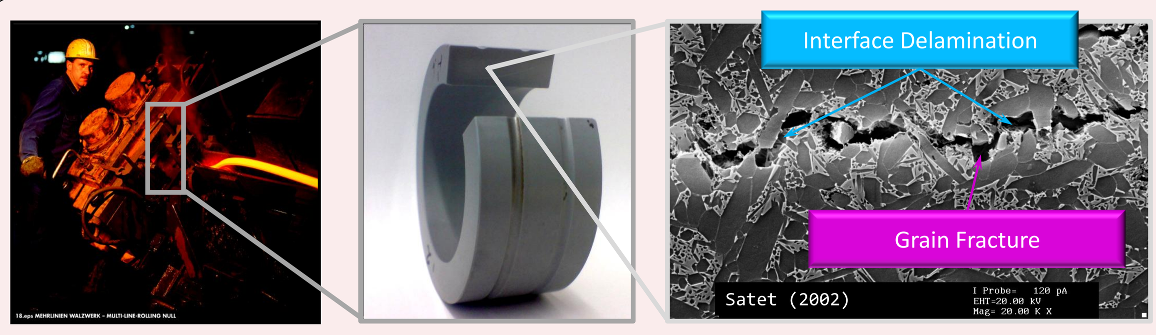
Karlsruhe Institute of Technology

Micromechanical Finite Element Simulation of Crack Propagation in Structural Reinforced Silicon Nitride

J. Wippler, T. Böhlke (Institute of Engineering Mechanics, Chair for Continuum Mechanics)

Motivation

The production of high strength wires needs extremly resistant forming rolls for a robust and efficient process.



Structural reinforced high performance ceramics like Si_3N_4 have a complex microstructure, which leads to a tough material behavior.

Reason: The microstructure leads to increasing crack resistance through long crack path

Concept

Generation of a 3D silicon nitride-like microstructure → Finite element mesh generation

Assumptions for thermo-elastic and fracture behavior → Implementation of the constitutive assumptions into FE-code

→ Finite element calculations on the microstructural level → Calculation of the effective material behavior

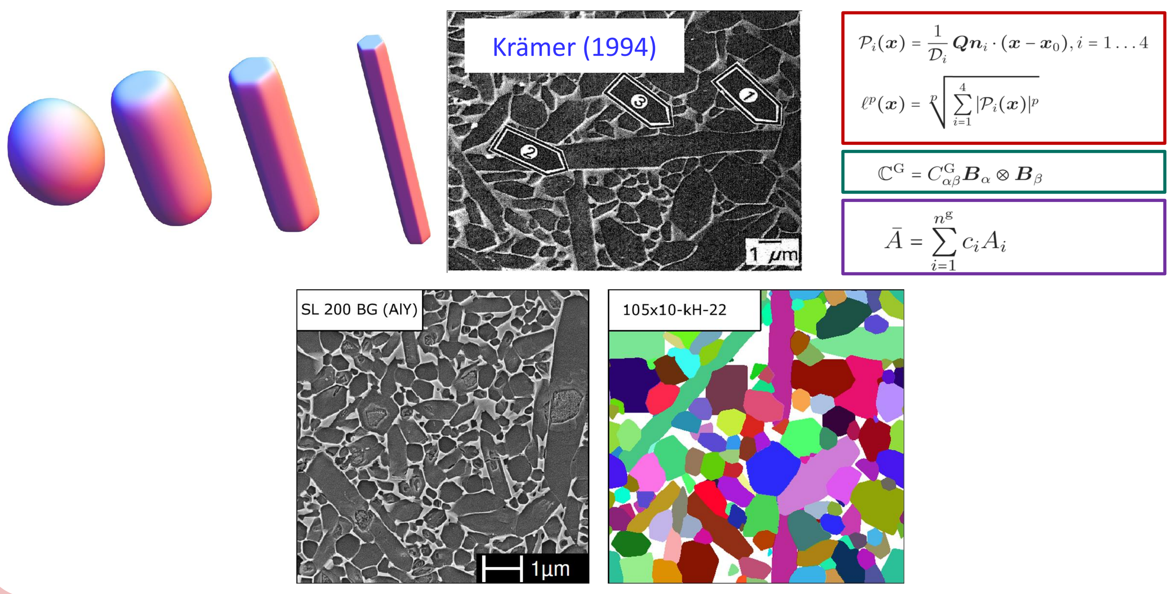
Structure Generator with Grain Growth and Pinning

