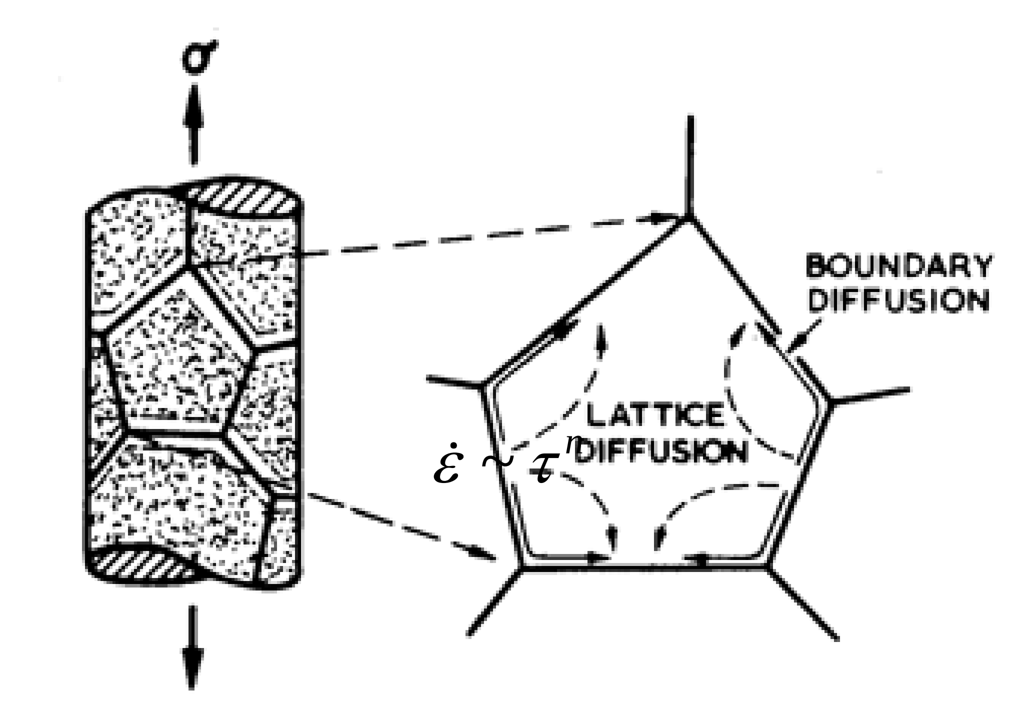
- Involves the sliding of grains past each other - enhanced by films on the grain boundaries.



$$\tau_{II} = c + \mu \cdot P$$

Diffusion Creep

- Involves the transport of material from one site to another within a rock body
- The material transfer may be intracrystalline, intercrystalline or both.
- Newtionian rheology:



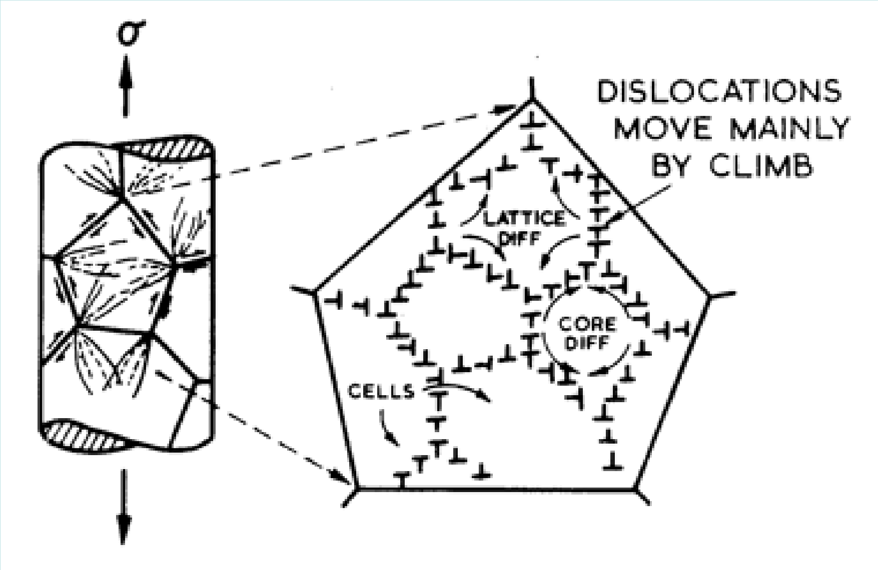
$\dot{\varepsilon} \sim \tau^n$

$$\dot{\varepsilon} \sim \tau$$

$$\dot{\varepsilon}_L = B_L \, \tau_{II} \exp\left(-\frac{H_L}{RT}\right)$$

Dislocation Creep

- Involves processes internal to grains and crystals of rocks.
- In any crystalline lattice there are always single atoms (i.e. point defects) or rows of atoms (i.e. line defects or dislocations) missing. These defects can migrate or diffuse within the crystalline lattice.
- Motion of these defects that allows a crystalline lattice to strain or change shape without brittle fracture.
- Power-law rheology :



