

VORLESUNG 7

Vorlesung
Humboldt-Universität zu Berlin
Institut für Physik

Biologische Physik

Die Dynamik biologischer Prozesse im menschlichen Körper

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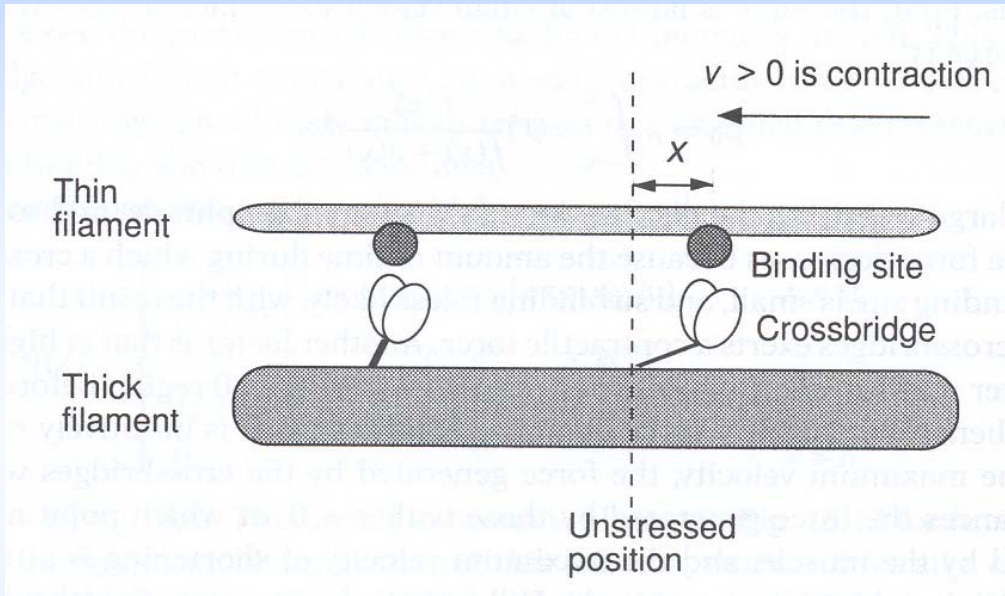


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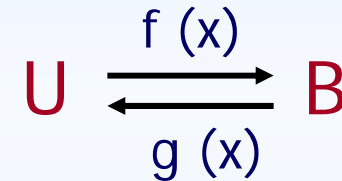
4.4 The Huxley Model

schematic diagram of the crossbridge model:



crossbridge can be only in one of two states:

- U ... unbound
- B ... bound



$n(x, t)$... the fraction of crossbridges with displacement x that are bound

$$\frac{\partial n}{\partial t} - v(t) \frac{\partial n}{\partial x} = (1 - n)f(x) - ng(x)$$

total force exerted by the muscle:

steady state, $v = \text{const}$:

$$-v \frac{dn}{dx} = (1 - n)f(x) - ng(x)$$

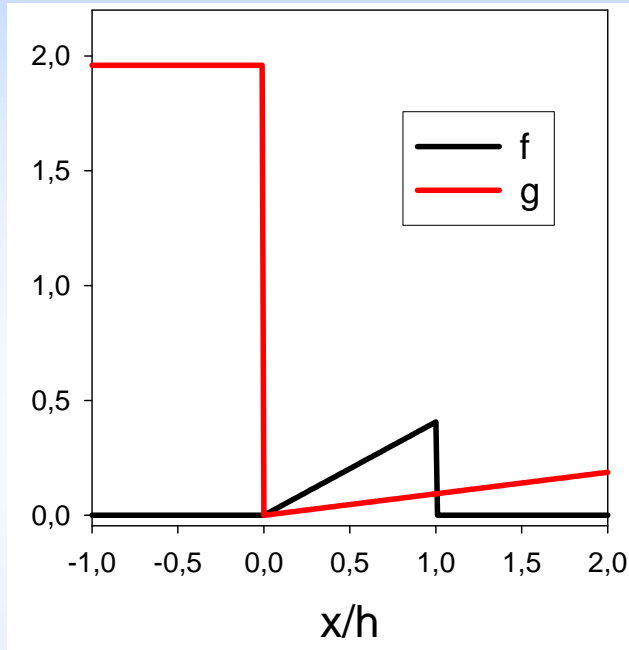
$$p = \rho \int_{-\infty}^{+\infty} r(x) n(x, t) dx$$