Idea: Generation of a periodic 3D geometry model of the complex Si_3N_4 structure

Requires: Representation of the most important geometric features (aspect ratio, grain volume fraction, grain dimensions)

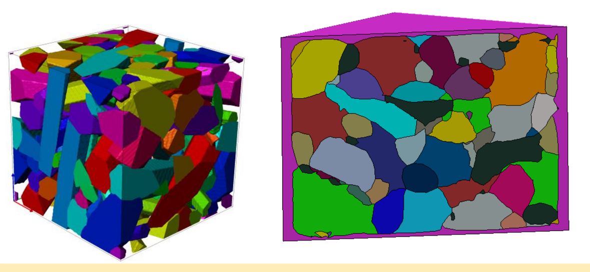
Procedure:

- Seeding of grains with statistical homogenous distributions of locations, orientations and growth relations
- Pinning check under consideration of experimental observations (Krämer 1994)
- Determination of images for mesh generation, data for the material models and statistical quantities for structure evaluation



Finite element mesh generation

- Calculation of an image stack
- Smoothening and meshing of the geometry with Simpleware™
- Export of the discretized geometry , selection of pairsings for PBC, interface relations



Technical Details:

- 64 periodic grains + matrix (transverse-isotropic/isotrop)
- > 1'500 eqs. for PBC
- > 600 contact relations
- > 150,000 elements & DoF

Thermoelasticity

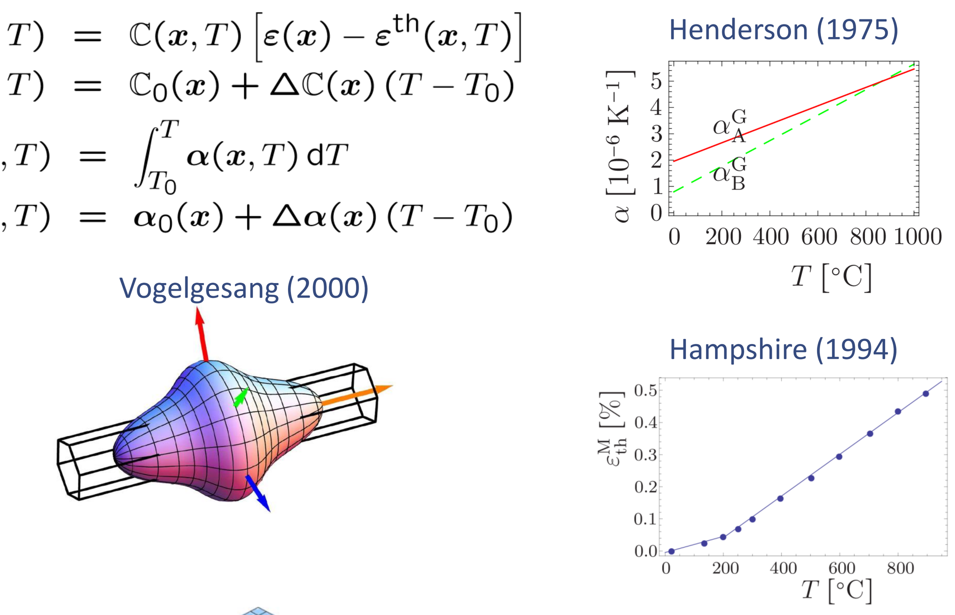
Wippler et al. (2011), accepted for publication in Acta Materialia

