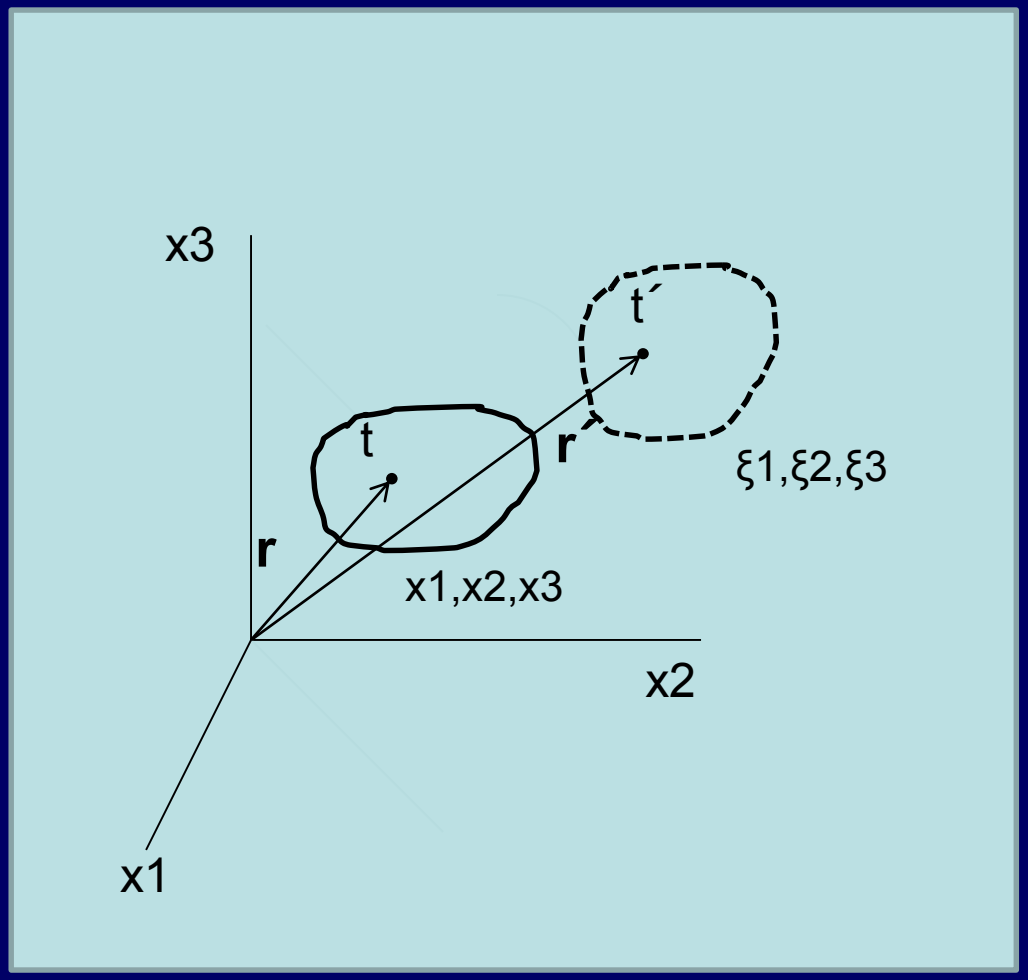
# Lecture 1. How to model: physical grounds

**Outline**

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

# Physical grounds: displacement, strain and stress tensors

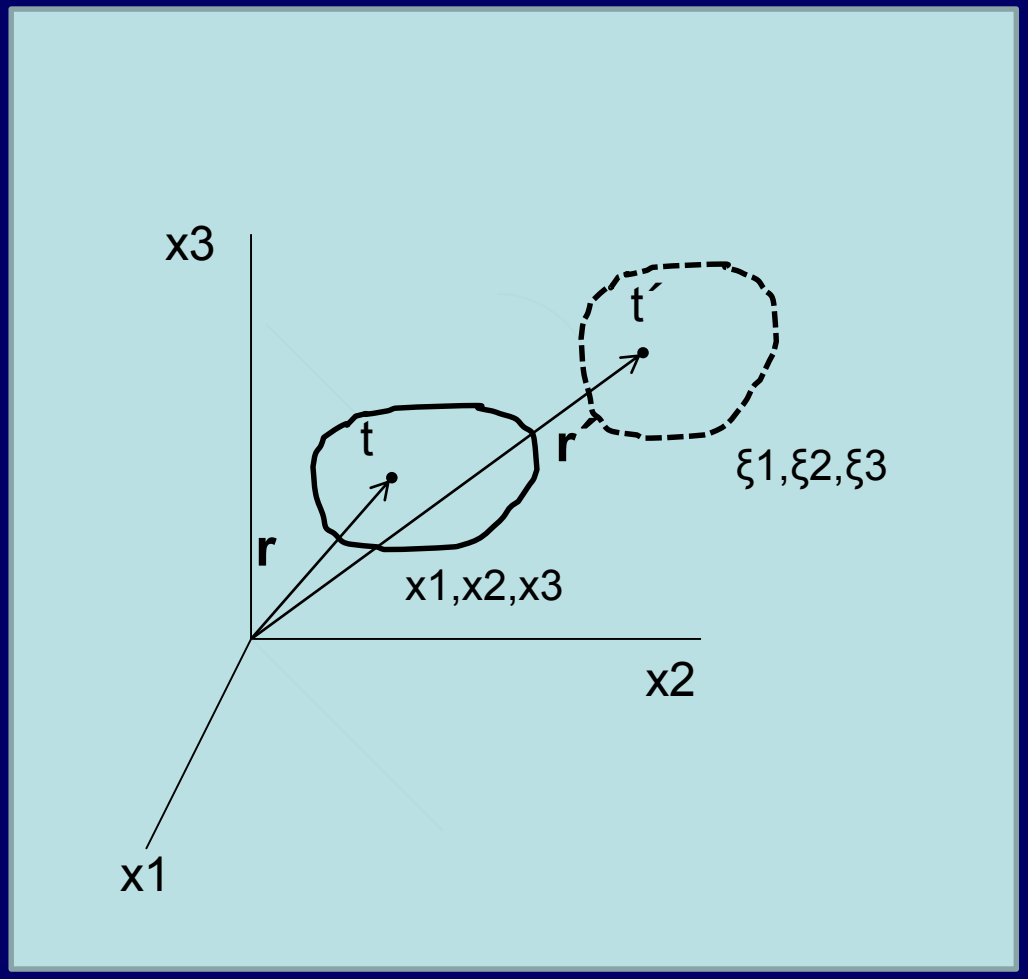
# Strain




$\xi_i = \xi_i (x_1, x_2, x_3, t)$

$i = 1, 2, 3$

# Strain




Lagrangian

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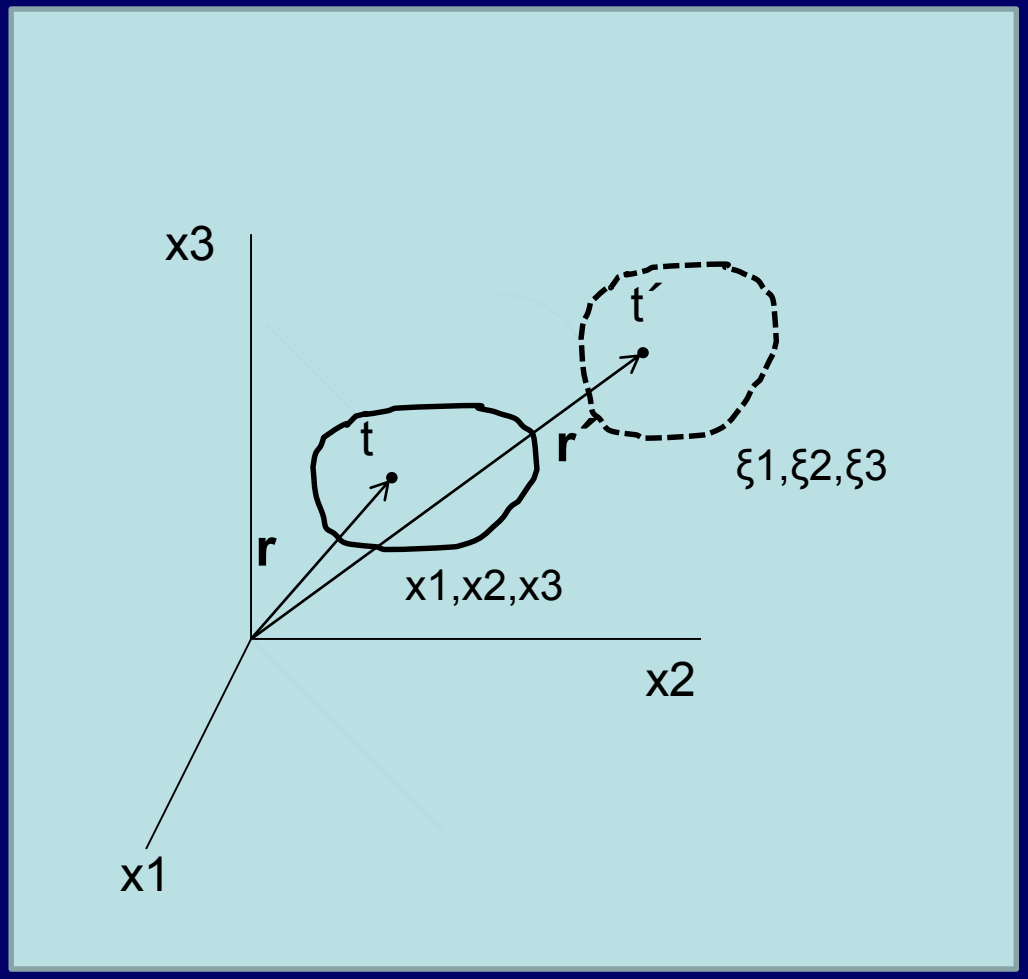


