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Recent progress and future trends in the crystal plasticity finite element method

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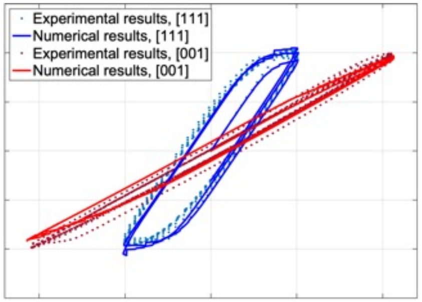

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INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

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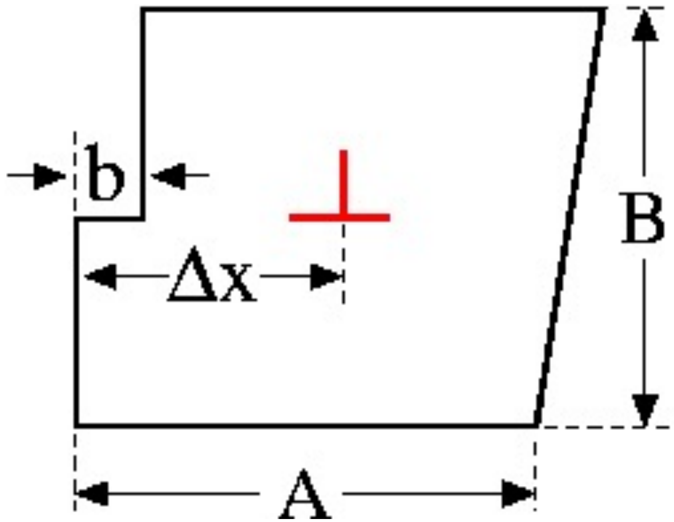
Outline

- Introduction to crystal plasticity (CP)
- Empirical and phenomenological CP models
- Example 1: High-temperature fatigue
- Example 2: Ultrafine-grained metals
- Example 3: Martensitic phase transformation

Orowan law (scalar form)

Plastic strain



plastic (irreversible) strain generated by motion of dislocations

$$\gamma_{pl} = \frac{b}{AB}\sum_{i=1}^{N}\Delta x_i = \frac{N}{AB} b \Delta \bar{x}$$

strain rate: $\dot{\gamma}_{pl} = \rho_{mob} b \bar{v}$ Orowan law

Orowan law (tensorial form)

Plastic slip increment on slip system α produced by N dislocation segments of length l_i Burgers vector $b^{(\alpha)}$ and slip plane normal vector $n^{(\alpha)}$ in volume $V=A_0\,H$

$$\Delta\gamma_{pl}^{(\alpha)} = \sum_{i=1}^{N} \frac{\Delta A_i}{A_0}\,\frac{b^{(\alpha)}}{H} = \frac{b^{(\alpha)}}{V}\sum_{i=1}^{N} \Delta x_i l_i$$

with $\Delta A_i = \Delta x_i l_i$

area swept by dislocation segment i moving over distance Δx_i

$$\dot{\gamma}_{pl}^{(\alpha)} = \frac{b^{(\alpha)}}{V}\sum_{i=1}^{N} v_i l_i = b^{(\alpha)}\,\frac{L_{\mathrm{tot}}\,\bar{v}^{(\alpha)}}{V} = b^{(\alpha)}\rho_{\mathrm{mob}}\;\bar{v}^{(\alpha)}$$

plastic slip rate

where $\bar{v}^{(\alpha)} = \frac{1}{N}\sum_{i=1}^{N} v_i$ and $\mathrm{L}_{\mathrm{tot}} = N\,l_i$, $\rho_{\mathrm{mob}} = \frac{L_{\mathrm{tot}}}{V}$

with $\mathbf{M}^{(\alpha)} = \frac{\boldsymbol{b}^{(\alpha)}}{b_0} \otimes \boldsymbol{n}^{(\alpha)}$

Schmid tensor

$$\dot{\boldsymbol{\varepsilon}}_{pl} = \sum_{\alpha=1}^{P} \dot{\gamma}_{pl}^{(\alpha)}\,\mathbf{M}^{(\alpha)} = \sum_{\alpha=1}^{P} b^{(\alpha)}\rho_{\mathrm{mob}}\;\bar{v}^{(\alpha)}\,\mathbf{M}^{(\alpha)}$$

plastic strain rate

Constitutive modeling

Microstructure-sensitive constitutive models are typically based on the Orowan law:

$$\dot{\gamma}_{pl}^{(\alpha)} = b^{(\alpha)} \rho_{\mathrm{mob}} \ \bar{v}^{(\alpha)}(\tau_{\mathrm{RSS}}, T, \Xi_{\mathrm{microstructure}})$$

evolution equation for dislocation density evolution (Kocks-Mecking model)

$$\dot{\rho} = \left(A\sqrt{\rho} - B\rho + C \right) \dot{\gamma}_{pl}$$

Note: Mobile dislocations are usually only a very small fraction of the total number of dislocations!