$$\dot{\varepsilon} \sim \tau^n$$

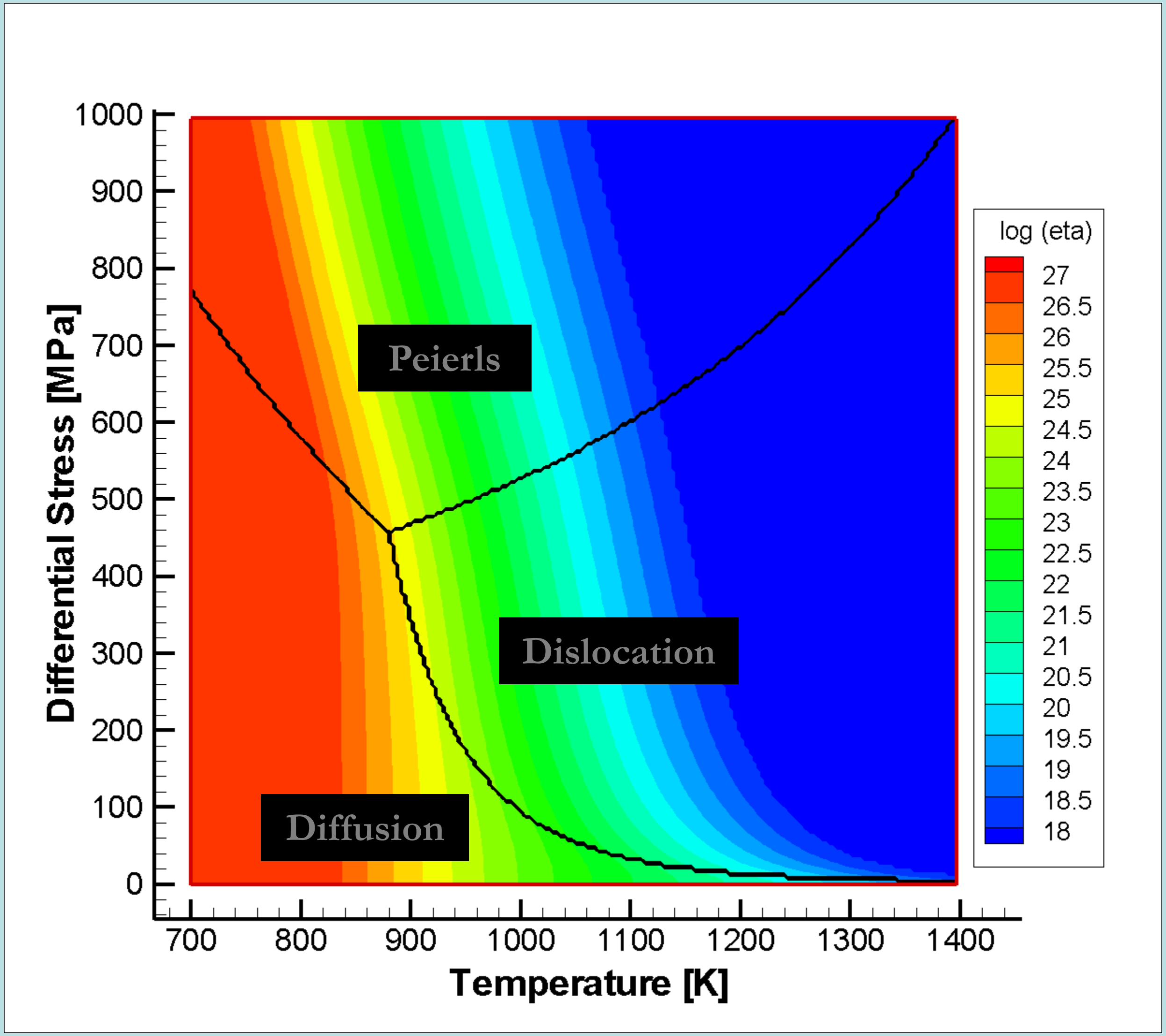
$$\dot{\varepsilon}_N = B_N (\tau_{II})^n \exp\left(-\frac{H_N}{RT}\right)$$

