Applications of Machine Learning in Mechanics of Materials

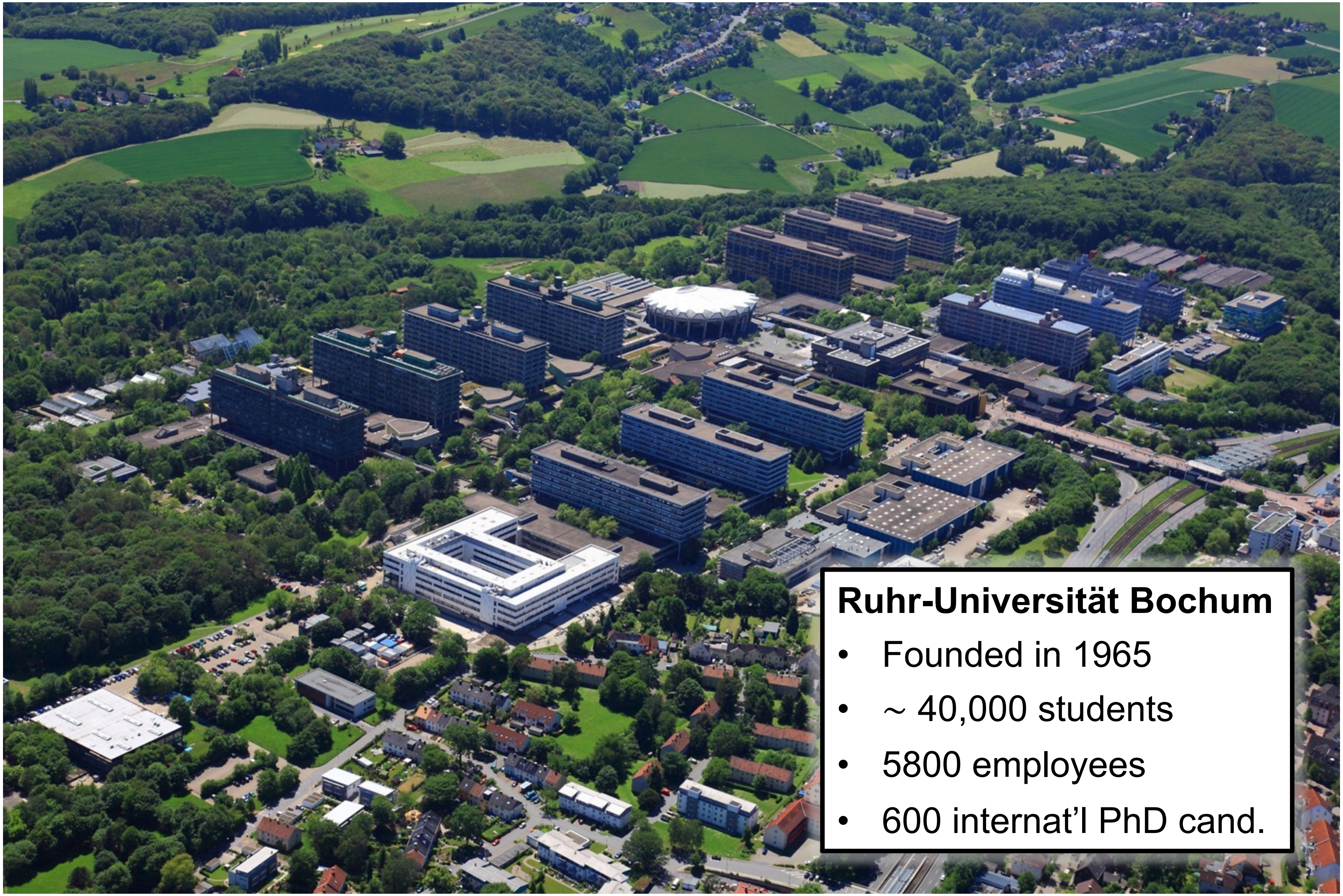
Alexander Hartmaier

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)

Ruhr-Universität Bochum
alexander.hartmaier@rub.de

Where Ruhr University is

Ruhr University Bochum, Germany



Ruhr-Universität Bochum, Germany

Chinese garden gifted by Tongji University, Shanghai

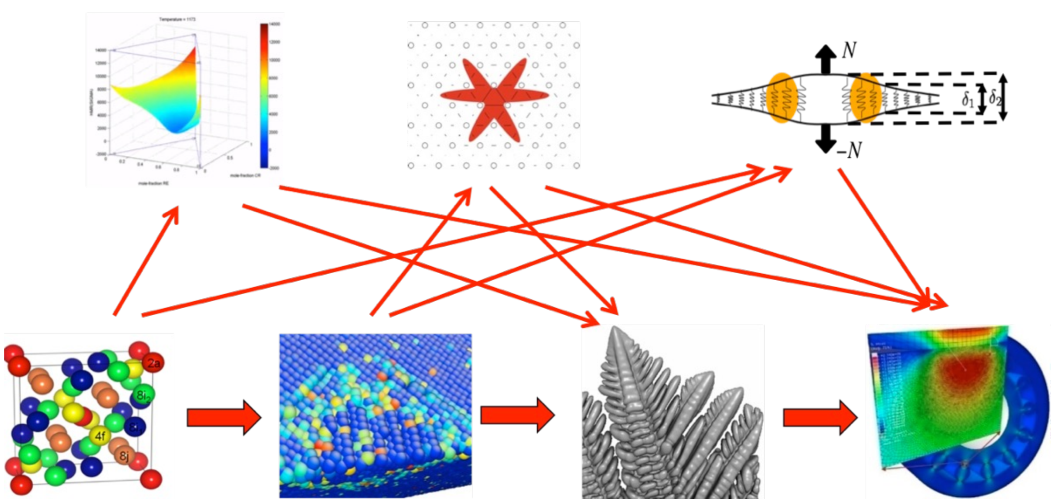
ICAMS

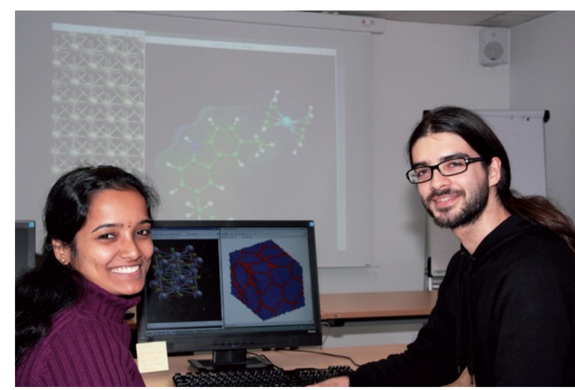
ICAMS has been founded in 2008 as private-public partnership of RUB with industrial consortium; since 2013 it is scientific unit of RUB

ICAMS develops scalebridging methods for materials modelling

ICAMS supports the design of technical materials

ICAMS educates talented students and young scientists





International Master’s course

MATERIALS SCIENCE AND SIMULATION (MSS)

- Combines materials science, physics, numerical methods, and programming
- Promotes practical implementation of knowledge
- International and interdisciplinary environment

https://mss.rub.de

Literature

Course material including numerical examples:

[Link to Binder]

[GitHub repository]

PDF's of lecture slides under docs.

Further reading:

- Nemat-Nasser, Hori:
  Micromechanics: Overall Properties of the Heterogeneous Materials
- Shaofan, Wang:
  Introduction to Micromechanics and Nanomechanics

Outline

Applications of Machine Learning in Mechanics of Materials

Part I
- Theoretical homogenization rules
- Micromechanical modeling

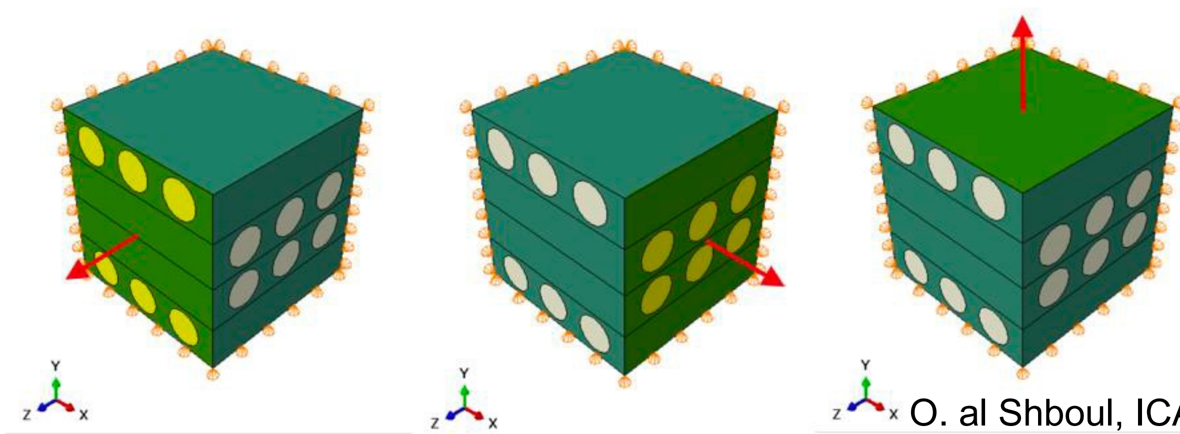
Part II
- Theory of Finite Element Analysis (FEA)
- Data generation

Part III
- Training of machine learning models
- Analysis of results

Theoretical homogenization rules

Motivation

- Effective properties of heterogeneous multiphase and polycrystalline materials can be calculated numerically by micromechanical modeling
- There exist also theoretical homogenization rules to estimate effective material properties of heterogeneous materials
- Theoretical homogenization rules are typically applied to composite materials with two distinctly different phases, e.g. glass or carbon fiber-reinforced plastics