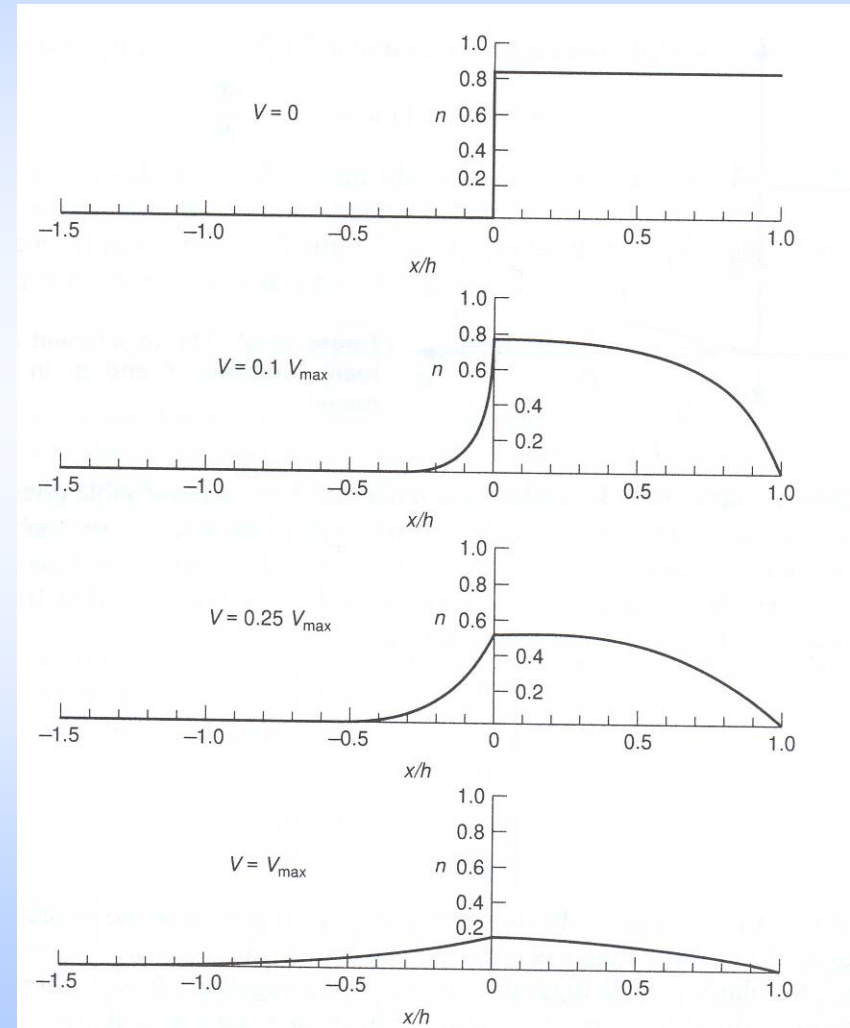
4.4 The Huxley Model

attachment and detachment functions, f and g :



solution:

$$n(x) = \begin{cases} \frac{f_1}{f_1 + g_1} [1 - \exp(-\phi/v) \exp(g_2 x / v)] & x < 0 \\ \frac{f_1}{f_1 + g_1} \left[1 - \exp\left(\left(\frac{x^2}{h^2} - 1\right) \frac{\phi}{v}\right) \right] & 0 < x < h \\ 0 & x > h \end{cases}$$

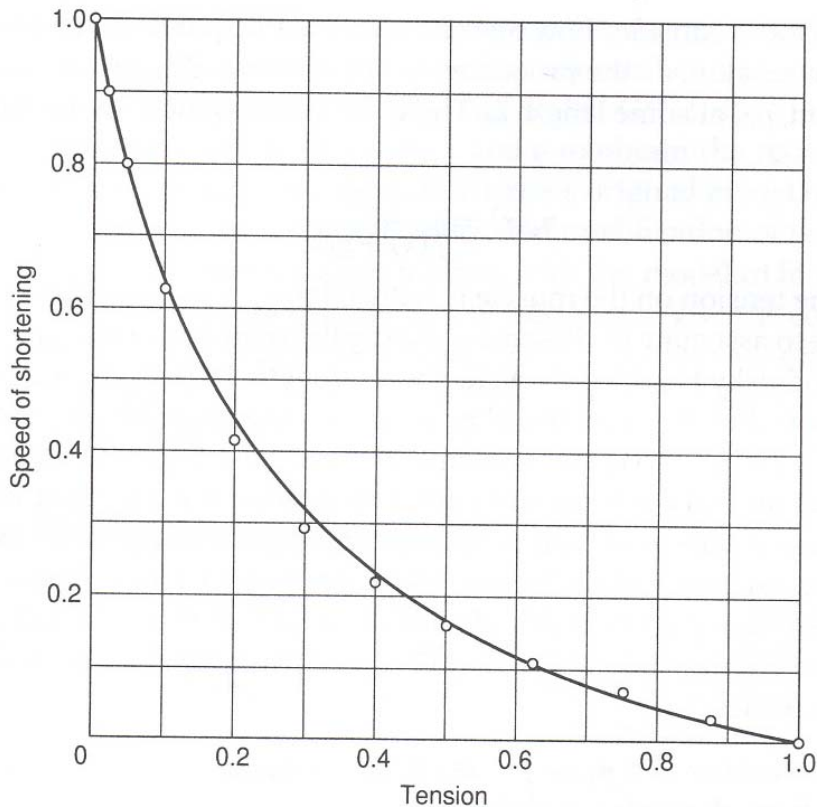




4.4 The Huxley Model

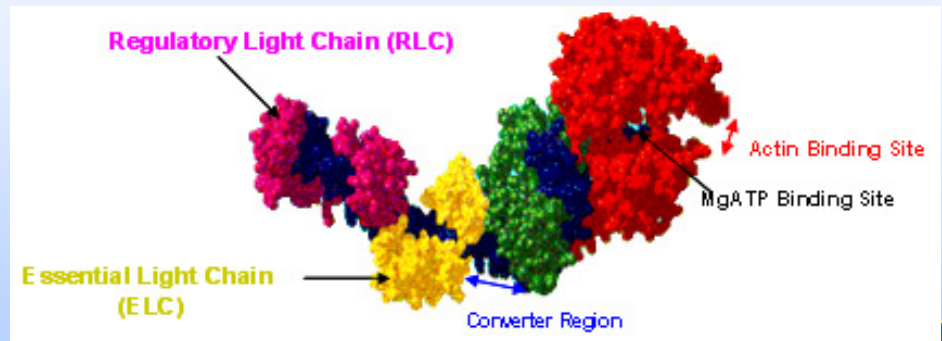
force-velocity equation calculated from the Huxley model:

$$\rho = \frac{\rho k f_1}{f_1 + g_1} \frac{h^2}{2} \left\{ 1 - \frac{v}{\phi} (1 - \exp(-\phi/v)) \left(1 + \frac{1}{2} \left(\frac{f_1 + g_1}{g_2} \right)^2 \frac{v}{\phi} \right) \right\}$$



OUTLOOK:

- inverse problem:
experimental data given –
calculate f, g
- using structural data to calculate f, g