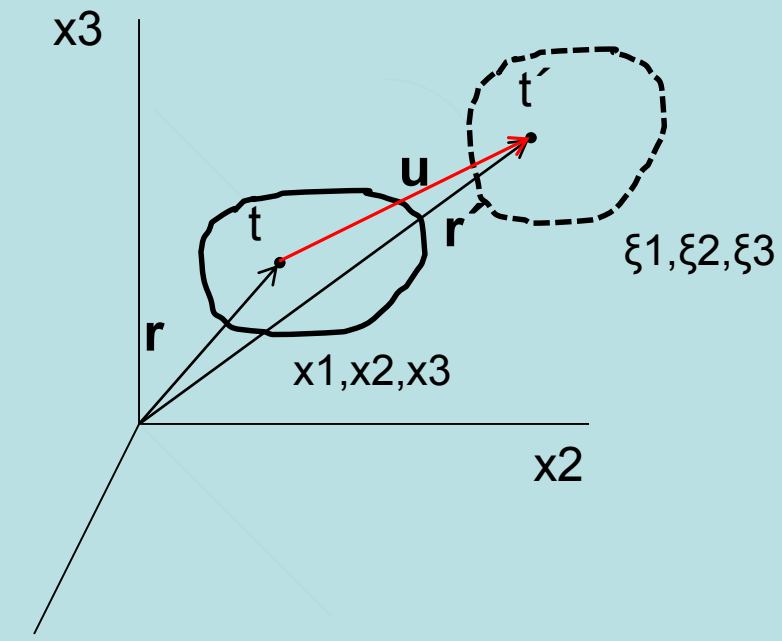

Lagrangian

$\xi i = \xi i\ (x1, x2, x3, t)$
$i = 1,2,3$

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

$xi = xi\ (\xi 1, \xi 2, \xi 3, t)$
$i = 1,2,3$

# Strain




**u**= **r´**-**r** -displacement vector

Lagrangian

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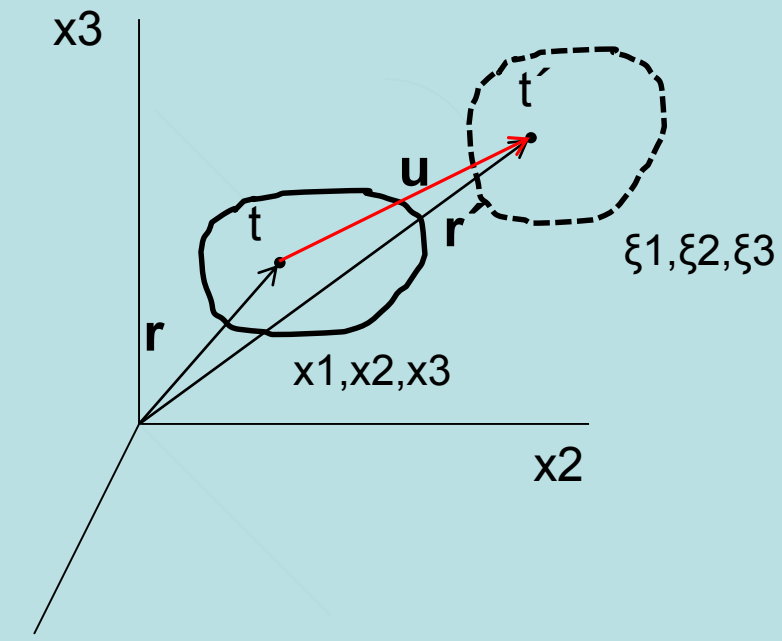


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Lagrangian

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$i=1,2,3$

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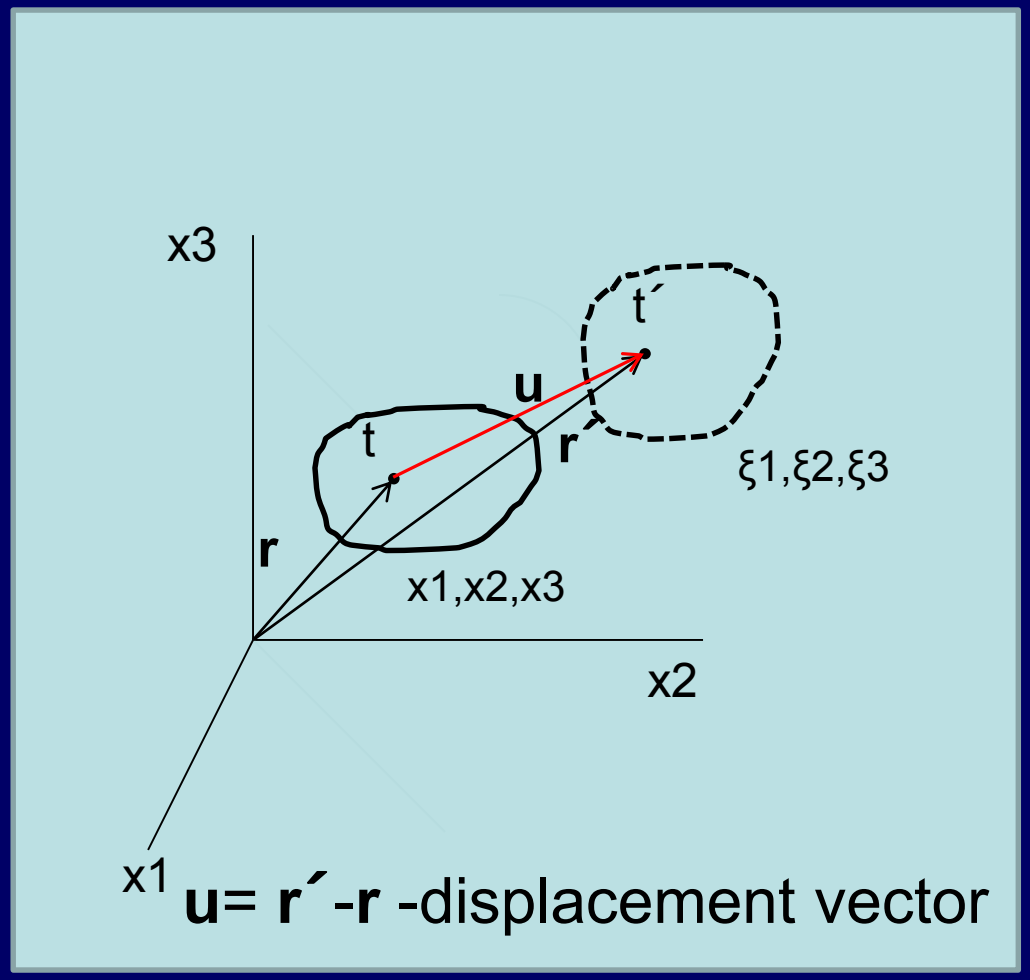
$xi = xi\ (\xi 1, \xi 2, \xi 3, t)$
$i=1,2,3$