O. al Shboul, ICAMS

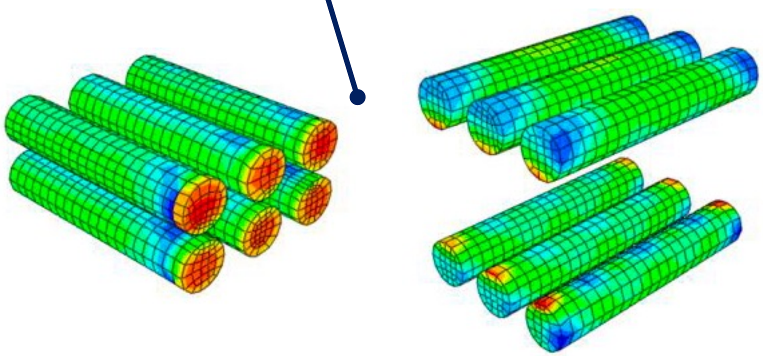
Example: Homogenization of density

Density

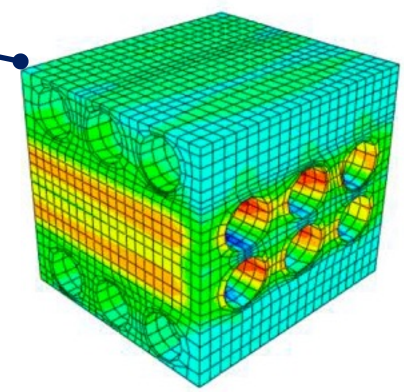
Mass: $m_c = m_f + m_m$

$$\rho_c = \frac{m_c}{V_c} = \frac{m_f + m_m}{V_c} = \frac{\rho_f V_f + \rho_m V_m}{V_c}$$

$$\boldsymbol{\rho_c = \rho_f f_f + \rho_m (1 - f_f)}$$ **(homogenization rule for density)**



fibers / filler



matrix

Theoretical homogenization rules

Elastic constants

- Rule of mixture for long fiber reinforced materials (iso-strain or Voigt model)
- Appropriate for properties along fiber direction

$$\varepsilon_f = \varepsilon_m = \varepsilon_c = \frac{\Delta L}{L} \quad \text{(iso-strain)}$$

$$F_c = F_f + F_m$$

Definition stress: $\sigma = F/A$

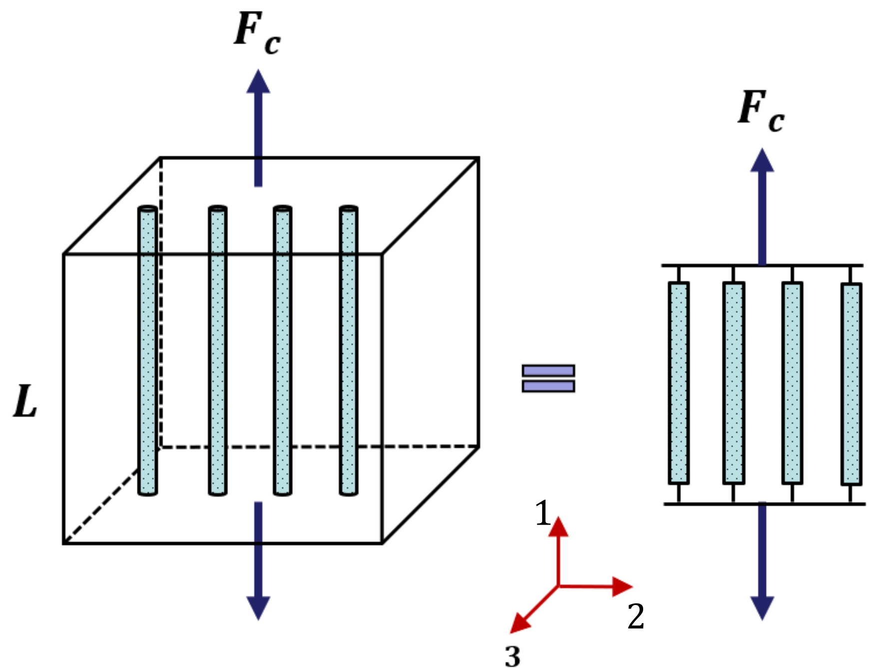
$$\sigma_c^l A_c = \sigma_f A_f + \sigma_m A_m$$

Assumption: $f_f = V_f/V_c \approx A_f/A_c$

Hooke's law and iso-strain:

$$\frac{\sigma_c^l}{\varepsilon_c^l} = E_c^l = \frac{\sigma_f\ f_f + \sigma_m f_m}{\varepsilon_c^l}$$

$$E_c^l = E_f f_f + E_m\left(1 - f_f\right) = E_{11}$$



(homogenization rule for elastic stiffness under iso-strain conditions)

Theoretical homogenization rules

Elastic constants

- Rule of mixture for long fiber reinforced materials (iso-stress or Reuss model)
- Rigorous derivation for laminates, lower bound for fiber reinforced materials

$\sigma_c^t = \sigma_f = \sigma_m$ (iso-stress)

$\Delta t_c = \Delta t_f + \Delta t_m$

Definition strain: $\varepsilon = \Delta t / t$

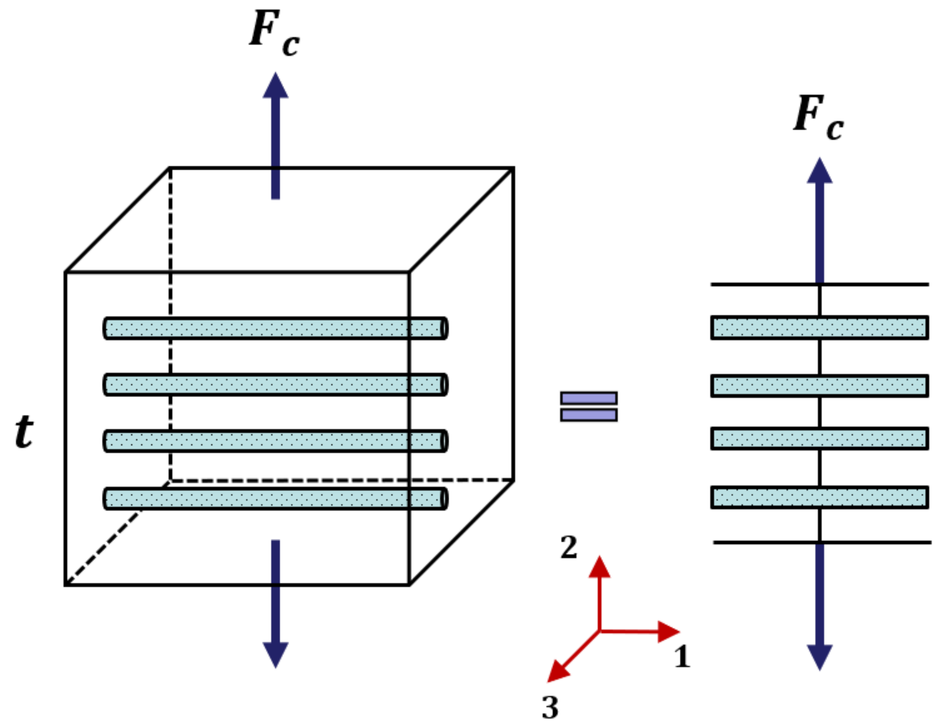
$\varepsilon_c^t t_c = \varepsilon_f t_f + \varepsilon_m t_m$

Assumption: $f_f = V_f / V_c \approx t_f / t_c$

Hooke's law and iso-stress:

$$\frac{\varepsilon_c^t}{\sigma_c^t} = \frac{1}{E_c^t} = \frac{\varepsilon_f \ f_f + \varepsilon_m f_m}{\sigma_c^t}$$

$$\frac{1}{E_c^t} = \frac{f_f}{E_f} + \frac{1 - f_f}{E_m} = \frac{1}{E_{22}}$$

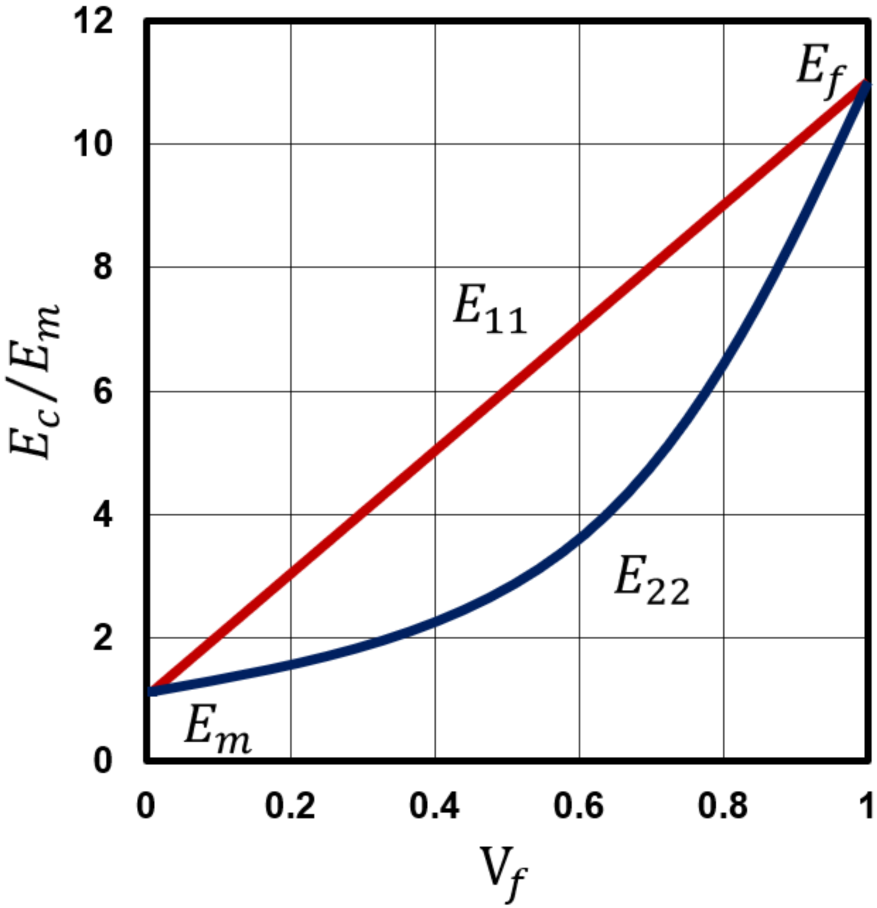


(homogenization rule for elastic stiffness under iso-stress conditions)