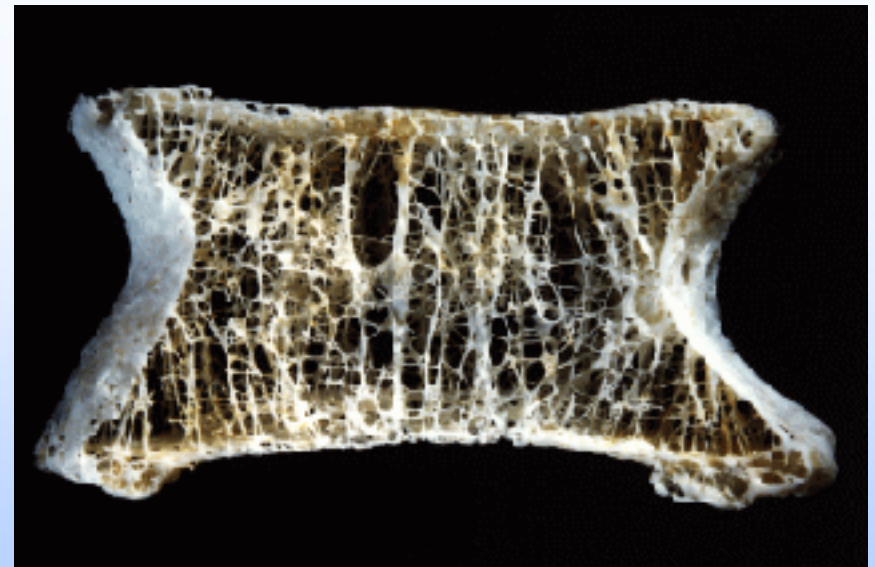
5 Bone

Why studying bone?

MEDICAL ISSUES

aging and bone diseases (like osteoporosis) lead to a

- loss in bone volume
- deterioration of the bone architecture
- deterioration of the bone material properties





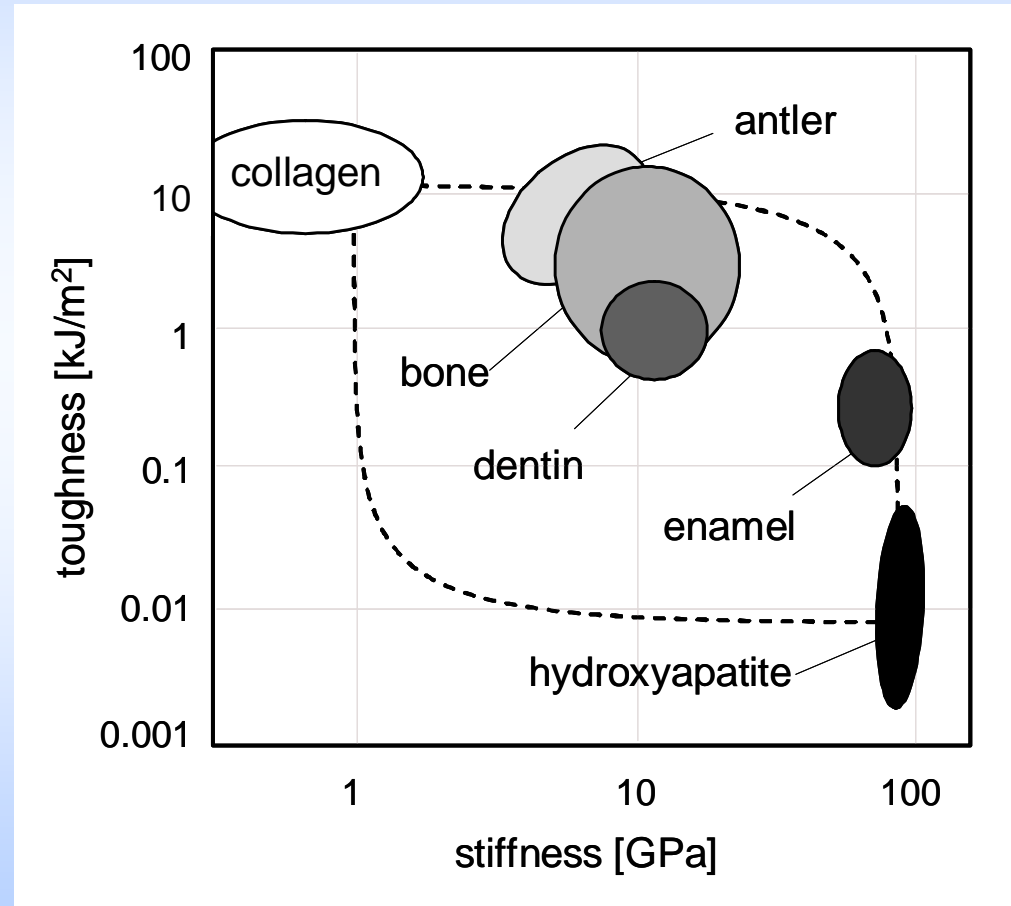
5 Bone

Why studying bone?

MATERIAL ISSUES

bone as a stiff and tough material

- hierarchical structured
- living
- intelligent/adaptive
- self-healing

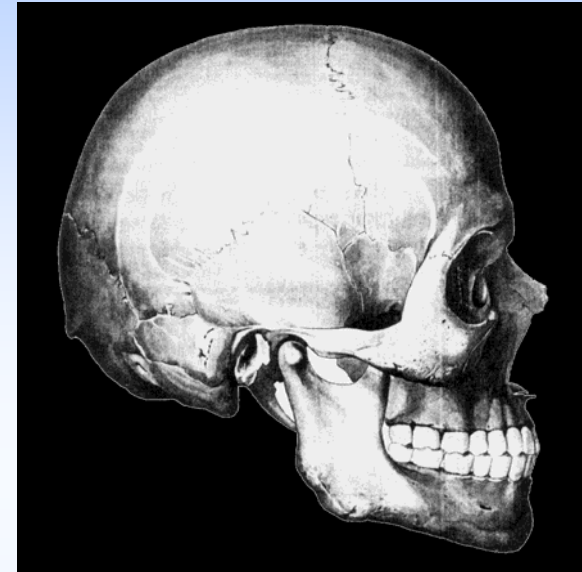
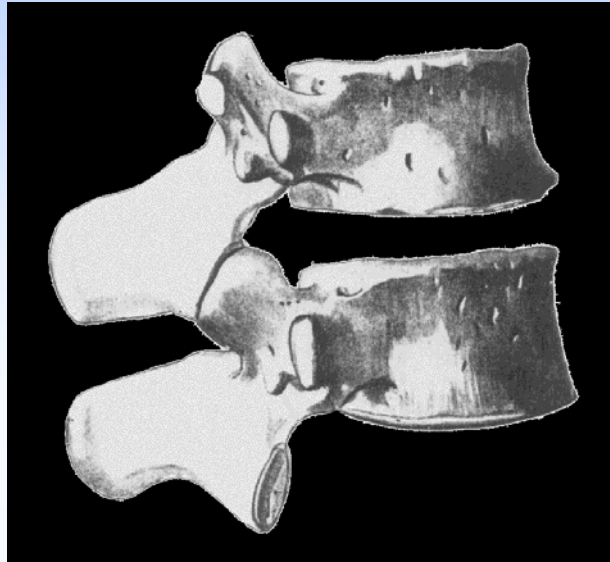