$ui = \xi i - xi = ui\ (x1, x2, x3, t)$
$i=1,2,3$

# Strain




$\xi i = \xi i\ (x1,x2,x3,t)$
$i=1,2,3$

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

$xi = xi\ (\xi 1,\xi 2,\xi 3,t)$
$i=1,2,3$ Lagrangian

$ui = \xi i - xi = ui\ (x1,x2,x3,t)$
$i=1,2,3$

$ui = \xi i - xi = ui\ (\xi 1,\xi 2,\xi 3,t)$
$i=1,2,3$

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

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

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

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

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

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

# 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

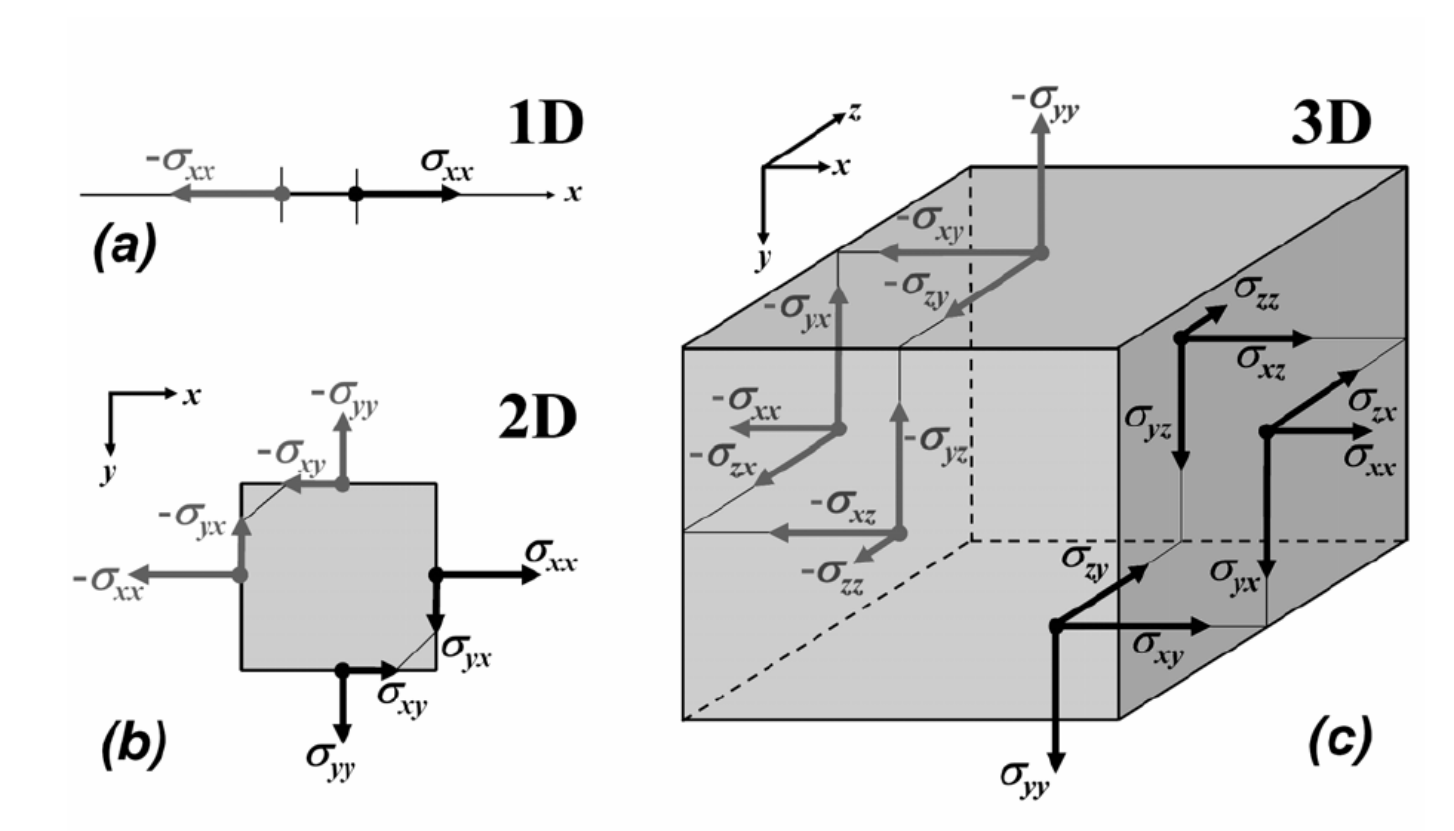
$$\cos\varphi_{12} = 0$$
$$\cos\varphi'_{12} = \varepsilon_{12}$$

Changing angle

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

Changing volume

# Stress tensor




$\sigma_{ij}$ 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

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

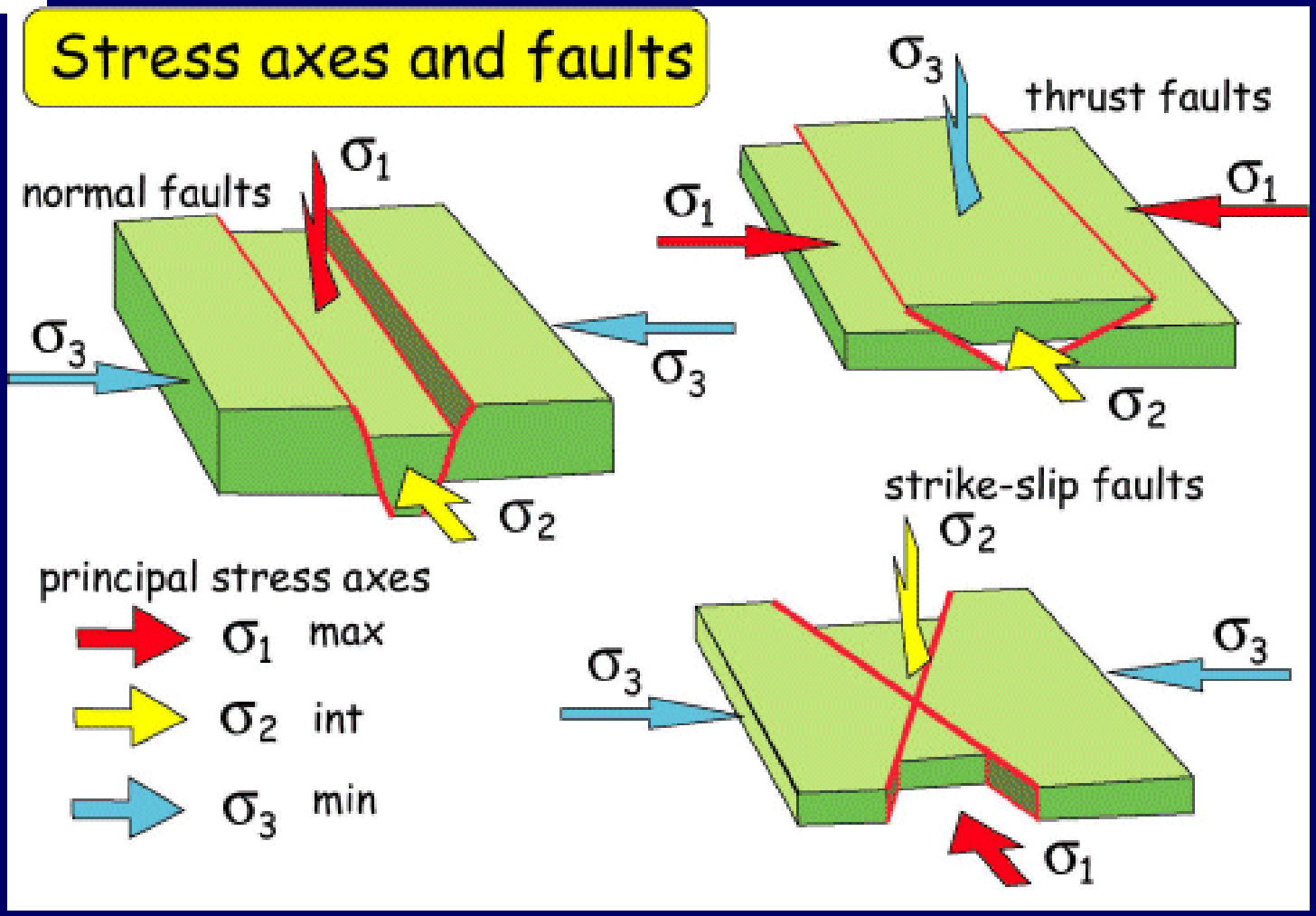
*P* is pressure

$$\tau_{II} = \sqrt{\tau_{ij} \tau_{ij} / 2}$$

*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

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

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# 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