- Significant phase contrasts in the thermoelastic properties of silicon nitride
- Elastic stiffness in the grains higher than in the glassy phase and anisotropic
- Thermal expansion in the grains lower than in the glassy phase and anisotropic

$$\sigma(x,T) = \mathbb{C}(x,T)\left[\varepsilon(x) - \varepsilon^{\text{th}}(x,T)\right]$$
$$\mathbb{C}(x,T) = \mathbb{C}_0(x) + \Delta\mathbb{C}(x)(T-T_0)$$
$$\varepsilon^{\text{th}}(x,T) = \int_{T_0}^{T}\alpha(x,T)\,\mathrm{d}T$$
$$\alpha(x,T) = \alpha_0(x) + \Delta\alpha(x)(T-T_0)$$

=> Significant tensile stresses in the glassy phase (Peterson and Tien (1995))

=> Influence on the fracture behavior



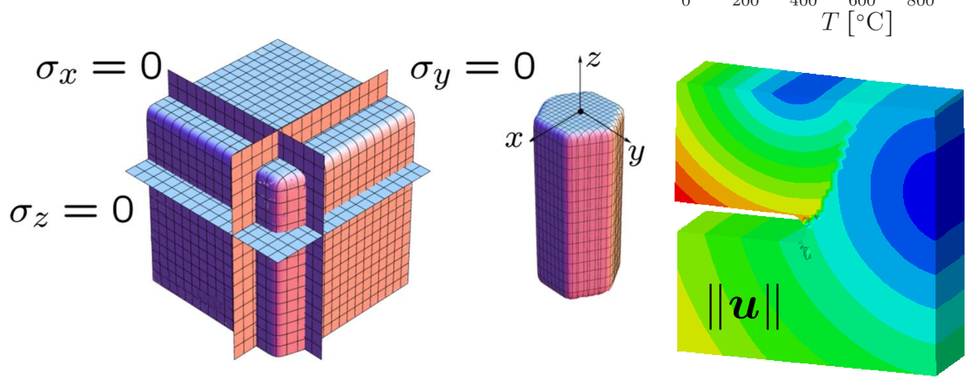
Fracture Behavior of the Phases

The glassy phase and the β-Si_3N_4 grain exhibit a brittle fracture behavior.

Tensile stress tensor: $\sigma^z = \sum_{\alpha=1}^{\beta} \langle\sigma^{\text{H}}_{\alpha}\rangle \mathbb{P}_\alpha$ mit $\langle\cdot\rangle = \max(0,\cdot)$

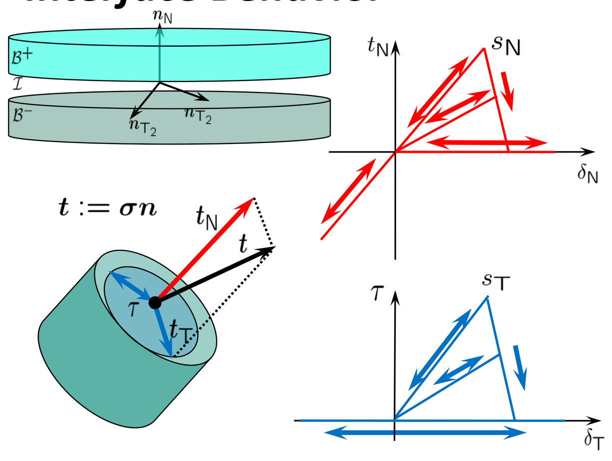
Glassy phase: Isotropic maximum principle stress criterion $\varphi^{\text{glas}}(\sigma^z,\sigma^{\text{B}}) = \sqrt[p]{\sum_\alpha \left[\frac{\langle\sigma^{\text{H}}_\alpha\rangle}{\sigma^{\text{B}}}\right]^p} - 1 = 0$

β-Si_3N_4 grains: Anisotropic maximum principle stress criterion $\varphi^{\beta}(\sigma^z,\sigma^{\text{B}}) = \sqrt[p]{\sum_\alpha \left[\frac{\sigma^z\cdot\mathbb{P}^{\text{B}}_\alpha}{\sigma^{\text{B}}_\alpha}\right]^p} - 1 = 0$