Fratzl, Weinkamer, Progress in Materials Science 52 (2007)





5.1 Bone – hierarchical structure



short

plate-like

long

Fratzl, Weinkamer,
Progress in Materials Science 52 (2007)

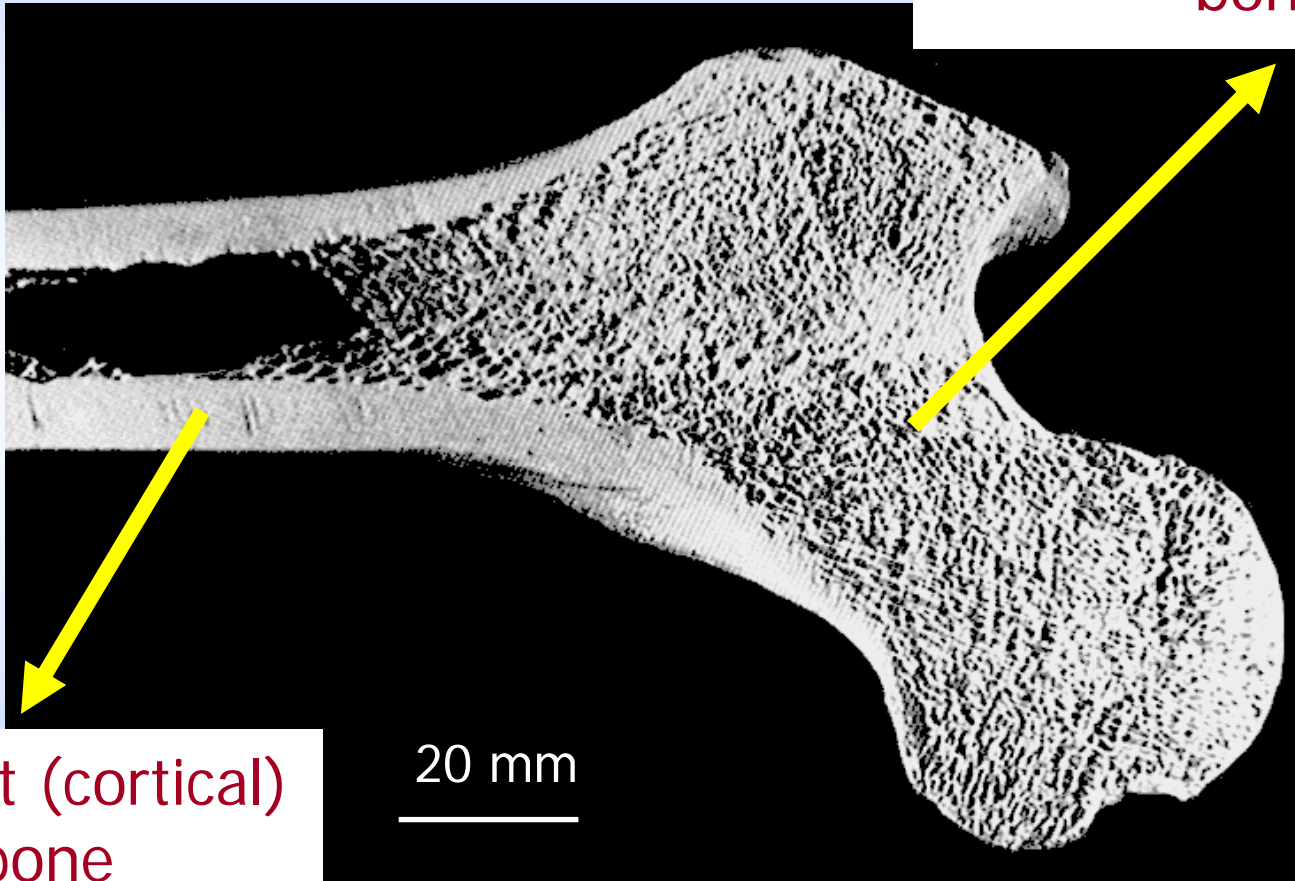




5.1 Bone – hierarchical structure

human femur (cross-section):

trabecular (cancellous)
bone



compact (cortical)
bone

20 mm

Fratzl, Weinkamer,
Progress in Materials Science 52 (2007)