# Geodynamic modelling

## *Basic conservation laws*

Mass conservation law:

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

Momentum conservation law:

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

Energy conservation law:

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

# Geodynamic modelling

## *Basic conservation laws*

Mass conservation law:

1 equation

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

Momentum conservation law:

3 equations

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

Energy conservation law:

1 equation

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

# Geodynamic modelling

*Basic conservation laws*

**Only 5 equations for 11 unknowns!**

# Geodynamic modelling

## *Rheological (constitutive) equations*

Equation of state for density:

1 equation

$$\rho = F(P,T)$$

Deformation mechanisms:

5 equations

$$\dot{\varepsilon}_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) = \Phi(P,T,\tau_{ij})$$

# All conservation equations

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

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

$$\rho = F(P, T)$$

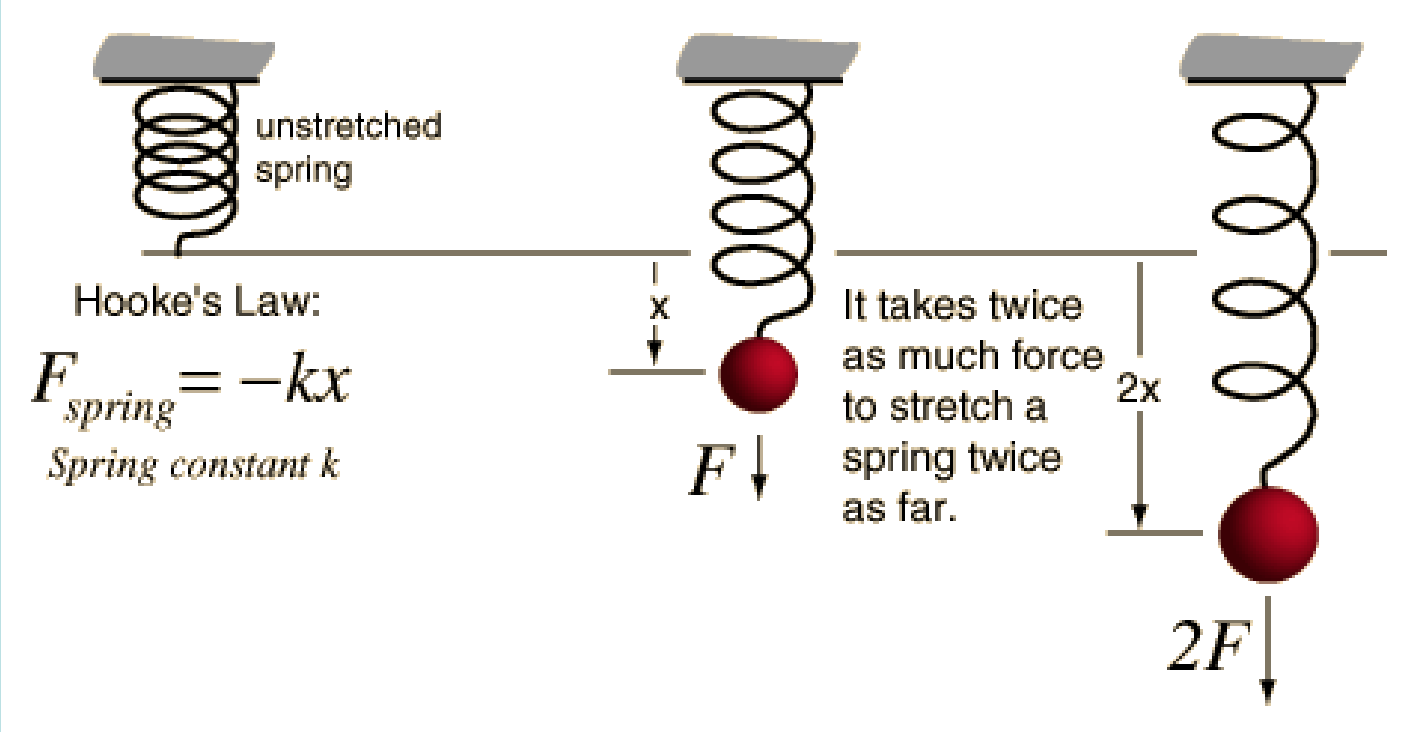
# Physical grounds: constitutive laws

# 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

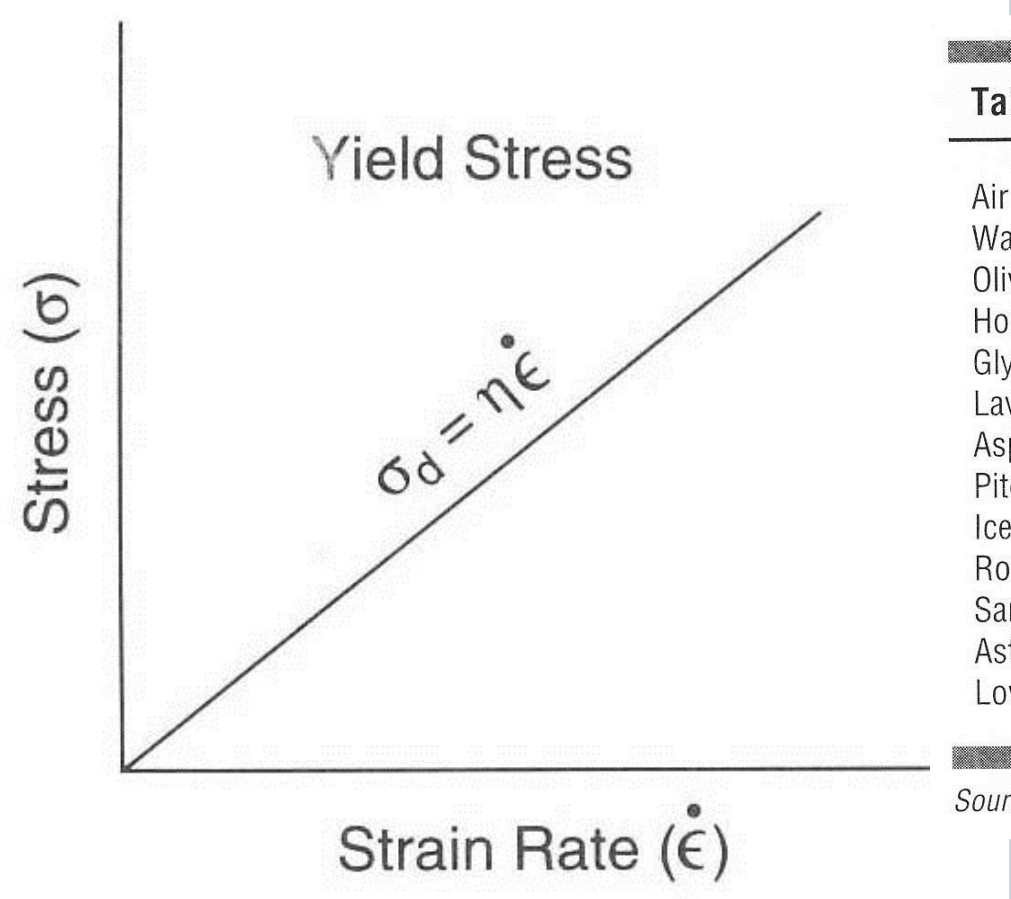
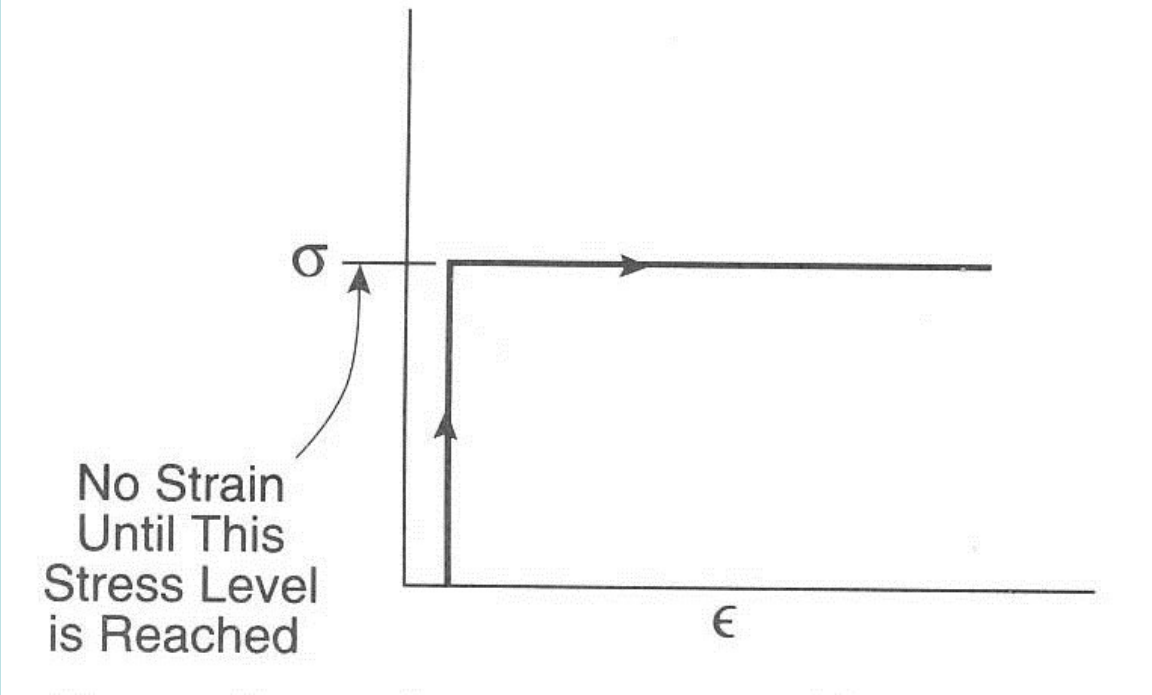