Peierls Creep

For high differential stresses (about 0.002 times Young's modulus as a threshold), mixed dislocation glide and climb occurs. This mechanism has a finite yield stress (Peierls stress,) at absolute zero temperature conditions.

$$\dot{\varepsilon}_P = B_P \exp(-\frac{H_P}{RT}(1-\frac{\tau_{II}}{\tau_P}))$$

Three creep processes



$$\eta_{eff} = \frac{1}{2}\tau_{II}\left(\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P\right)^{-1}$$

Diffusion creep

$$\dot{\varepsilon}_L = B_L \tau_{II} \exp\left(-\frac{E_L}{RT}\right)$$

Dislocation creep

$$\dot{\varepsilon}_N = B_N \left(\tau_{II}\right)^n \exp\left(-\frac{E_N}{RT}\right)$$

Peierls creep

$$\dot{\varepsilon}_P = B_P \exp\left[-\frac{E_P}{RT}\left(1-\frac{\tau_{II}}{\tau_P}\right)^2\right]$$

(Kameyama *et al.* 1999)

Full set of equations

$$\frac{1}{K}\frac{DP}{Dt}-\alpha\frac{DT}{Dt}+\frac{\partial v_i}{\partial x_i}=0$$

mass

$$-\frac{\partial P}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\rho g_i=\rho\frac{Dv_i}{Dt}$$

momentum

$$\rho C_p\frac{DT}{Dt}=\frac{\partial}{\partial x_i}(\lambda\frac{\partial T}{\partial x_i})+\frac{1}{\eta_{eff}}\tau_{ij}\tau_{ij}+\rho A+\Delta H_{chem}$$

energy

$$\dot{\varepsilon}_{ij}^{d}=\frac{1}{2}(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i})-\frac{1}{3}\delta_{ij}\frac{\partial v_k}{\partial x_k}=\frac{1}{2G}\frac{D\tau_{ij}}{Dt}+\frac{1}{2\eta_{eff}(P,T,\tau_{II})}\tau_{ij}$$

Final effective viscosity

$$\frac{1}{2\eta_{eff}} = (\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P + \dot{\gamma}) / \tau_{II}$$

$$\dot{\varepsilon}_L = B_L \, \tau_{II} \exp\left(-\frac{H_L}{RT}\right)$$

$$\dot{\varepsilon}_N = B_N \left(\tau_{II}\right)^n \exp\left(-\frac{H_N}{RT}\right)$$

$$\dot{\varepsilon}_P = B_P \exp\left(-\frac{H_P}{RT}\left(1 - \frac{\tau_{II}}{\tau_P}\right)\right)$$

Plastic strain

$$\frac{1}{2\eta_{eff}} = (\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P + \dot{\gamma}) / \tau_{II}$$

$$\dot{\gamma} = 0 \quad \text{if} \quad \tau_{II} < c + \mu \cdot P$$

$$\dot{\gamma} \neq 0 \quad \text{if} \quad \tau_{II} = c + \mu \cdot P$$

Drucker-Prager yield criterion

$$\text{if} \quad \mu = 0, c \neq 0 \quad \tau_{II} = c$$

Von Mises yield criterion

$$c, \mu = a - b \cdot \gamma$$

softening

Final effective viscosity

$$\frac{1}{2\eta_{eff}} = (\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P + \dot{\gamma}) / \tau_{II}$$

$$\dot{\varepsilon}_L = B_L \, \tau_{II} \exp\left(-\frac{H_L}{RT}\right)$$

$$\dot{\varepsilon}_N = B_N \left(\tau_{II}\right)^n \exp\left(-\frac{H_N}{RT}\right)$$

$$\dot{\varepsilon}_P = B_P \exp\left(-\frac{H_P}{RT}\left(1-\frac{\tau_{II}}{\tau_P}\right)\right)$$

$\dot{\gamma} = 0$ if $\tau_{II} < c + \mu \cdot P$

$\dot{\gamma} \neq 0$ if $\tau_{II} = c + \mu \cdot P$

Strength envelope