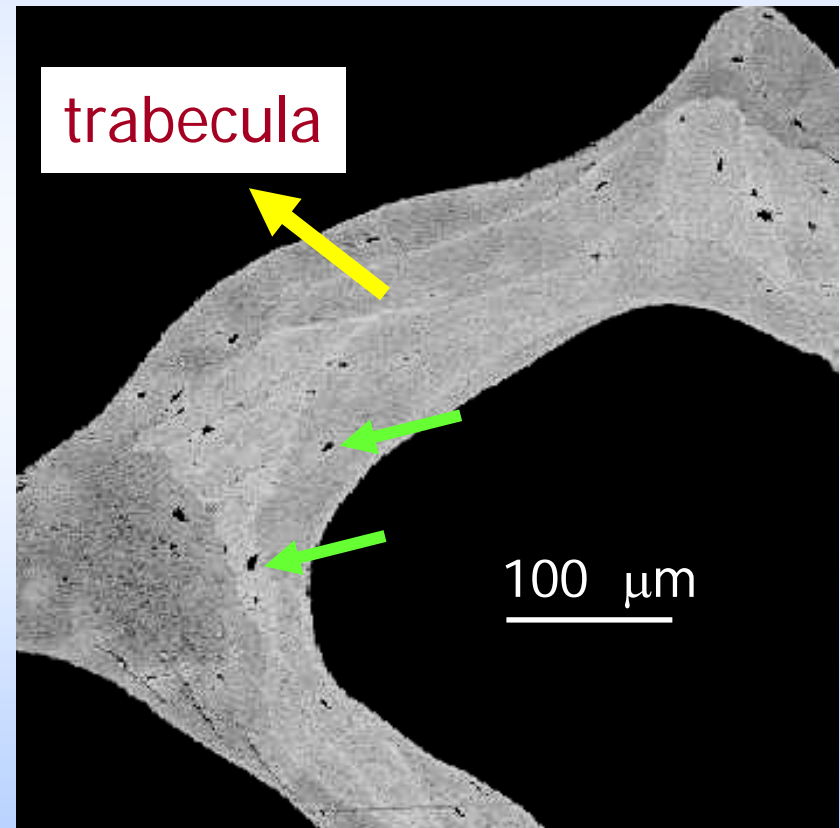
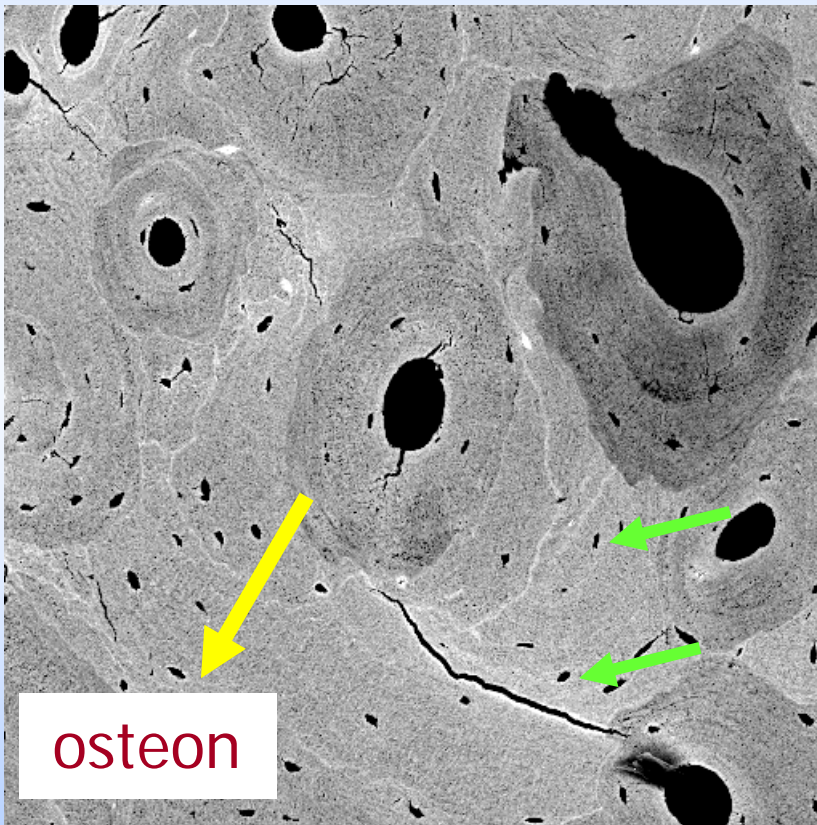




5.1 Bone – hierarchical structure

compact (cortical)
bone

trabecular (cancellous)
bone



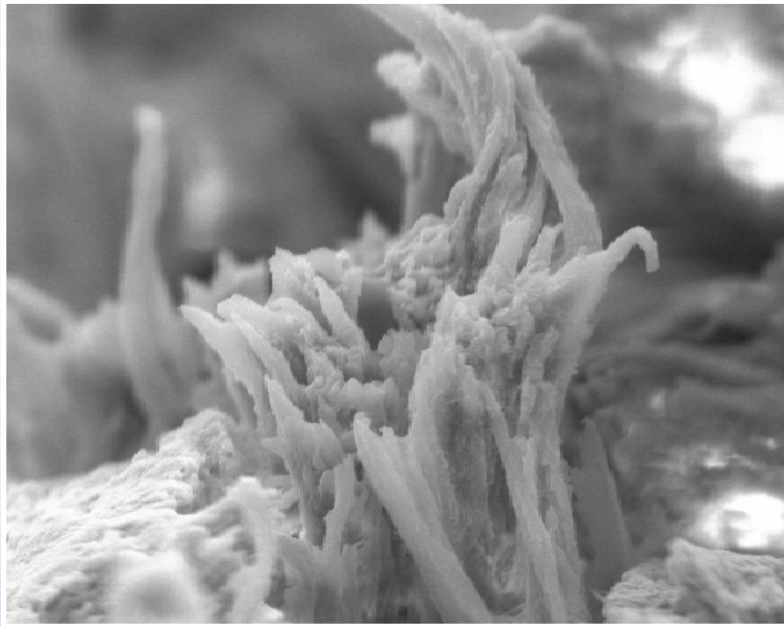
Fratzl, Weinkamer,
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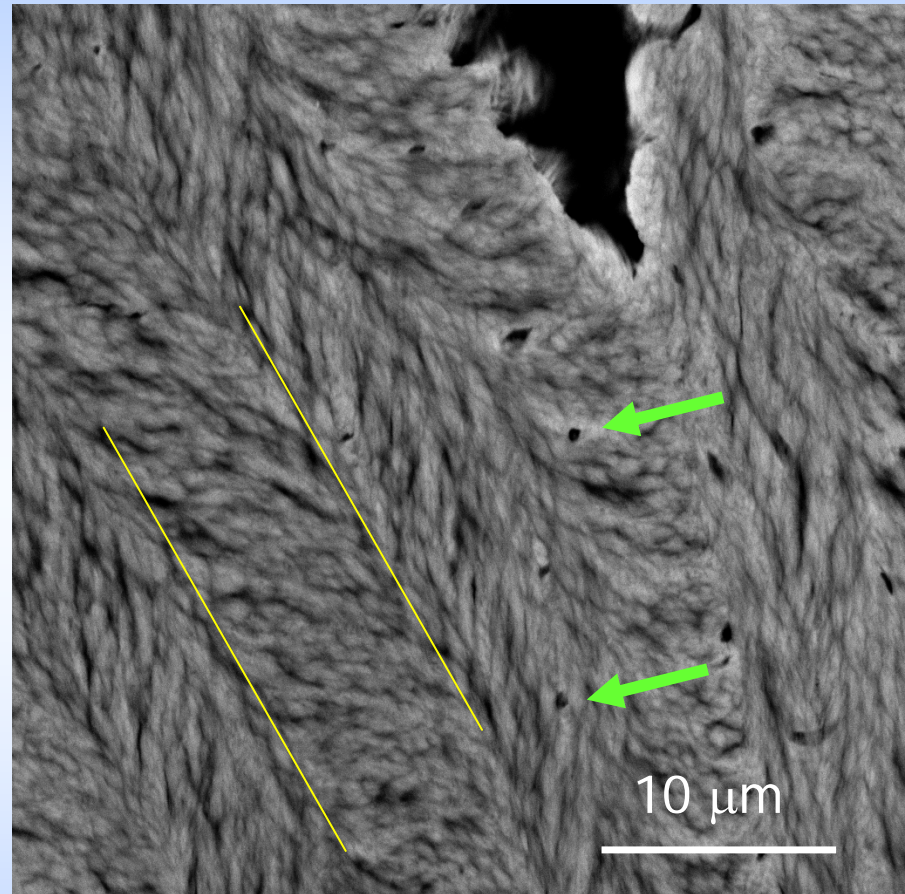