**Table 5.5** Some Representative Viscosities (in Pa · s)

| | |
|---|---|
| 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

$$\tau_{II} = \sqrt{\frac{1}{2}\tau_{ij}\tau_{ij}}$$

# Superposition of constitutive laws

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

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

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

# 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

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

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

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$$\uparrow$$

$$\dot{\varepsilon}^d_{ij}$$

# Full set of equations

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

mass

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

momentum

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

$$\tau_{ij} = \eta\left(\frac{\square v_i}{\square x_j} + \frac{\square v_j}{\square x_i}\right) - \cancel{\frac{2}{3}\eta\delta_{ij}\frac{\square v_k}{\square x_k}}$$

# Navier -Stokes equations

Continuity equation

$$\frac{\partial v_i}{\partial x_i} = 0$$

mass

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

momentum

Navier- Stokes equations

# Stokes equations

Continuity equation

$$\frac{\partial v_i}{\partial x_i} = 0$$

mass

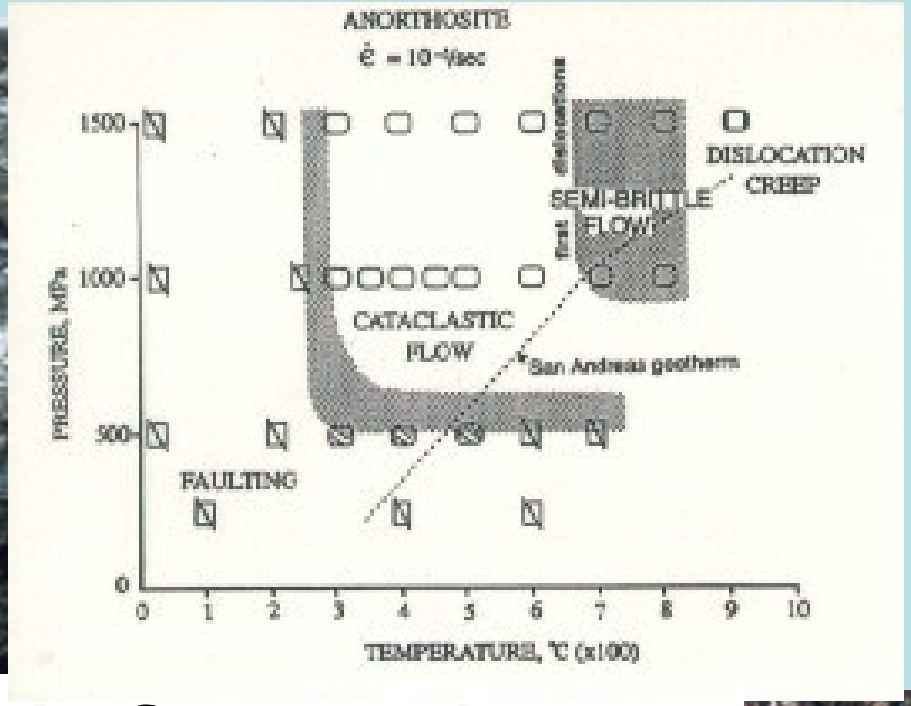
$$-\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right) + \rho g_i = 0$$

momentum

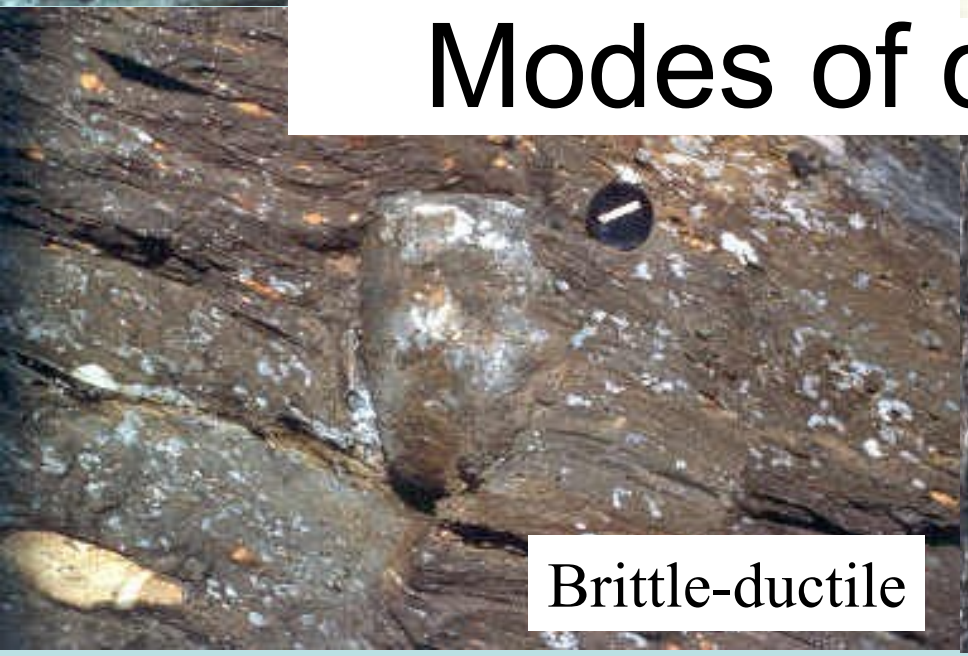
Stokes equations

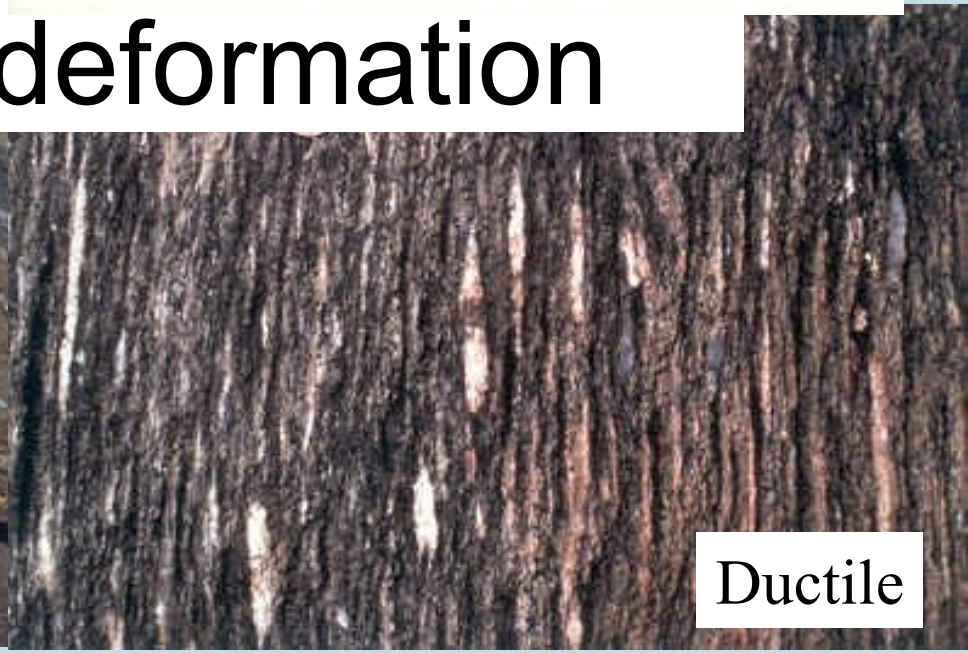
# How Does Rock Flow?