Interface Behavior

Govindjee (1994), Wei & Anand (2004)



Separation and Traction

$\delta = [\![u]\!]\ \forall\, x\in\mathcal{I}$, $\delta_{\text{N}} = (\delta\cdot n_{\text{N}})n_{\text{N}}$, $\delta_{\text{T}} = \delta - \delta_{\text{N}}$

$t = t_{\text{N}} + t_{\text{T}}$, $t_{\text{N}} = t_{\text{N}}n_{\text{N}}$, $t_{\text{N}} = t\cdot n_{\text{N}}$, $t_{\text{T}} = t - t_{\text{N}}$, $\tau = \|t_{\text{T}}\|$

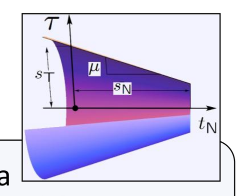
Normal Behavior

- Tensile loading => elastic damage
- Compressive behavior remains unaffected

Tangential Behavior

- Shear load => elastic damage
- Post-failure => Coulomb friction

$\tau = \begin{cases}\tau_0 & \text{if } \tau_0 < \mu\langle -t_{\text{N}}\rangle \\ \mu\langle -t_{\text{N}}\rangle & \text{else}\end{cases}$, $\langle\cdot\rangle = \max\{0,\cdot\}$



Delamination Criteria

$\phi_{\text{N}} = t_{\text{N}} - s_{\text{N}} + k_{\text{N}}q$

$\phi_{\text{T}} = \tau + \mu t_{\text{N}} - s_{\text{T}} + k_{\text{T}}q$

Stiffness and Compliance

$K = \begin{pmatrix} K_{\text{N}} & 0 & 0\\ 0 & K_{\text{T}} & 0\\ 0 & 0 & K_{\text{T}}\end{pmatrix}$, $K^{-1} := S$, $\dot{S}_{\text{N}} \geq 0$, $\dot{S}_{\text{T}} \geq 0$

Helmholtz Free Energy (due to elasticity and degradation)

$\psi = \frac{1}{2}t\cdot St + S(\alpha)$

Dissipation

$\mathscr{D} = \dot{\psi} - t\cdot\dot{\delta} \geq 0$

$= \frac{1}{2}t\cdot\dot{S}t + q\dot{\alpha}$, $q = -\frac{\partial S(\alpha)}{\partial\alpha}$

Lagrange Formalism

$\mathscr{L} = -\mathscr{D} + \sum_{i=1}^{2}\dot{\gamma}_i\phi_i$

$\frac{\partial\mathscr{L}}{\partial t} \stackrel{!}{=} 0 \Rightarrow \dot{S} = \sum_{i=1}^{2}\dot{\gamma}_i\frac{\partial_t\phi_i\otimes\partial_t\phi_i}{\partial_t\phi_i\cdot t}$

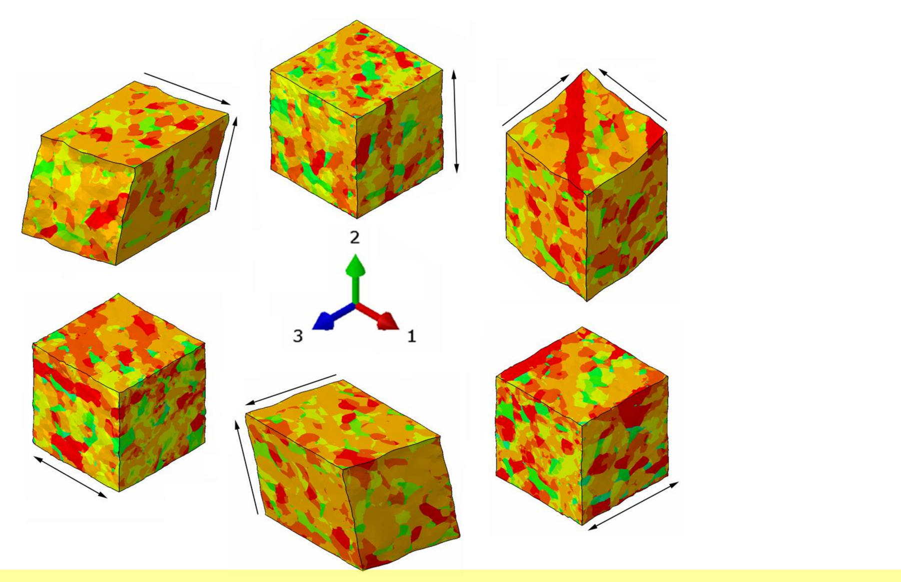
$\frac{\partial\mathscr{L}}{\partial q} \stackrel{!}{=} 0 \Rightarrow \dot{\alpha} = \sum_{i=1}^{2}\dot{\gamma}_i\frac{\partial\phi_i}{\partial q}$