5.1 Bone – hierarchical structure

fracture surface:



mineralized collagen fibril



lamellar arrangement

SEM images courtesy of Paul Roschger, LBIO, Vienna;
Fratzl, Weinkamer, Prog Mat Sci 52 (2007)





5.1 Bone – hierarchical structure

nano-composite:



calcium-phosphate
particles with
thickness = 2 – 4 nm

collagen molecules
(triple-helices)
300 nm long

adapted from Landis et al.,
Microsc Res Tech 33 (1996)



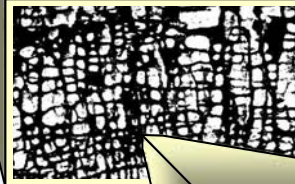


10 cm



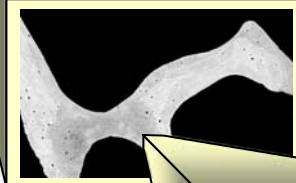
human vertebra

5.1 Bone – hierarchical structure



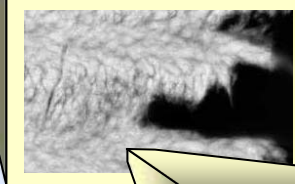
10 mm

trabecular bone



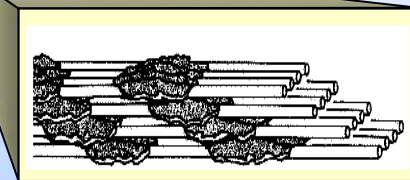
500 μm

trabecula



20 μm

lamellar structure



100 nm

nano-composite:
collagen fibrils +
mineral crystals

different motifs:

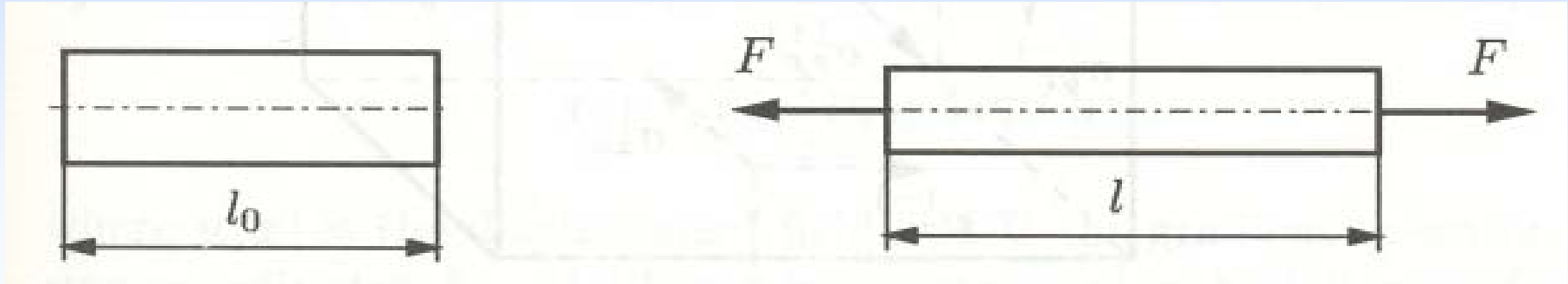
- cellular structure
- fiber structure
- nano-composite





mechanics: elasticity theory

uniaxial tension test:



relation between „forces“ and „deformations“

(uniaxial) stress, i.e.,
an internal force F per unit area

$$\tau_{11} = \frac{F}{A}$$

dimensionless strain reflecting
the relative elongation

$$\varepsilon_{11} = \frac{(l - l_0)}{l_0}$$



generalization to multi-axial loading





stress

isolating a parallelepiped with dimensions $dx \times dy \times dz$

stress tensor:

$$\tau(x) = \begin{pmatrix} \tau_{11}(x) & \tau_{12}(x) & \tau_{13}(x) \\ \tau_{12}(x) & \tau_{22}(x) & \tau_{23}(x) \\ \tau_{13}(x) & \tau_{23}(x) & \tau_{33}(x) \end{pmatrix}$$

$$t^{(x)} = \frac{f}{dy dz} =$$

$$= \tau_{11} e_1 + \tau_{12} e_2 + \tau_{13} e_3 = \tau \cdot e_1$$

in general: traction vector t ,

i.e. the force per unit area acting on a facet with unit normal n

$$t = \tau \cdot n$$

σ in the figure corresponds to the stress τ

deviatoric stress tensor s (traceless)

$$\tau_{xx}^{(\pm)} = \tau_{xx} \pm \frac{\partial \tau_{xx}}{\partial x} \frac{dx}{2}$$