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




# Modes of deformation



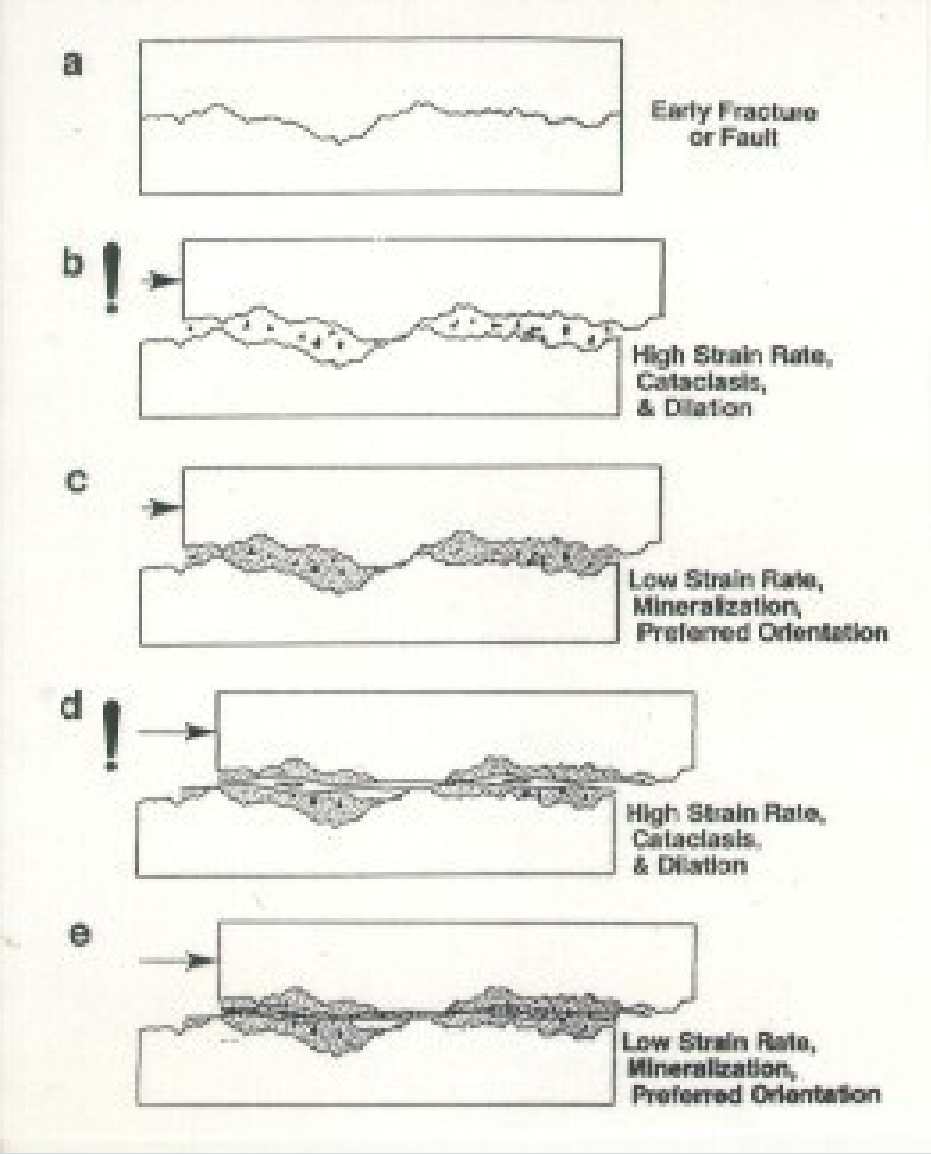



# Deformation Mechanisms

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

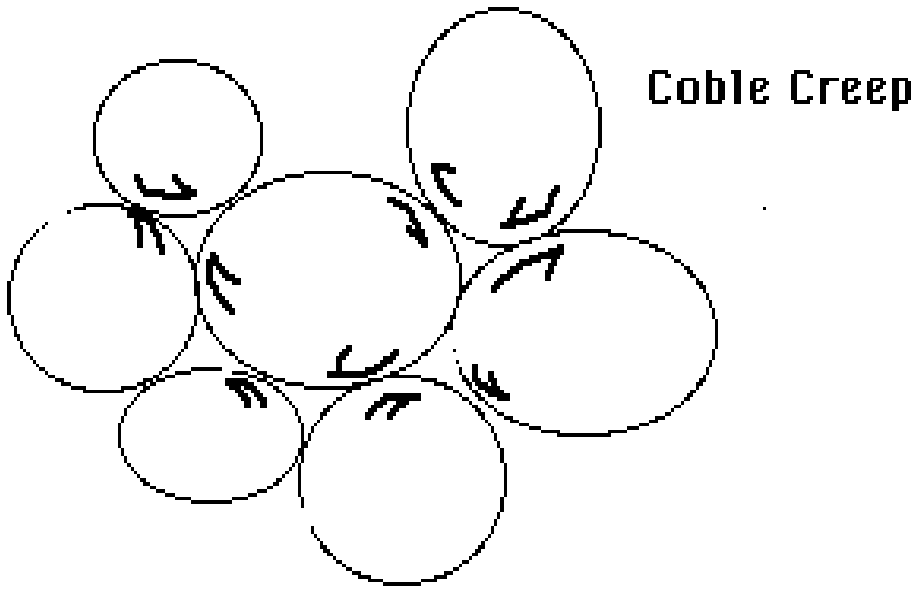
# Cataclasis

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



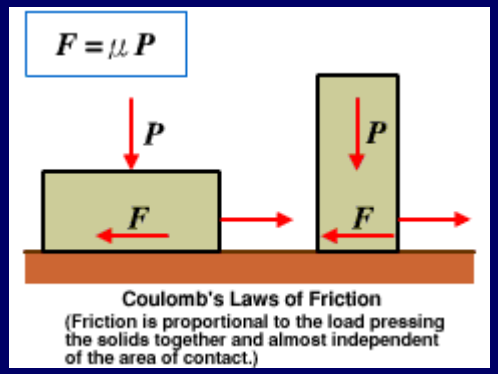
# Frictional grain-boundary sliding

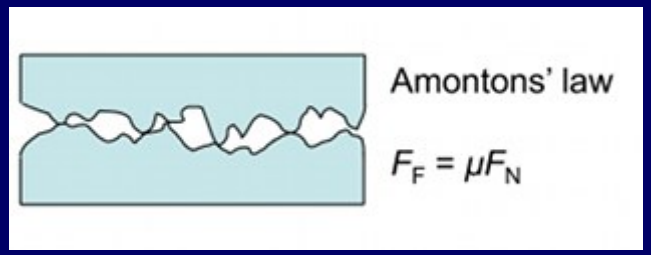
- Involves the sliding of grains past each other - enhanced by films on the grain boundaries.