Theoretical homogenization rules

Rule of mixture

Variation of effective Young's modulus (E_c) *in* longitudinal (E_{11}) and transversal direction (E_{22}) with fiber volume fraction (v_f)

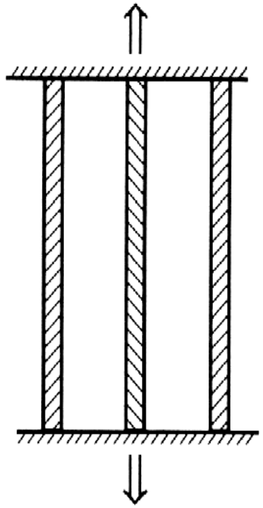


General form for all aggregates

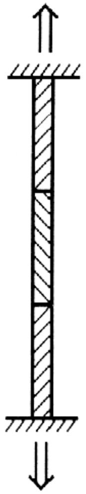
Upper bound (Taylor model)
Iso-strain assumption

$$\varepsilon^{(i)} = \varepsilon_{tot} \qquad \sigma_0 = \sum_{i=1}^{N} f_i \sigma^{(i)}(\varepsilon_{tot})$$

Real case is softer than upper bound
and harder than lower bound



(b)

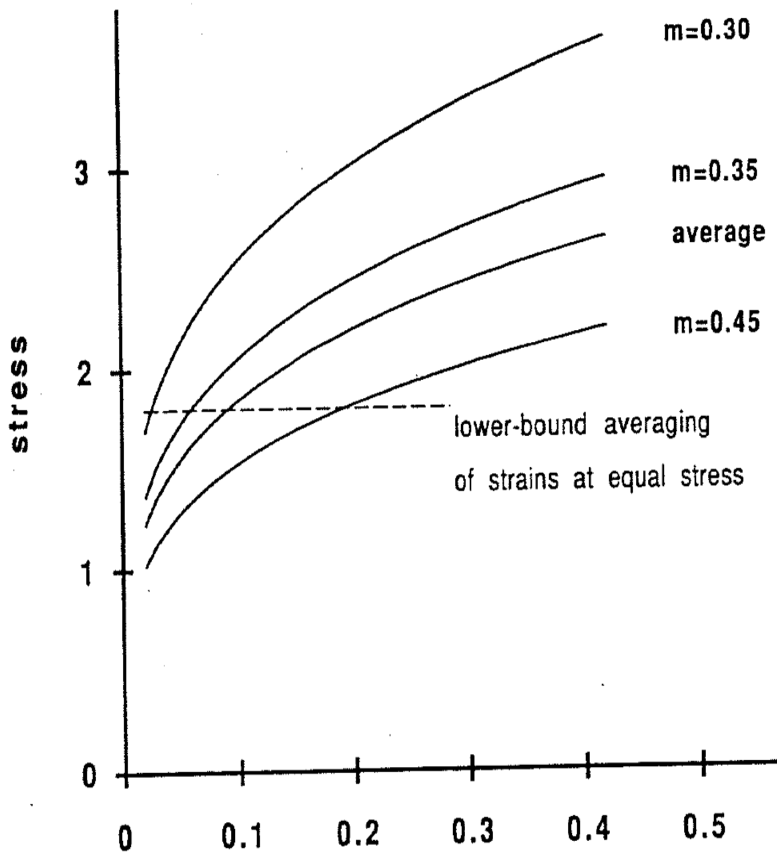


(a)

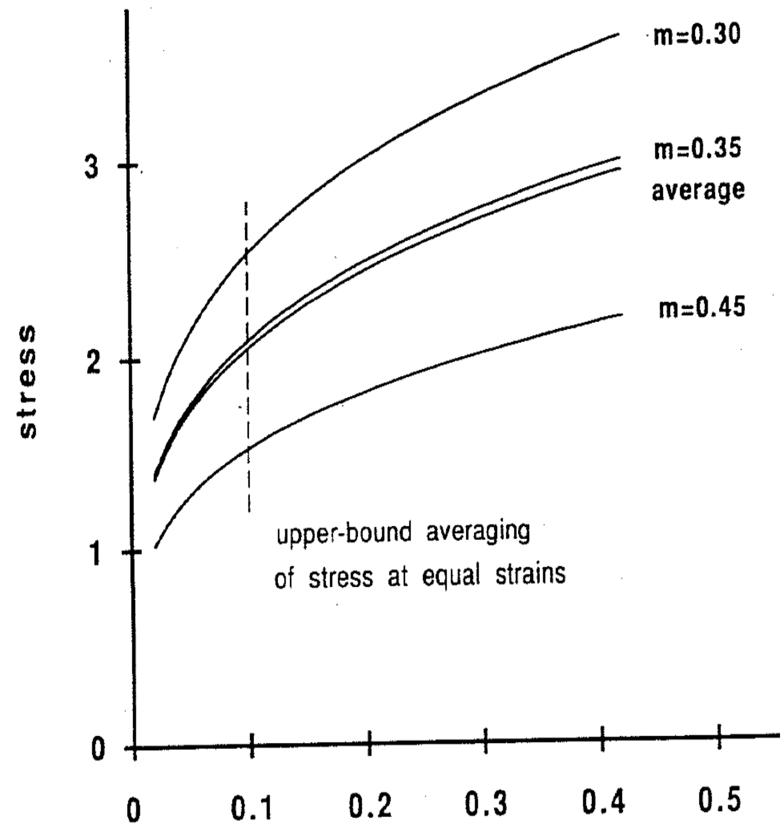
Lower bound (Sachs model)
Iso-stress assumption

$$\sigma^{(i)} = \sigma_0 \qquad \varepsilon_{tot} = \sum_{i=1}^{N} f_i \varepsilon^{(i)}(\sigma_0)$$

Polycrystalline aggregates: Analytical homogenization



(a)

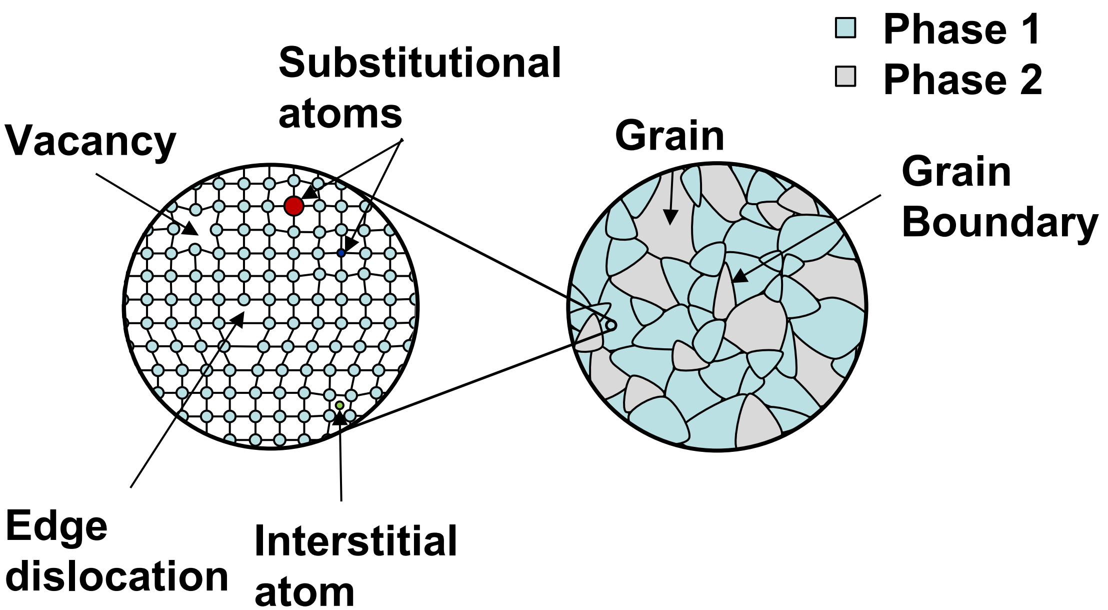


(b)

Micromechanical Modeling

Elements of Microstructure:

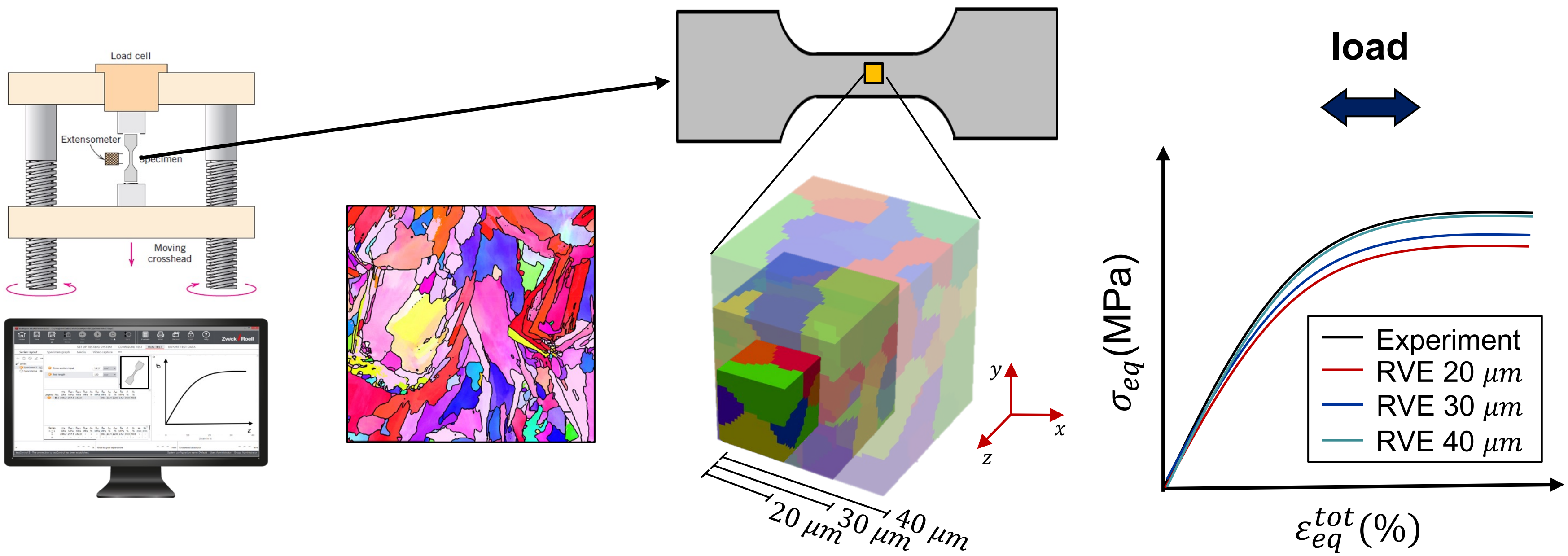
- Phases
- Grains
- Grain boundaries
- Dislocations
- Atomic defects



Micromechanical Modeling

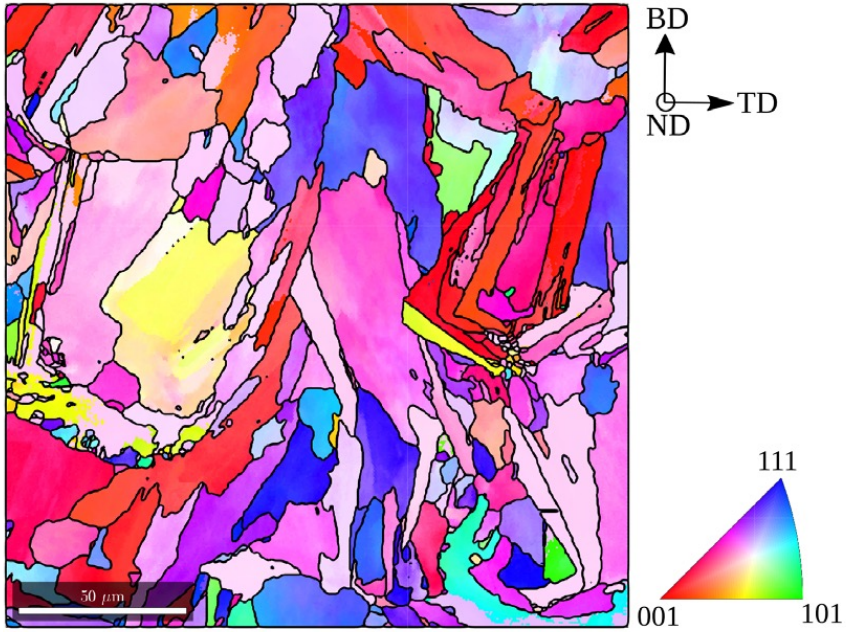
RVE (Representative Volume Element): Microstructure model

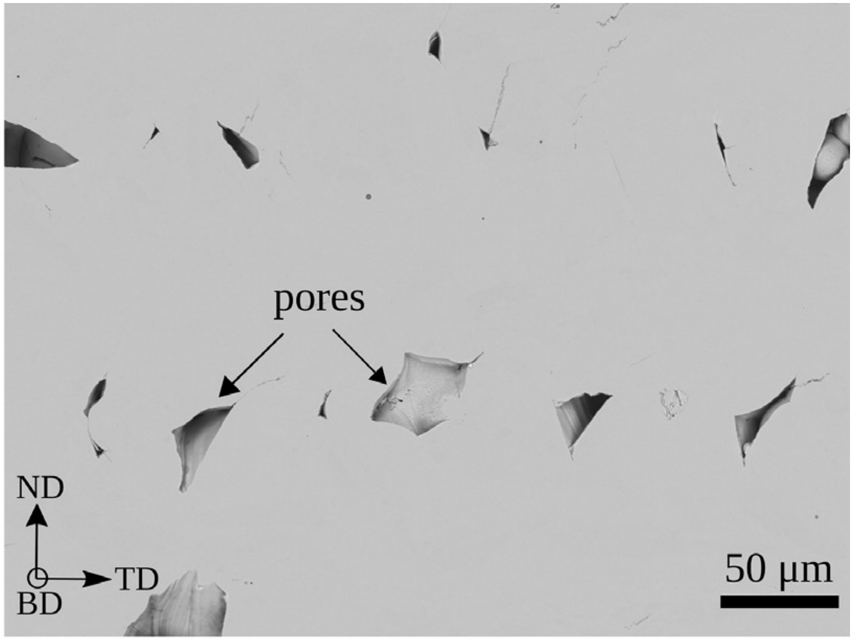
- RVE captures microstructural features in statistical sense (volume fraction of phases, size and shape distribution of grains)
- RVE size influences the efficiency and accuracy of mechanical property prediction



Experimental Test | EBSD Scan | RVE Reconstruction (Kanapy) | Finite Element Simulation (Abaqus)

Micromechanical Modeling



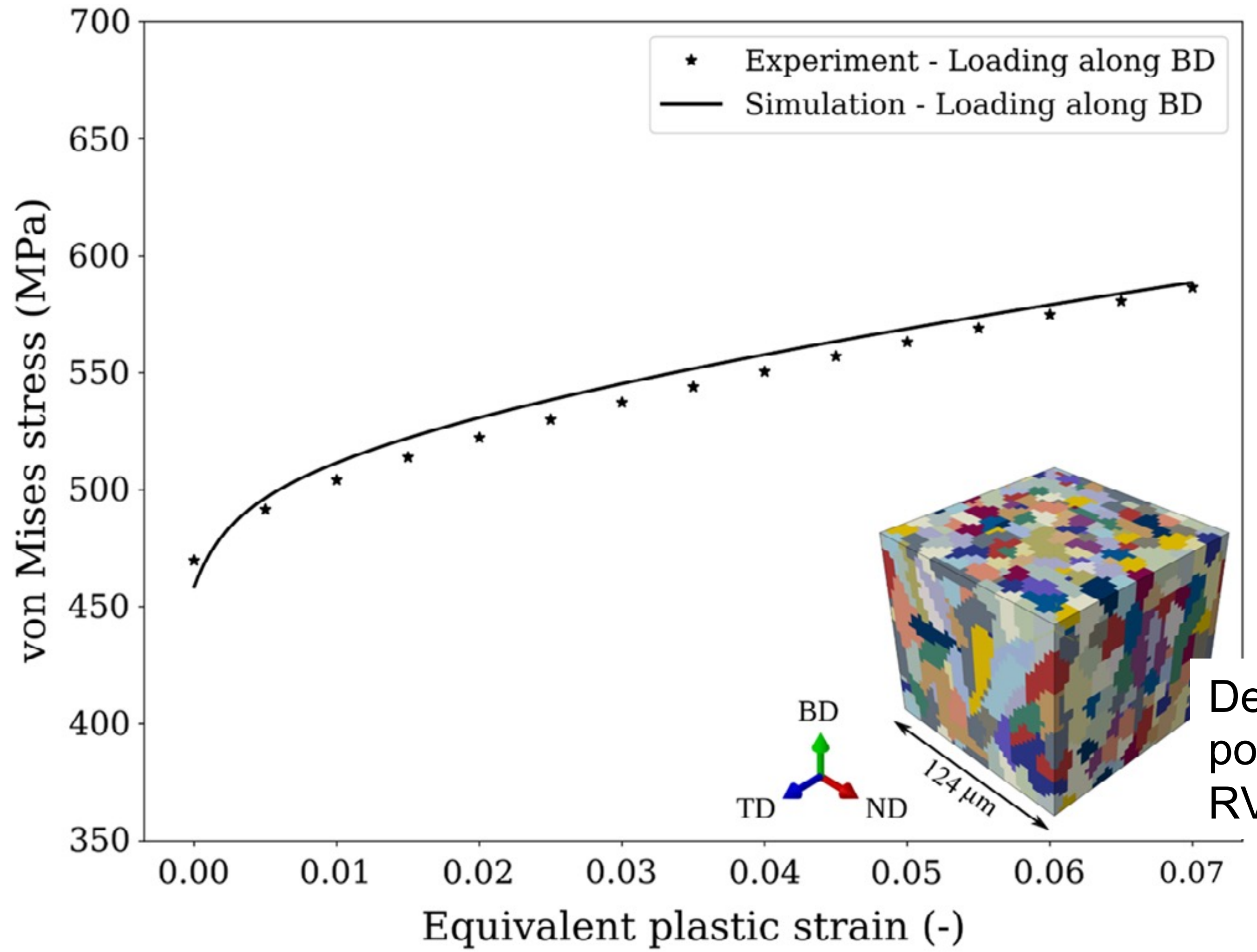


Additively (PBF-LB/M) manufactured sample of austenitic steel (316L): elongated grains and porosity