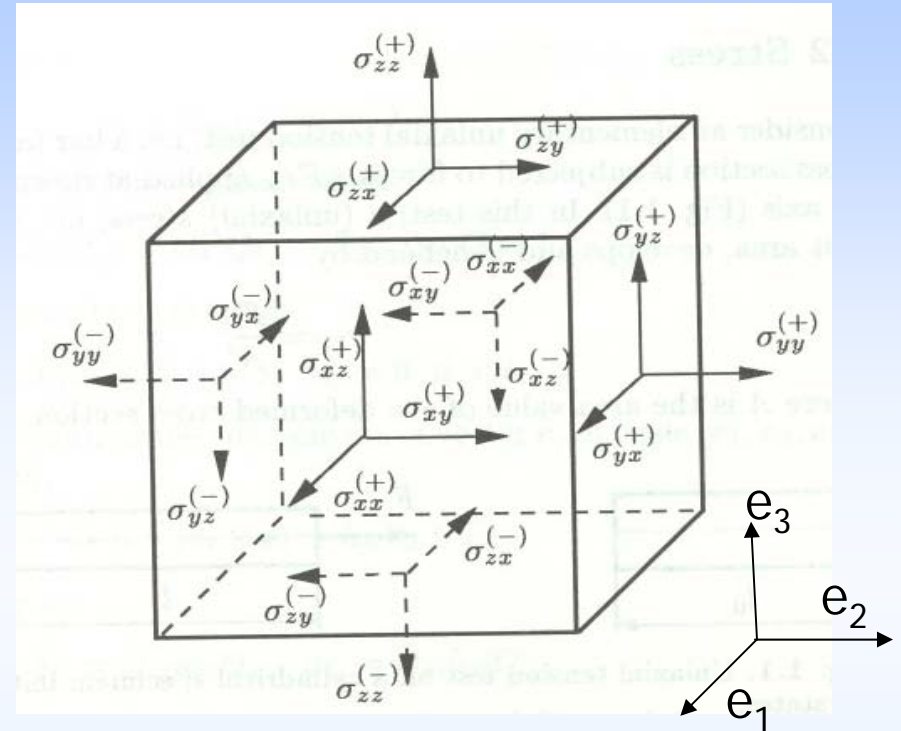
$$s \equiv \tau - \frac{1}{3} (tr \tau) I \quad \text{i.e.,} \quad s_{ij} \equiv \tau_{ij} - \frac{1}{3} (\tau_{mm}) \delta_{ij}$$

equilibrium

(without volume forces)

$$\nabla \cdot \tau = 0 \quad \text{or} \quad div \tau = 0$$

$$\text{i.e.,} \quad \frac{\partial \tau_{ij}}{\partial x_j} = 0$$





strain

(infinitesimal case)

$$\varepsilon(x) = \frac{1}{2} \left[\nabla u(x) + \nabla u(x)^T \right] \quad \text{i.e.,} \quad \varepsilon_{ij} = \frac{1}{2} \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right]$$

strain tensor:

$$\varepsilon(x) = \begin{pmatrix} \varepsilon_{11}(x) & \varepsilon_{12}(x) & \varepsilon_{13}(x) \\ \varepsilon_{12}(x) & \varepsilon_{22}(x) & \varepsilon_{23}(x) \\ \varepsilon_{13}(x) & \varepsilon_{23}(x) & \varepsilon_{33}(x) \end{pmatrix}$$

interpretation:

diagonal strain components: $\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}$

relative length variation in the directions of the coordinate system

non-diagonal strain components – shear strain: $\varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}$

angle variation

e_1, e_2 transforms onto e'_1, e'_2 \rightarrow $\varepsilon_{12} = \frac{1}{2} e'_1 \cdot e'_2$

$tr \varepsilon$ measures the variation of the volume: $tr \varepsilon \approx \frac{dV - dV_0}{dV_0}$

deviatoric strain tensor e (traceless)

$$e \equiv \varepsilon - \frac{1}{3} (tr \varepsilon) I \quad \text{i.e.,} \quad e_{ij} \equiv \varepsilon_{ij} - \frac{1}{3} (\varepsilon_{mm}) \delta_{ij}$$





local formulation of the elastic problem:

boundary conditions: (well posed)

$$u_i = U_i \quad \text{on } \partial N_U$$

$$\tau_{ij} n_j = F_i \quad \text{on } \partial N_F$$

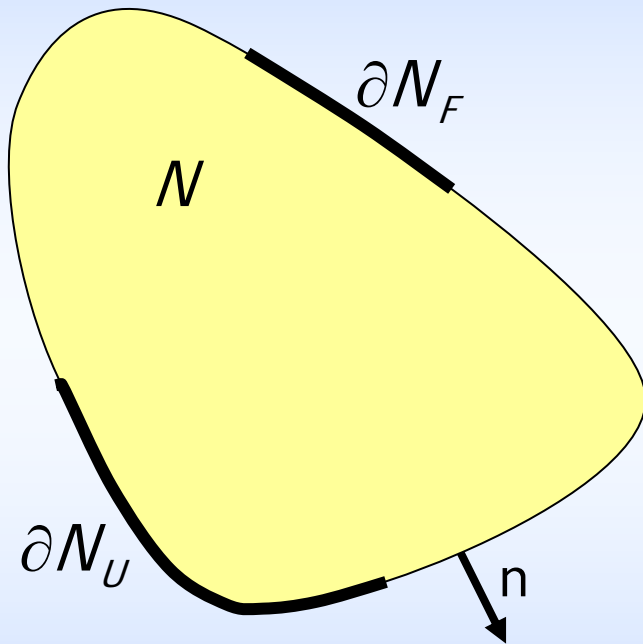
equilibrium:

$$\frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad \text{in } N$$

infinitesimal strains:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \equiv u_{(i,j)}$$

„constitutive equations“





constitutive equations: linear elasticity

$$\begin{aligned}\tau(X) &= C(X) : \varepsilon(X) & \tau_{ij} &= C_{ijkl} \varepsilon_{lk} \\ \varepsilon(X) &= C^{-1}(X) : \tau(X) & C(X) &= C_1 I^{(1)}(X) + C_2 I^{(2)}(X)\end{aligned}$$

in N

stiffness tensor C_{ijkl} (Hooke's operator)

$$\tau_{ij} = C_{ijkl} \varepsilon_{lk}$$

C_{ijkl} fourth-order tensor

$$d^4 = 3^4 = 81 \text{ components}$$

symmetries:

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$$



reduction to
21 components

strain energy density function u :

$$\tau_{ij} = \frac{\partial u}{\partial \varepsilon_{ij}} \quad \longrightarrow \quad u = \frac{1}{2} \tau_{ij} \varepsilon_{ij} = \frac{1}{2} \varepsilon_{kl} C_{ijkl} \varepsilon_{ij} \geq 0$$





stiffness tensor C_{ijkl} (Hooke's operator)

$$\begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \\ \tau_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

$$\tau_1 = \tau_{11}, \tau_2 = \tau_{22}, \tau_3 = \tau_{33}, \tau_4 = \tau_{23}, \tau_5 = \tau_{13}, \tau_6 = \tau_{12}$$

$$\varepsilon_1 = \varepsilon_{11}, \varepsilon_2 = \varepsilon_{22}, \varepsilon_3 = \varepsilon_{33}, \varepsilon_4 = 2\varepsilon_{23}, \varepsilon_5 = 2\varepsilon_{13}, \varepsilon_6 = 2\varepsilon_{12}$$

replacing the subscripts ij by p using the following rules:

$$11 \leftrightarrow 1, 22 \leftrightarrow 2, 33 \leftrightarrow 3, 13 \text{ or } 31 \leftrightarrow 5, 23 \text{ or } 32 \leftrightarrow 4, 12 \text{ or } 21 \leftrightarrow 6$$

➔ further reduction of independent components due to symmetries





isotropic elasticity

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(C_{11} - C_{12}) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(C_{11} - C_{12}) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(C_{11} - C_{12}) \end{bmatrix}$$

only two constants:

Lamé coefficients λ and μ : $\lambda = C_{12}$, $\mu = \frac{1}{2}(C_{11} - C_{12})$ ($C_{11} = \lambda + 2\mu$)

$$\tau = \lambda (tr \varepsilon) I + 2\mu \varepsilon \quad \text{or} \quad \tau_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij}$$

$$\varepsilon = -\frac{\lambda}{2\mu(3\lambda + 2\mu)} (tr \tau) I + \frac{1}{2\mu} \tau \quad \text{or} \quad \varepsilon_{ij} = -\frac{\lambda}{2\mu(3\lambda + 2\mu)} \tau_{kk} \delta_{ij} + \frac{1}{2\mu} \tau_{ij}$$





isotropic elasticity

only two constants: λ ... Lamé coefficient
 μ ... Lamé coefficient

E ... Young's modulus
 ν ... Poisson's ratio

$$E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \quad \nu = \frac{\lambda}{2(\lambda + \mu)}$$

$$\tau = \frac{E\nu}{(1+\nu)(1-2\nu)} (tr \varepsilon) I + \frac{E}{1+\nu} \varepsilon \quad \text{or} \quad \tau_{ij} = \frac{E\nu}{(1+\nu)(1-2\nu)} \varepsilon_{kk} \delta_{ij} + \frac{E}{1+\nu} \varepsilon_{ij}$$

$$\varepsilon = -\frac{\nu}{E} (tr \tau) I + \frac{1+\nu}{E} \tau \quad \text{or} \quad \varepsilon_{ij} = -\frac{\nu}{E} \tau_{kk} \delta_{ij} + \frac{1+\nu}{E} \tau_{ij}$$

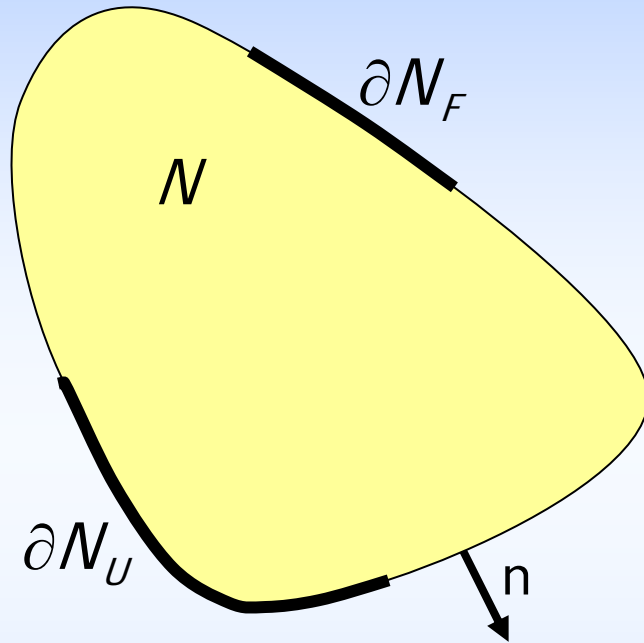
K ... bulk modulus
 G ... shear modulus

$$K = \frac{E}{3(1-2\nu)} \quad G = \frac{E}{2(1+\nu)} = \mu$$





local formulation of the elastic problem



unknowns:

- stress (6)
- strain (6)
- displacements (3)

boundary conditions: (well posed)

$$u_i = U_i \quad \text{on } \partial N_U$$

$$\tau_{ij} n_j = F_i \quad \text{on } \partial N_F$$

equilibrium:

$$\frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad \text{in } N$$

infinitesimal strains:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \equiv u_{(i,j)}$$

„constitutive equations“

$$\tau_{ij} = C_{ijkl} \varepsilon_{lk}$$

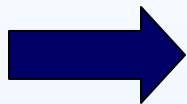




Navier equations

$$\frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad \tau_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} \quad \varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

$$\frac{\partial}{\partial x_j} \left[\lambda \delta_{ij} \frac{\partial u_k}{\partial x_k} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] = 0$$



$$(\lambda + \mu) \frac{\partial}{\partial x_i} \left(\frac{\partial u_k}{\partial x_k} \right) + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} = 0$$

or

$$(\lambda + \mu) \nabla (\nabla \cdot u) + \mu \Delta u = 0$$