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

# Friction law

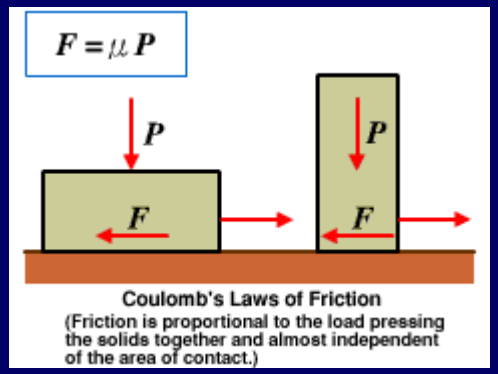


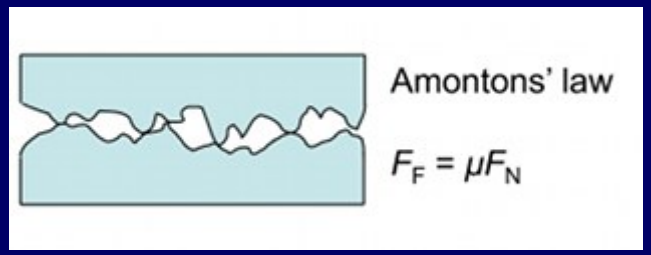




Brittle rheology:
Mohr-Coulomb (friction)
plasticity

$$\tau = c + \mu \cdot \sigma_n \approx c + \mu \cdot P$$

# Friction law



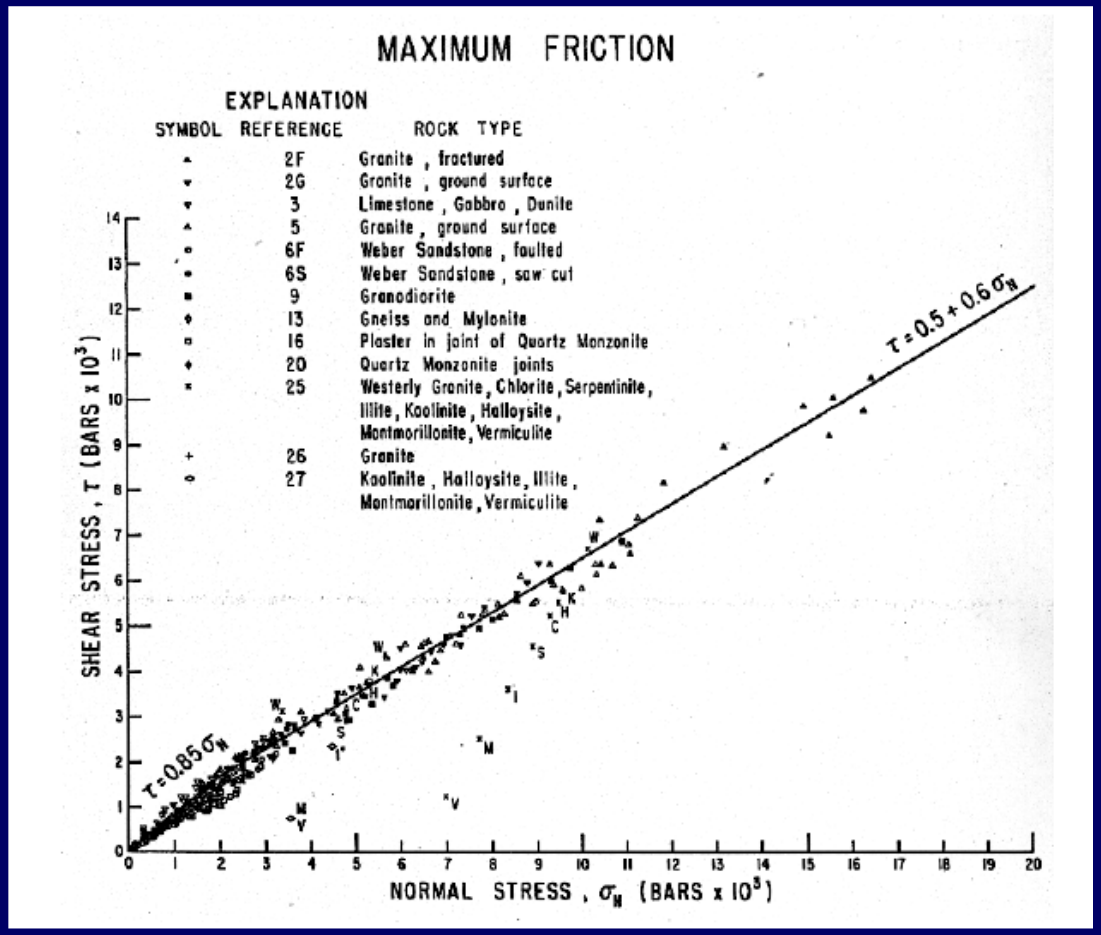

Brittle rheology:
Mohr-Coulomb (friction)
plasticity

$$\tau = c + \mu \cdot \sigma_n \approx c + \mu \cdot P$$

$\mu$ → Coefficient of friction

# Friction law

Byerlee, 1978




$\mu$ is about 0.6 for dry rocks

# Friction in presence of fluid

$$\tau = c + \mu \cdot (\sigma_n - P_f)$$

$$\tau = c + \mu_{eff} \cdot \sigma_n$$

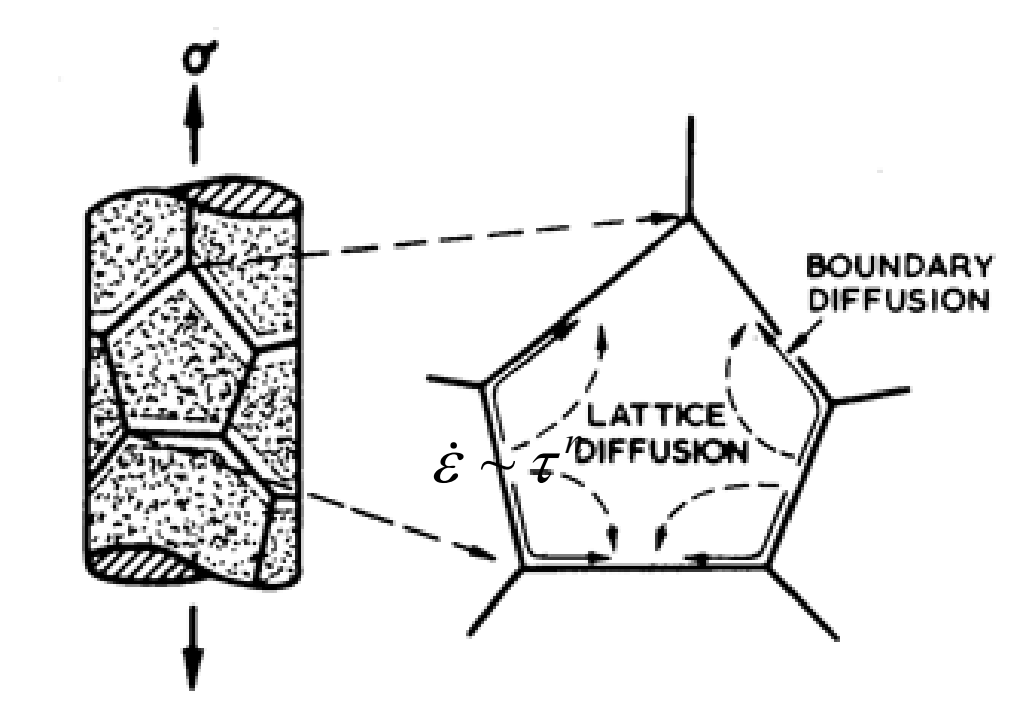
$$\mu_{eff} = \mu \cdot (1 - P_f / \sigma_n)$$