MRG Prasad, A Biswas, K Geenen, W Amin, S Gao, J Lian, A Röttger, N Vajragupta, A Hartmaier, Adv. Eng. Mater. 2020, 2000641

DOI: 10.1002/adem.202000641

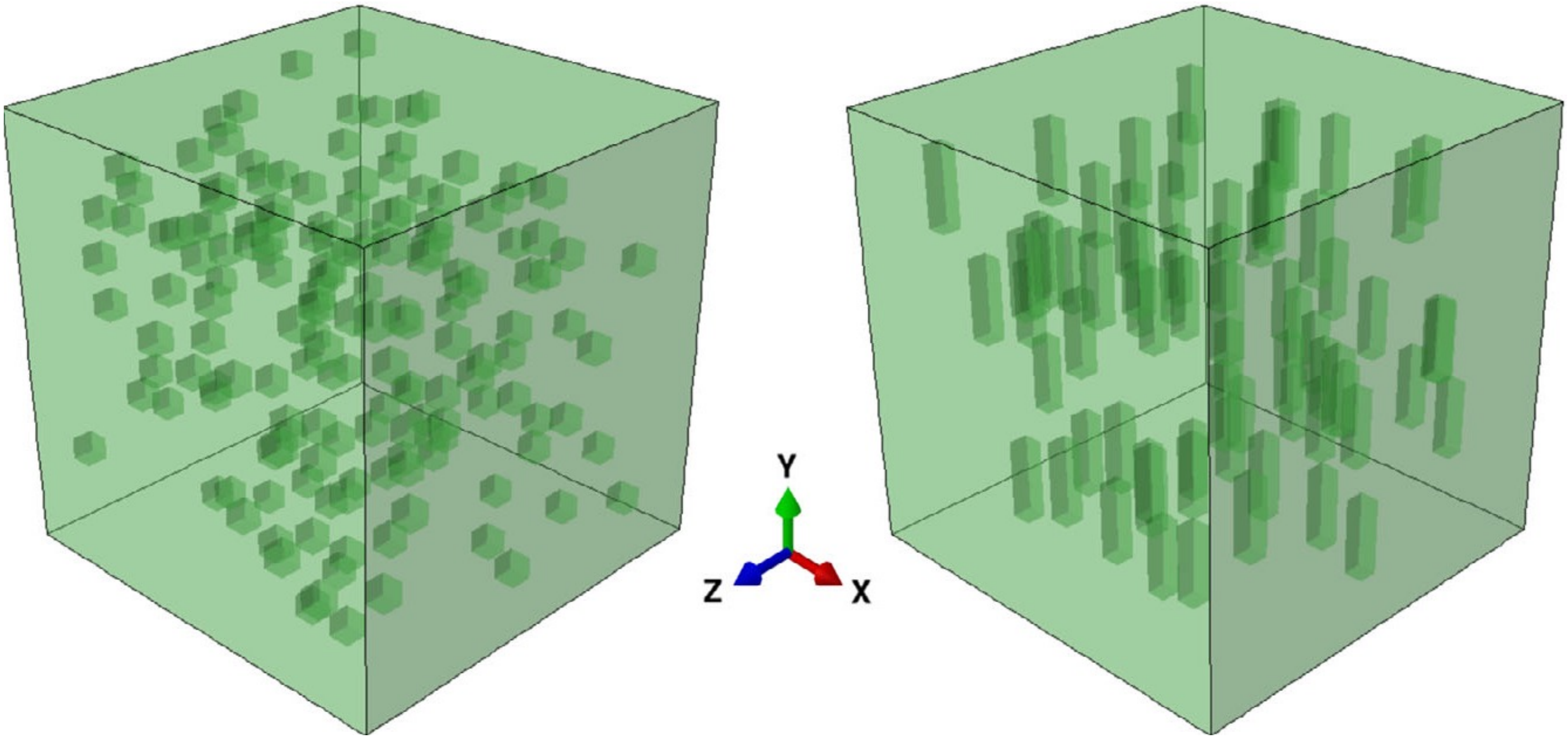
Micromechanical Modeling



Dense polycrystalline RVE

- Homogenized stress-strain curve of dense 316L polycrystal
- Experimental data used to determine material parameters