Elastic Law in Rate Form

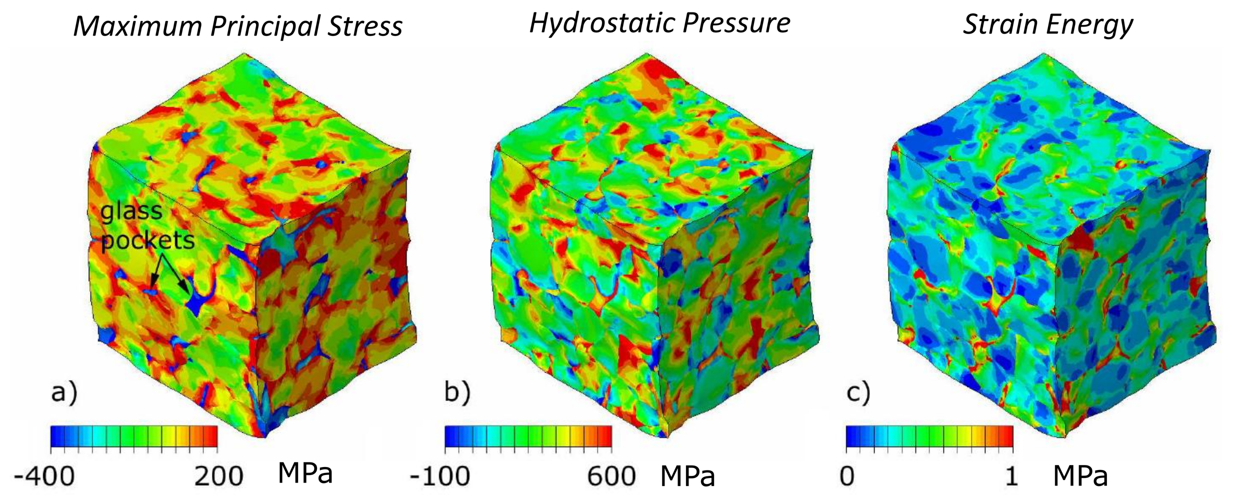
$\dot{t} = K\left[\dot{\delta} - \sum_{i=1}^{2}\dot{\gamma}_i\partial_t\phi_i\right]$