Assume $\mu$ = 0.6, $p_f$=0.95$\sigma_n$ ,

then $\mu_{eff}$ = 0.03

# 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:

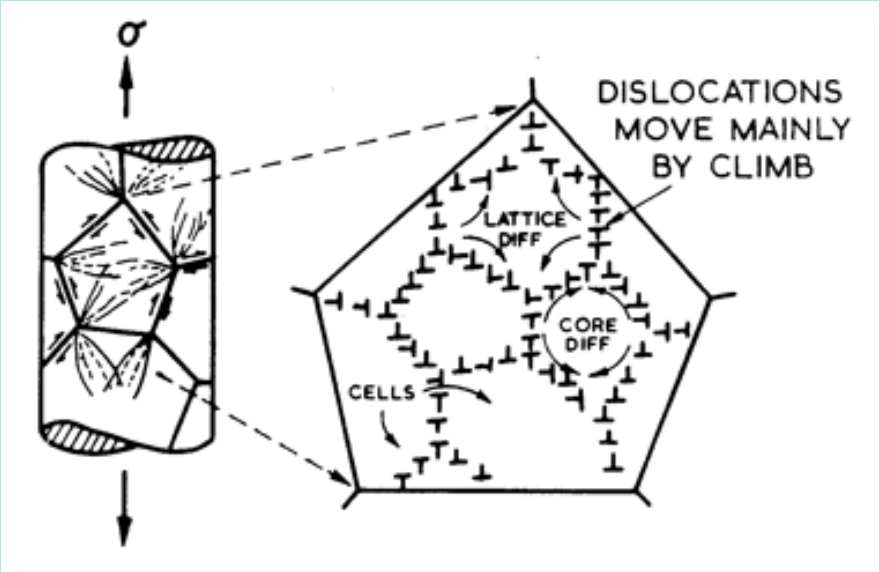



$$\dot{\varepsilon} \sim \tau$$

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

# 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 :




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

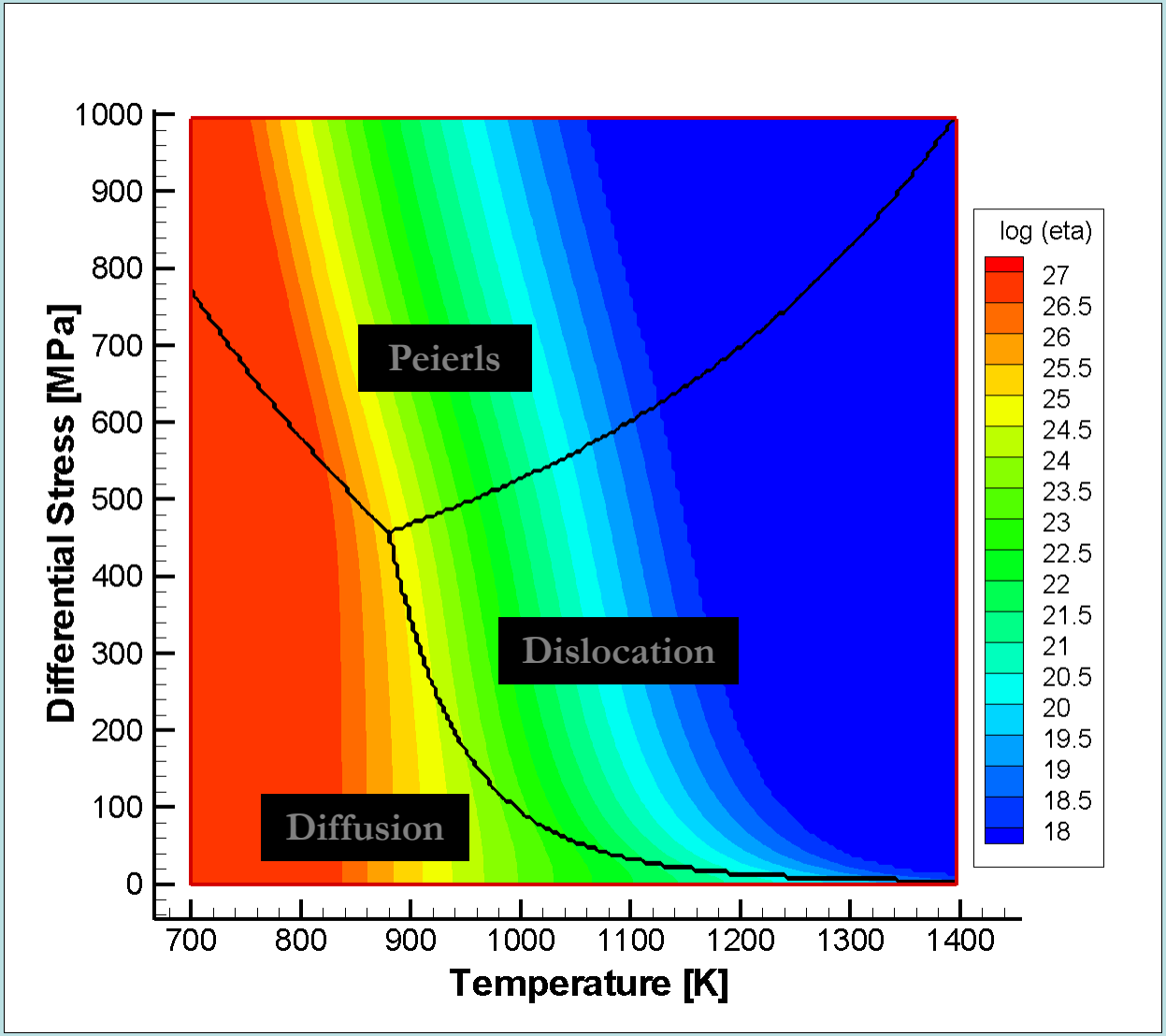
$$\dot{\varepsilon}_N = B_N \left(\tau_{II}\right)^n \exp\left(-\frac{H_N}{RT}\right)$$

# 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.

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

# Three creep processes




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

## 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

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

Von Mises yield criterion

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

softening

# Final effective viscosity

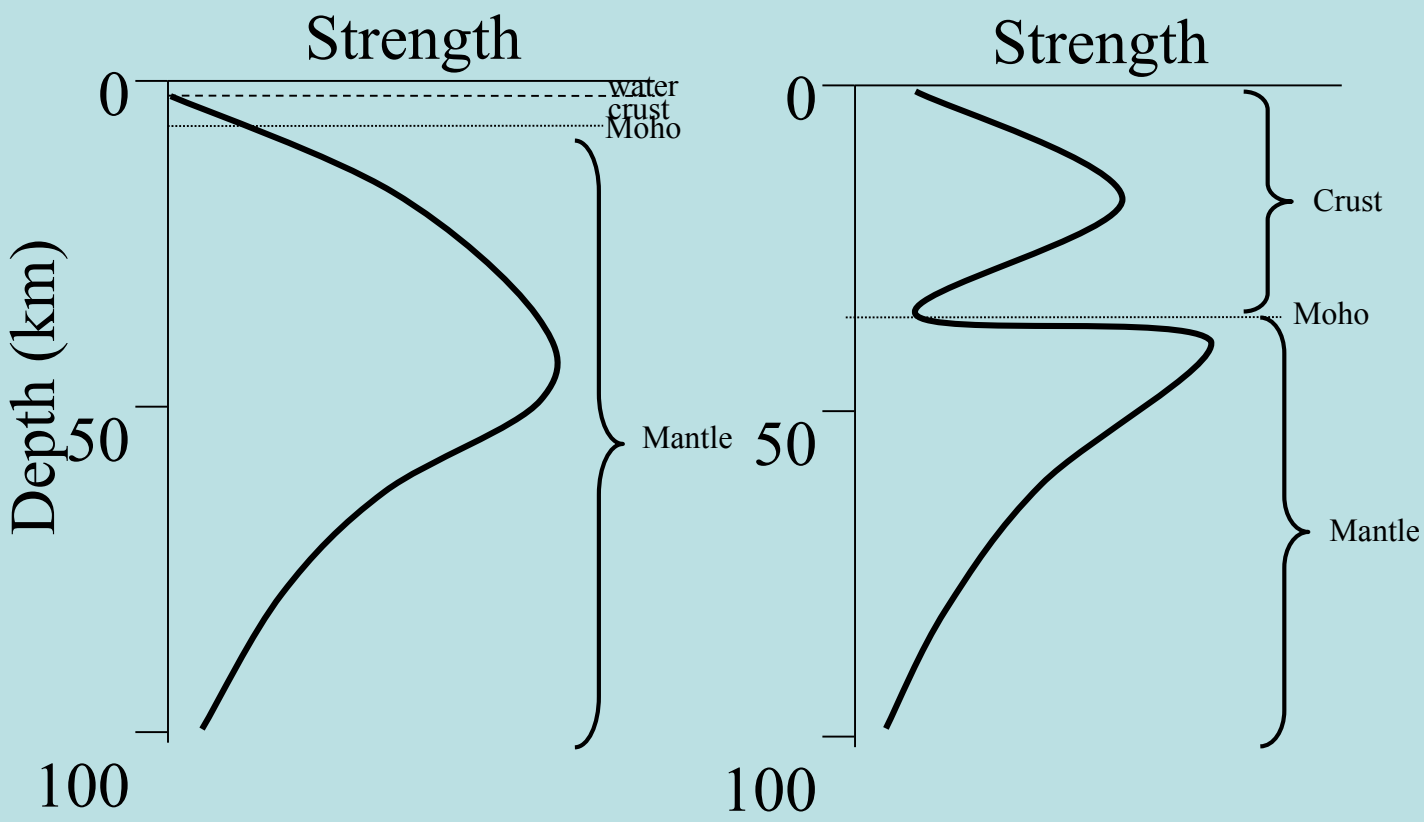
$$\frac{1}{2\eta_{eff}} = (\dot{\varepsilon}_L + \dot{\varepsilon}_N + \dot{\varepsilon}_P + \dot{\gamma}) / \tau_{II}$$

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

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

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

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

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

# Strength envelope