Micromechanical Modeling

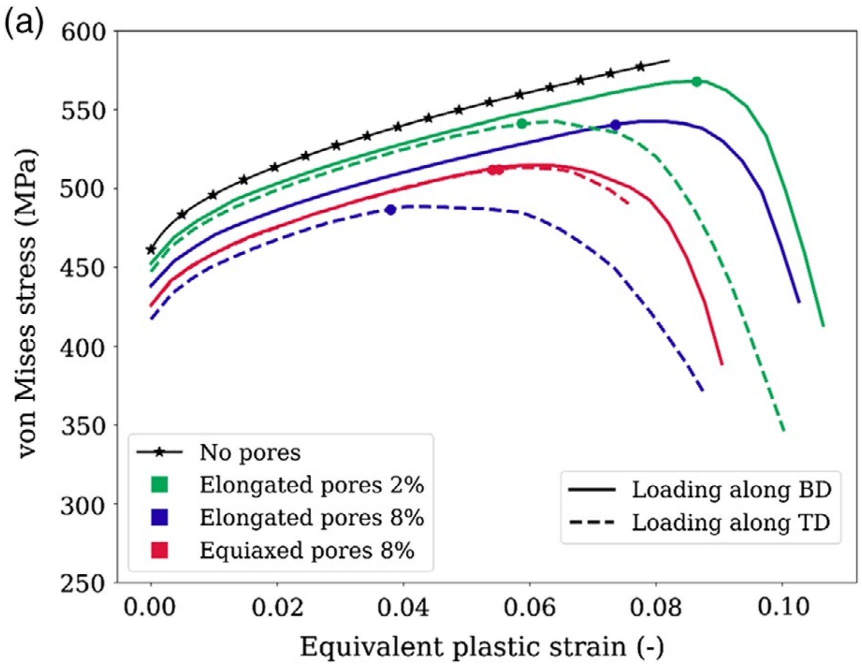


equiaxed pores

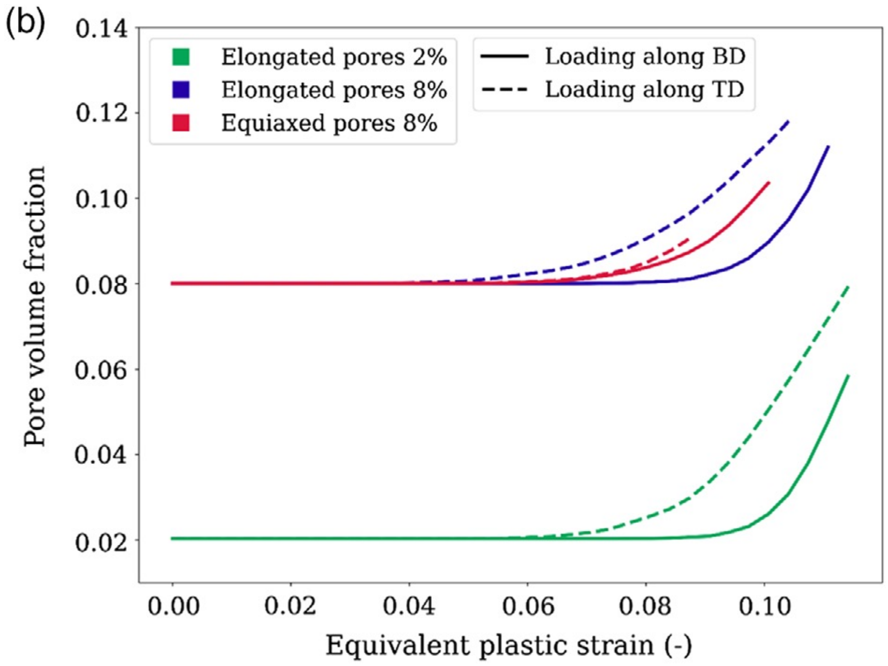
elongated pores

Representative volume elements (RVE) with porosity as second phase

Micromechanical Modeling



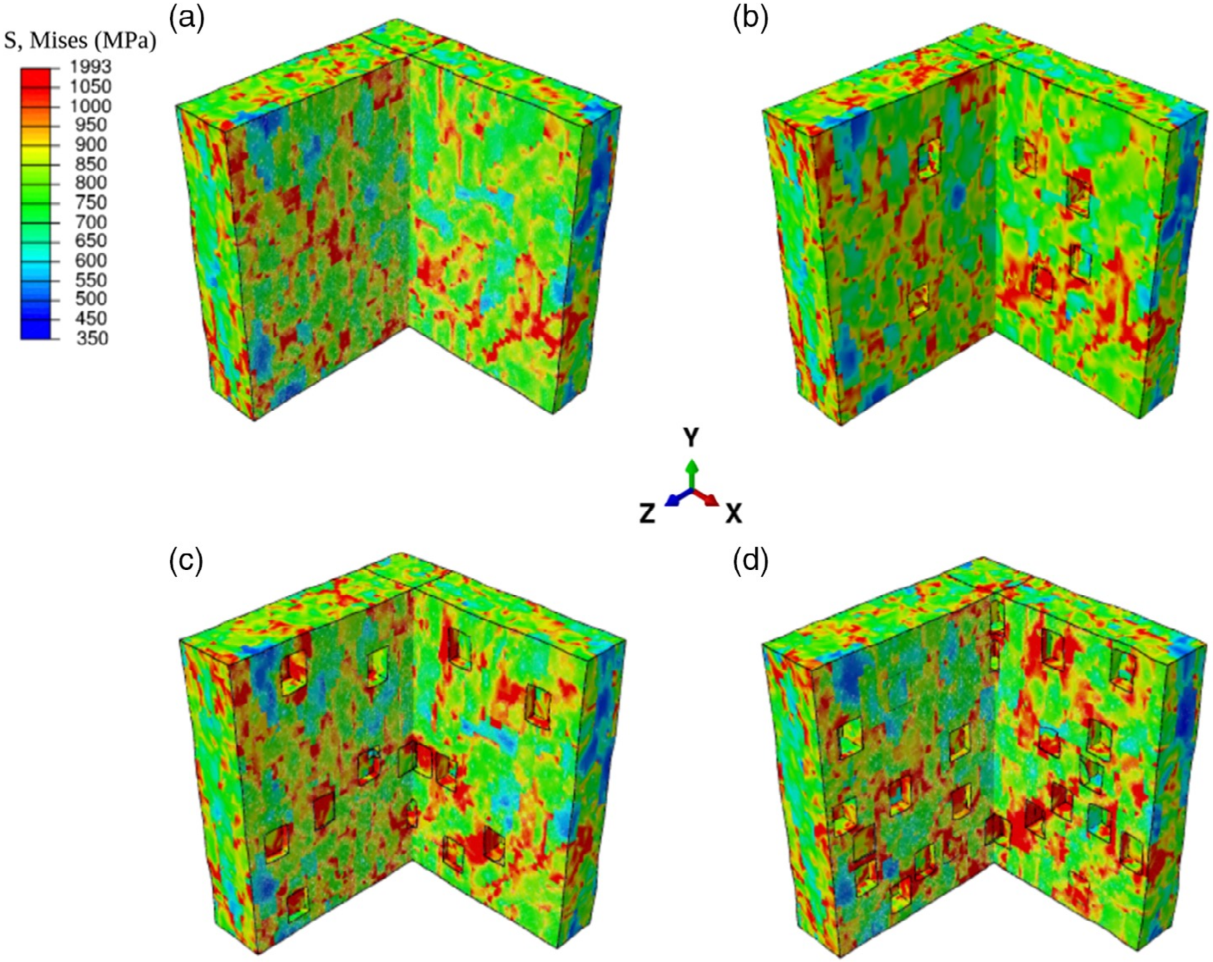
homogenized
stress vs. plastic strain curves



pore volume fraction as
function of plastic strain

- Comparison of RVEs with different pore shapes and volume fractions
- Point of instability calculated using the Considère criterion (filled circles)

Micromechanical Modeling



Cross-sectional views of stress contours inside the RVEs
a) nonporous, b) 2% porosity, c) 5% porosity, d) 8% porosity

Micromechanical material modeling

Micromechanical modeling = calculating the mechanical response of a simplified representation of a materials microstructure under mechanical loads

Representative Volume Elements (RVE)
as digital microstructure models

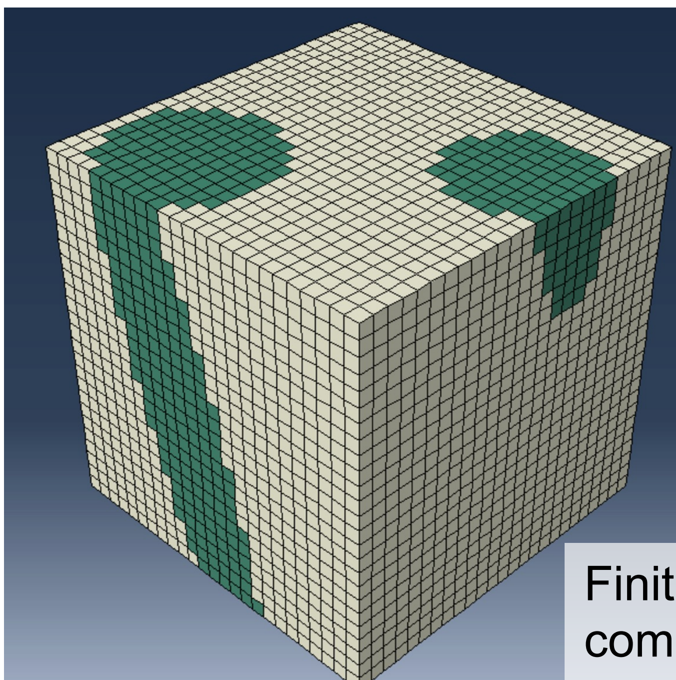
Calculation of effective **macroscopic properties** by numerical or theoretical **homogenization** methods

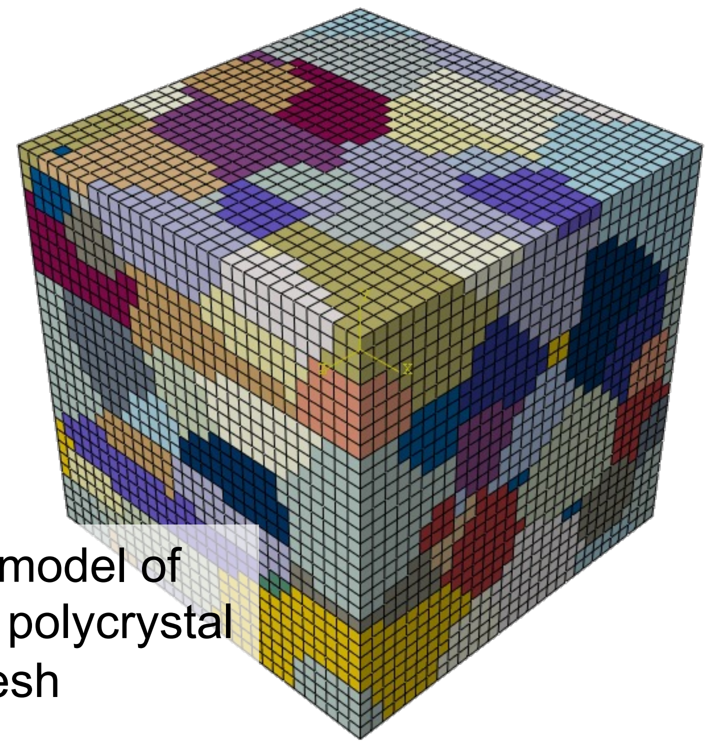
Recent advances in microscopic material description (crystal plasticity, cohesive zone models, etc.) and increasing computer power enables realistic RVE's and accurate prediction of microstructure-property relationships.

Introduction into the Finite Element Analysis

Basics of Finite Element Analysis (FEA):

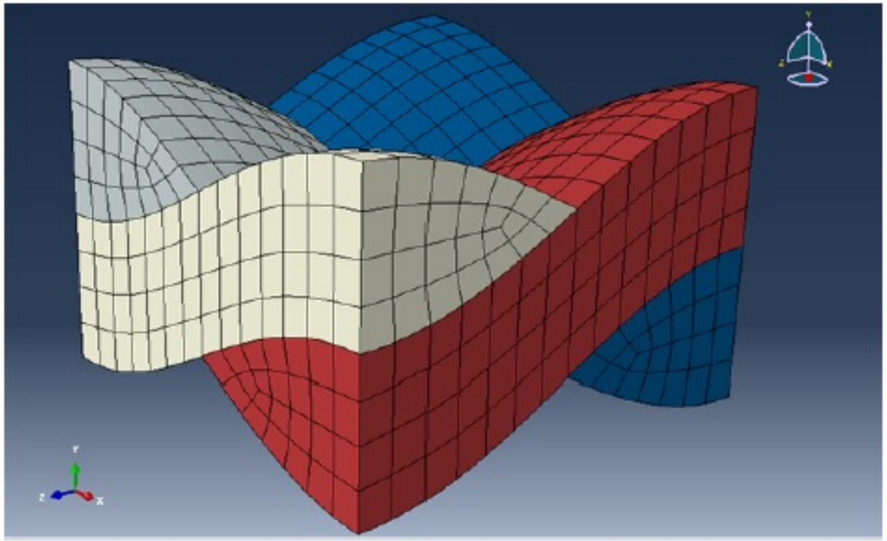
- Numerical method to calculate the **deformed shape** of a solid structure under mechanical boundary conditions (forces or distortions)
- **Mechanical equilibrium** is assumed: All forces on the structure are in balance, i.e. the sum of all forces acting on the surface is zero
- Discretization of the structure with **finite elements**





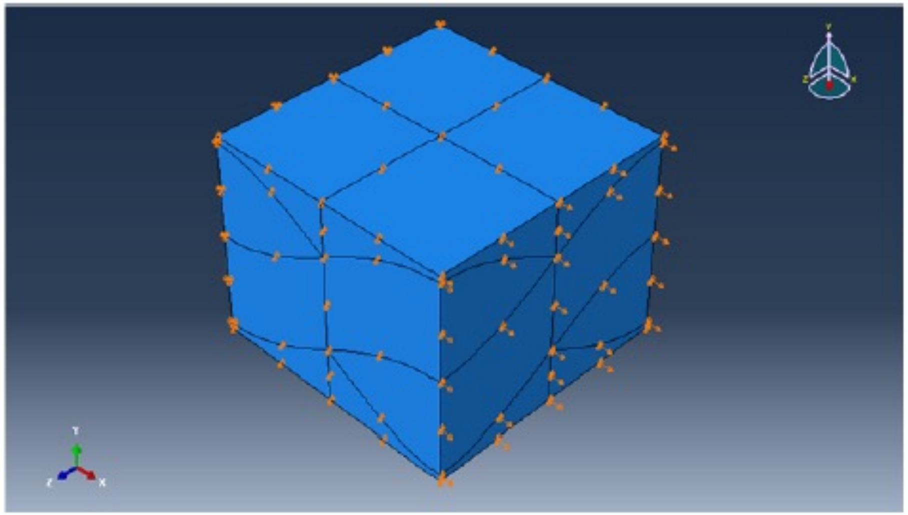
Finite element model of composite and polycrystal with regular mesh