Finite Element Simulations on the Microscale

Effective Stiffness from Six Orthogonal & Periodic Deformation Modes

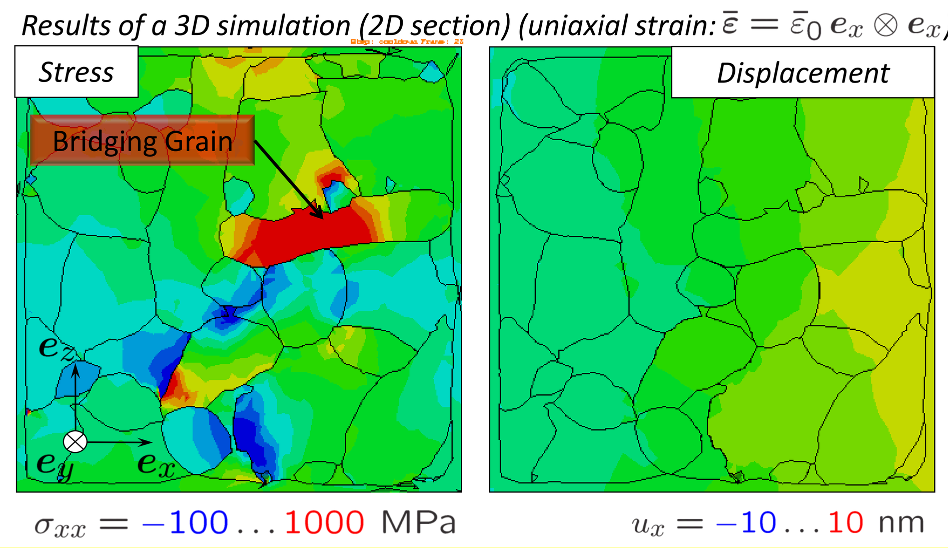


Cool Down Simulation with Different Field Solutions



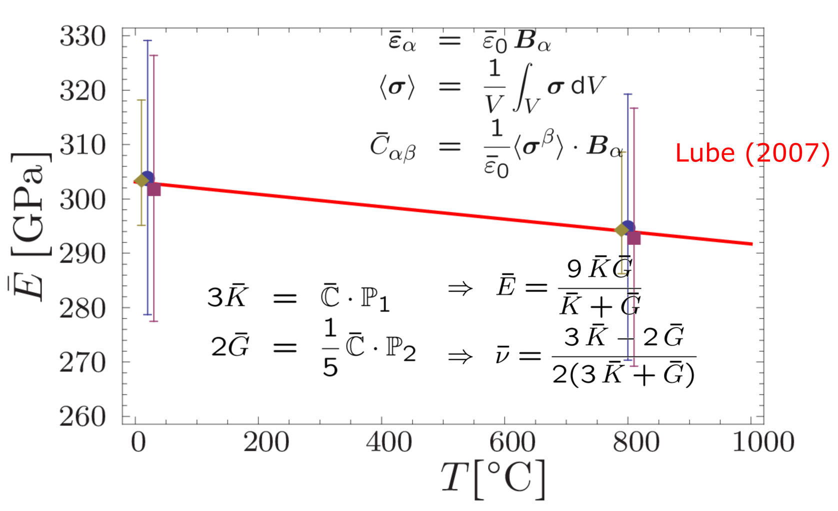
Fracture Simulation of a Unit Cell

Results of a 3D simulation (2D section) (uniaxial strain: $\bar{\varepsilon} = \bar{\varepsilon}_0\, e_x\otimes e_x$)



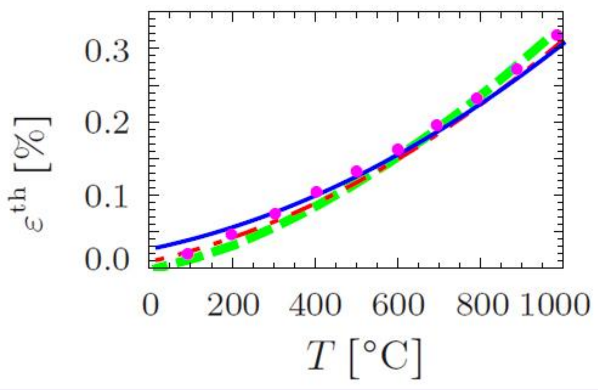
Calculation of the Effective Material Behavior

Effective Elastic Stiffness and Young's modulus



Effective Thermal Expansion

The unit cell is cooled down homogeneously from glass transition tempertature (950°C) to room temperature (25°C).



$$\langle\varepsilon^{\text{th}}(T)\rangle = \frac{1}{V}\int_V \varepsilon^{\text{th}}(T)\,\mathrm{d}V$$
$$\bar{\varepsilon}^{\text{th}}(T) = \frac{1}{3}\text{tr}(\langle\varepsilon^{\text{th}}(T)\rangle)$$

Effective Fracture Behavior