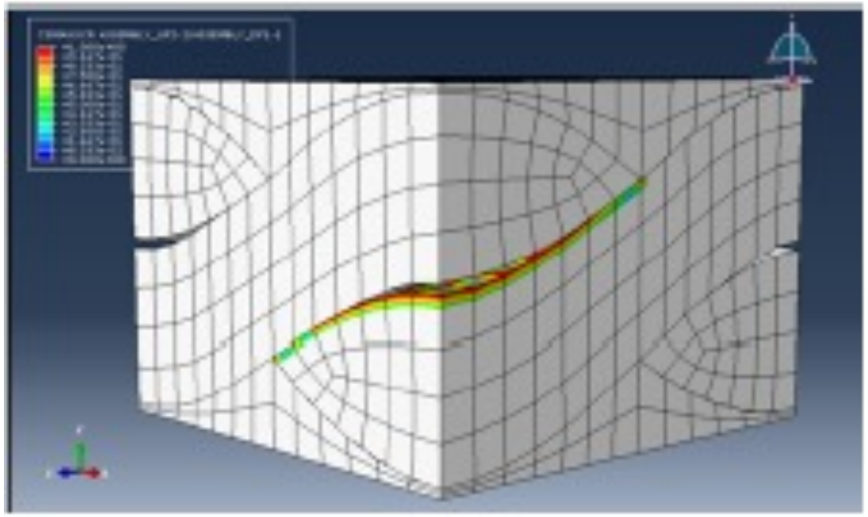
FEA of fiber reinforced polymers



RVE of plain weave composite

- plasticity in matrix
- damage at interfaces



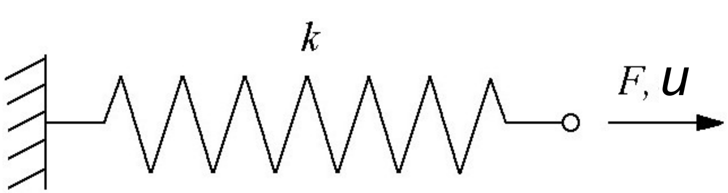


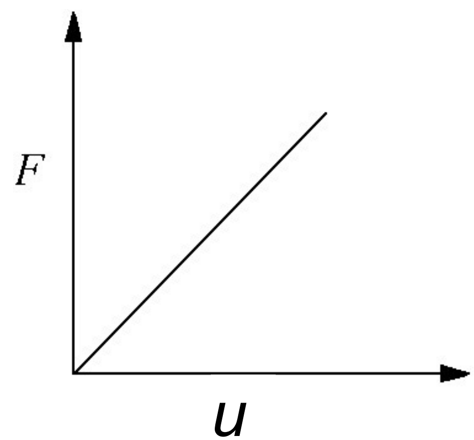
Introduction into the Finite Element Analysis

Basics of Finite Element Analysis (FEA):
In a simple 1-d finite element model, we can envision the finite elements as linear springs.
In mechanical equilibrium under given boundary conditions, the forces and the deformed shape of the system can be calculated.
Basic equation of FEA

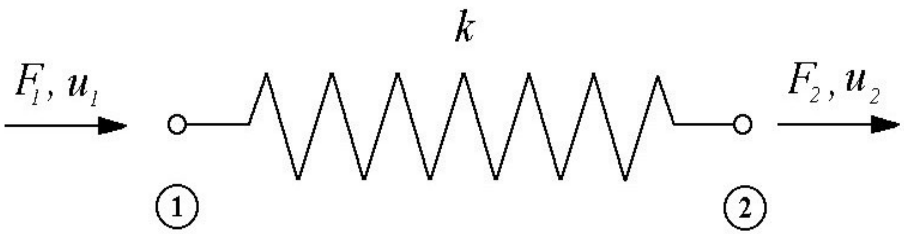
$$\underline{F} = \underline{\underline{K}}\;\underline{u}$$

Discretization (spring model)





Discretization (spring model)

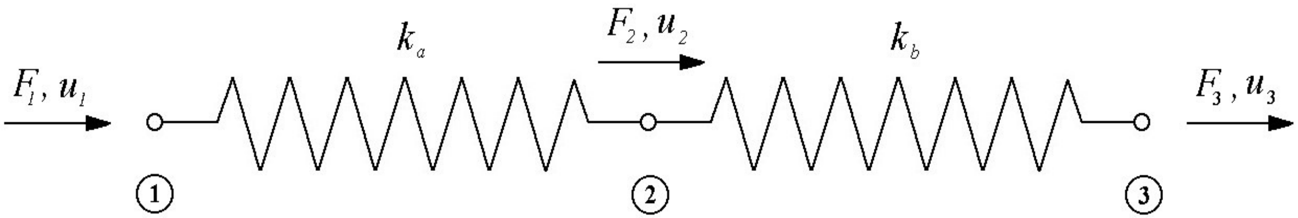


$$\begin{Bmatrix} F_1 \\ F_2 \end{Bmatrix} = k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix}$$

Element stiffness matrix for one-spring-system

$$[K] = k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

Introduction into the Finite Element Analysis



Element stiffness matrix

Element 1

$$\begin{Bmatrix} F_1 \\ F_2 \\ F_3 \end{Bmatrix} = \begin{bmatrix} k_a & -k_a & 0 \\ -k_a & k_a & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

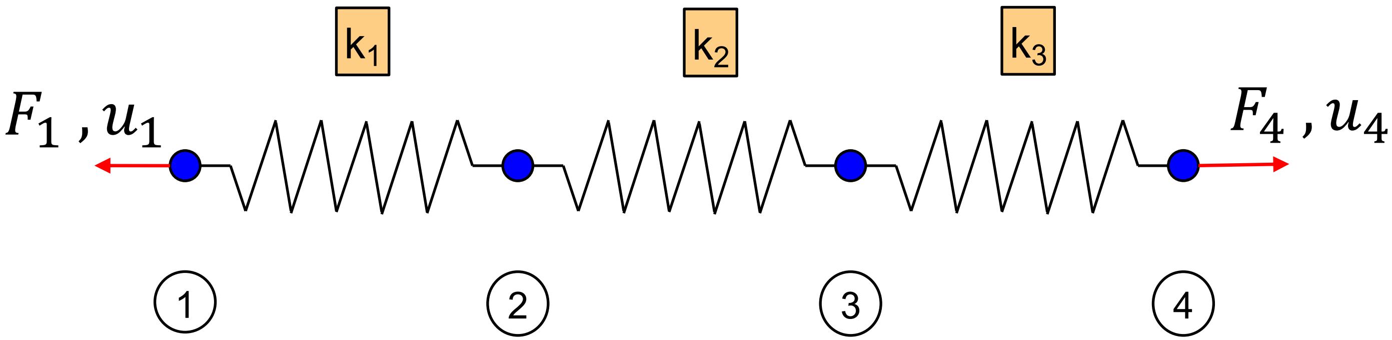
Element 2

$$\begin{Bmatrix} F_1 \\ F_2 \\ F_3 \end{Bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & k_b & -k_b \\ 0 & -k_b & k_b \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

system stiffness matrix

$$\begin{Bmatrix} F_1 \\ F_2 \\ F_3 \end{Bmatrix} = \begin{bmatrix} k_a & -k_a & 0 \\ -k_a & k_a + k_b & -k_b \\ 0 & -k_b & k_b \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix}$$

Basics of Finite Element Analysis



$$\{F\} = \begin{Bmatrix} F^{(1)} \\ F^{(2)} \\ F^{(3)} \\ F^{(4)} \end{Bmatrix} = \begin{bmatrix} K_{11} & K_{12} & K_{13} & K_{14} \\ K_{21} & K_{22} & K_{23} & K_{24} \\ K_{31} & K_{32} & K_{33} & K_{34} \\ K_{41} & K_{42} & K_{43} & K_{44} \end{bmatrix} \begin{Bmatrix} u^{(1)} \\ u^{(2)} \\ u^{(3)} \\ u^{(4)} \end{Bmatrix} = [K]\{u\}$$

Definition of stiffness matrix

[K]{u}={F}

Theoretical analysis of mechanical equilibrium yields

$$[K] = \frac{1}{2} \iiint_V [B]^T [C][B] dV$$

[C]: elasticity tensor, material property
[B]: strain-displacement-matrix: geometry, interpolation function

- Element stiffness matrix is calculated by volume integration over element
- System Stiffness matrix is assembled from element stiffness matrices

Computation of strain field

- Strain is calculated by using shape functions to interpolate nodal displacements u_j into finite element
- Conversion of displacement to strain is simple algebraic operation (B-matrix)

$$\varepsilon_\alpha(x,y,z) = B_{\alpha j}(x,y,z)\,u_j$$

$\alpha = 1,2,\ldots 6$ (tensor components in Voigt notation)

$j = 1,2,\ldots N$ (index over nodes of FE)

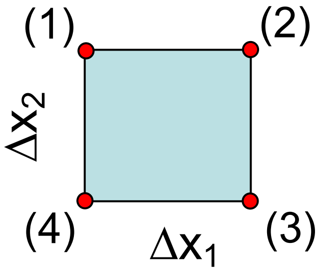
stress field (linear elasticity: Hooke's law)

$$\sigma_\alpha(x,y,z) = C_{\alpha\beta}\,\varepsilon_\alpha(x,y,z)$$

$C_{\alpha\beta}$ (stiffness tensor)

Strain tensor

- infinitesimally small volume element
- small strains



$\underline{u}^{(1)}$ displacement of point $\underline{x}^{(1)}$

$$\varepsilon_{11} = \lim_{\Delta x_1 \to 0} \frac{u_1^{(2)} - u_1^{(1)}}{\Delta x_1} = \frac{\partial u_1}{\partial x_1} = u_{1,1}$$

$$\gamma_{12} = \lim_{\Delta x_1 \to 0} \frac{u_2^{(2)} - u_2^{(1)}}{\Delta x_1} + \lim_{\Delta x_2 \to 0} \frac{u_1^{(1)} - u_1^{(4)}}{\Delta x_2} = \frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} = u_{2,1} + u_{1,2}$$

general:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \qquad \left(\gamma_{12} = 2\varepsilon_{12}\right)$$

Computation of strain fields

- derivation of interpolation function with respect to spatial coordinate
- linear elements $\rightarrow$ constant strain within elements

$$\varepsilon_\alpha^{(j)} = \begin{pmatrix} \frac{\partial}{\partial x} & & \\ & \frac{\partial}{\partial y} & \\ & & \frac{\partial}{\partial z} \\ & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & \end{pmatrix} \begin{pmatrix} u_x^{(j)} \\ u_y^{(j)} \\ u_z^{(j)} \end{pmatrix} = L_{\alpha i} u_i^{(j)}$$

$$\alpha = 1,\dots,6 \quad \text{(Voigt notation)}$$

$$j = 1,\dots,N$$

$$i = 1,\dots,3$$

Introduction into the Finite Element Method

Shape functions (interpolation functions) connect the displacement field within an element with the nodal displacements.

$$u_i(x,y,z) = N_{ij}(x,y,z)\, u_j \qquad i = 1,2,3 \qquad j = 1,\ldots,N$$

u_j is (1xN)-matrix of nodal displacements: $\{u\}=(u_x^{(1)}, u_y^{(1)}, \ldots, u_z^{(M)})$

M: number of nodes, N: degrees of freedom (3N)

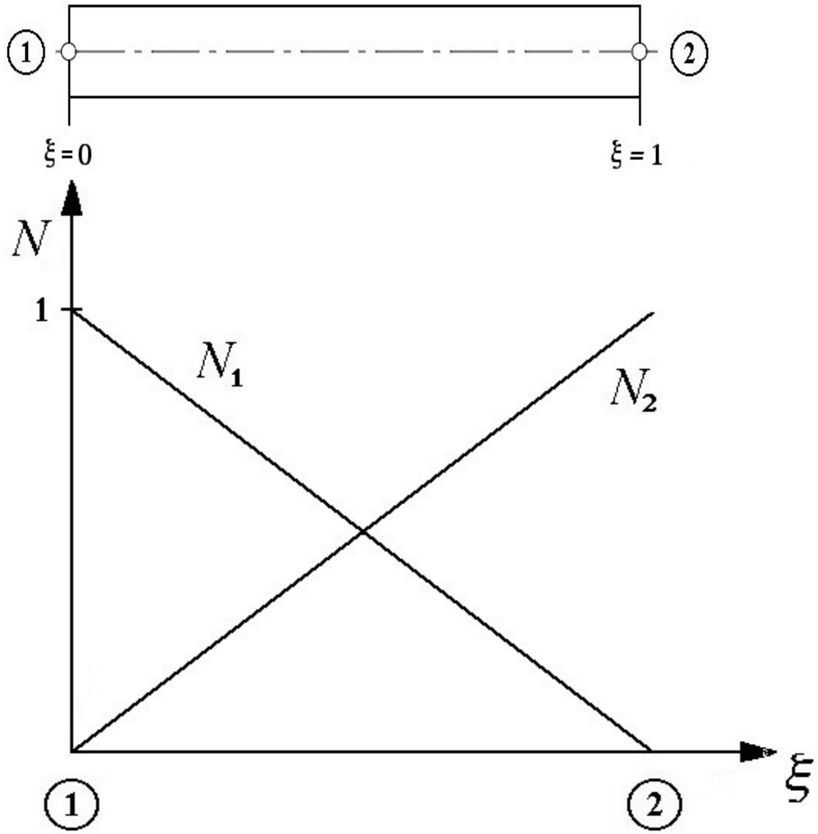
$u_i(x,y,z)$ is i-th component of continuous displacement field (i=1,2,3)

shape functions have the property

$$N_{ij}(x^{(k)}, y^{(k)}, z^{(k)}) = \delta_{jk} = \begin{cases} 1 & \text{für } j = k \\ 0 & \text{für } j \neq k \end{cases}$$

Linear (one-dimensional) shape functions

$$N_{11} = \frac{(\xi - 1)}{(0 - 1)} = 1 - \xi \qquad \text{und} \qquad N_{12} = \frac{(\xi - 0)}{(1 - 0)} = \xi$$

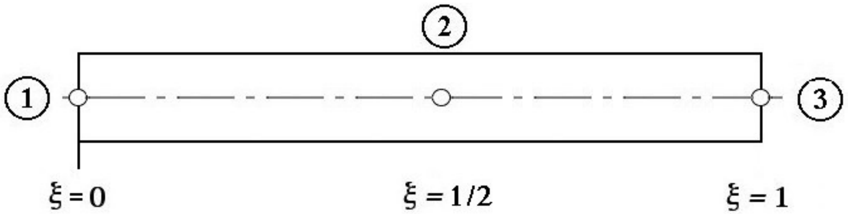


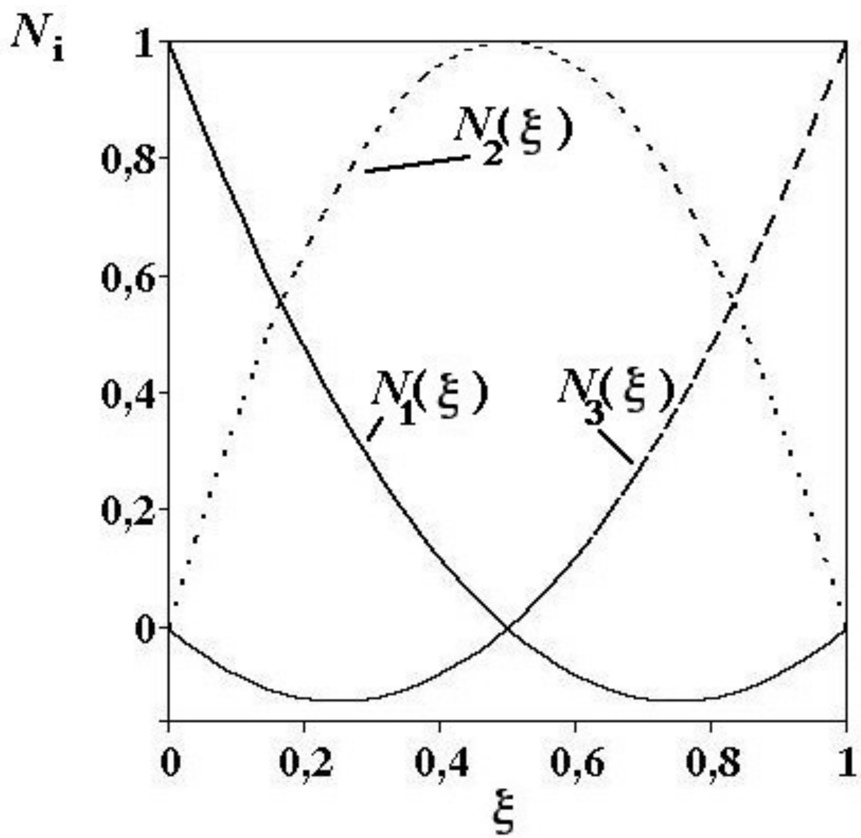
Quadratic (one-dimensional) shape functions

$$N_{11} = \frac{(\xi - 1/2)(\xi - 1)}{(0 - 1/2)(0 - 1)} = (1 - \xi)(1 - 2\xi) = 1 - 3\xi + 2\xi^2$$

$$N_{12} = \frac{(\xi - 0)(\xi - 1)}{(1/2 - 0)(1/2 - 1)} = 4\xi(1 - \xi)$$

$$N_{13} = \frac{(\xi - 0)(\xi - 1/2)}{(1 - 0)(1 - 1/2)} = -\xi(1 - 2\xi)$$





Computation of strain fields

- derivation of interpolation function with respect to spatial coordinate
- linear elements $\rightarrow$ constant strain within elements

$$\varepsilon_\alpha(x,y,z) = L_{\alpha k} N_{kj}\, u_j = B_{\alpha j}\, u_j \qquad \alpha = 1,\ldots,6 \quad \text{(Voigt notation)}$$

$$j = 1,\ldots,N; k = 1,2,3$$

stress field (linear elasticity: Hooke's law)

$$\sigma_\alpha(x,y,z) = C_{\alpha\beta}\, \varepsilon_\beta = C_{\alpha\beta}\, B_{\beta i}\, u_i$$

Elasticity

Hooke's law
(relation between stress and strain tensor)

$$\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl}$$

in Voigt Notation:
(NOTE: no rotations possible!)

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{13} \\ \gamma_{23} \end{pmatrix}$$

Elasticity

(Voigt) Elasticity matrix (isotropic or cubic)

$$C_{\alpha\beta} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix}$$

in case of isotropy: $C_{44} = \dfrac{C_{11} - C_{12}}{2}$

Normal strains create pure normal stresses
Shear strains create pure sheer stresses
No interference of normal/shear stresses and strains

Micromechanical Modeling

Micromechanical modeling is:

- Microstructure-based prediction of mechanical properties of multiphase and polycrystalline materials
- Virtual mechanical lab based on finite element analysis (or other solvers)

Micromechanical modeling requires:

- Microstructure description in form of Representative Volume Elements (RVE)
- Representation of volume fraction and geometrical features of all phases and grains, including crystallographic orientations
- Constitutive models and parameters for all phases and interfaces

Micromechanical modeling yields:

- Evolution of local stress, plastic strain and damage within microstructure
- Global values of mechanical and physical quantities through homogenization
- Insights into deformation and failure mechanisms of different microstructures