Microstructural influences on dislocation mobility: grain size, dislocation density (work hardening), precipitates, alloy element concentration, …

$$\Delta\sigma_{\mathrm{T}} = \alpha G b \sqrt{\rho}$$

work hardening (Taylor law) depends on total dislocation density

Dislocation density-based crystal plasticity

- Orowan law (connecting macroscopic plastic slip rate with microscopic quantities.

$$\dot{\gamma}_{pl}^{(\alpha)} = b^{(\alpha)} \rho_{\mathrm{mob}} \, \bar{v}^{(\alpha)}(\tau_{\mathrm{RSS}}, T, \Xi_{\mathrm{microstructure}})$$

- dislocation velocity law

$$\bar{v} = \bar{v}(\tau, T, \Xi) = v_0 \left(\frac{\tau - \tau_{back}}{\tau_0} \right)^m \exp\left(-\frac{Q}{k_B T} \right)$$

- with shear resistance τ_0 and back stress τ_{back}

$$\tau_0 = \hat{\tau} + \alpha \mu b \sqrt{\rho} + \text{other hardening mechanisms}(\Xi)$$

- yields

$$\dot{\gamma}^{(\mathrm{pl})} = A \left(\frac{\tau - \tau_{\mathrm{back}}}{\hat{\tau} + \alpha \mu b \sqrt{\rho}} \right)^m \exp\left(-\frac{Q}{k_B T} \right)$$

Phenomenological crystal plasticity

Viscous law:

(Peirce et la., 1982; Asaro and Needleman, 1985; Harren et al., 1989; Teodosiu et al., 1993; Forest, 1996)

$$\dot{\gamma} = \dot{\gamma}_0 \left|\frac{\tau}{\tau_0}\right|^m \operatorname{sign}(\tau)$$

Viscous law with backstresses:

(Méric and Cailletaud, 1992; Méric, 1994;Forest, 1996)

$$\dot{\gamma} = \dot{\gamma}_0 \left|\frac{|\tau - \tau_B| - \tau_C}{\tau_D}\right|^m \operatorname{sign}(\tau - \tau_B)$$

Viscous law based on thermal activation of slip:

(Kocks, 1975; Balasubramanian et al, 2002)

$$\dot{\gamma} = \dot{\gamma}_0 \exp\left\{-\frac{Q_{\text{slip}}}{kT}\left[1 - \left(\frac{\tau - \tau_b}{\tau_c}\right)^p\right]^q\right\} \operatorname{sign}(\tau) \quad \text{with} \quad \begin{array}{l} 0 \le p \le 1 \\ 1 \le q \le 2 \end{array}$$

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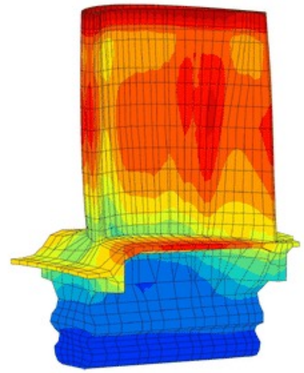
Motivation & objective

Turbine

Turbine blade

temperature gradients on a turbine blade



Long-term thermal & mechanical load → Creep; Isothermal fatigue; Thermo-mechanical fatigue (TMF)

Crystal plasticity finite element approach

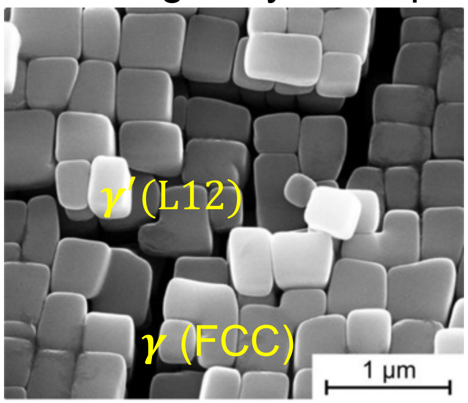
- To model plastic deformation behavior
- Widespread application
- Robust theoretical framework

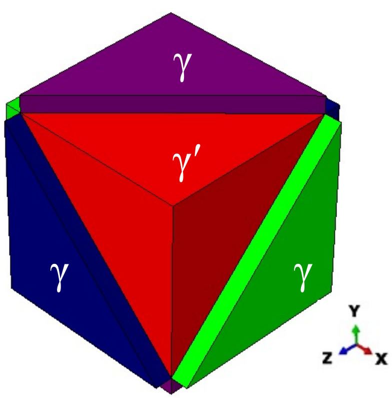
Objective:

Development a material model to describe cyclic creep and TMF behavior

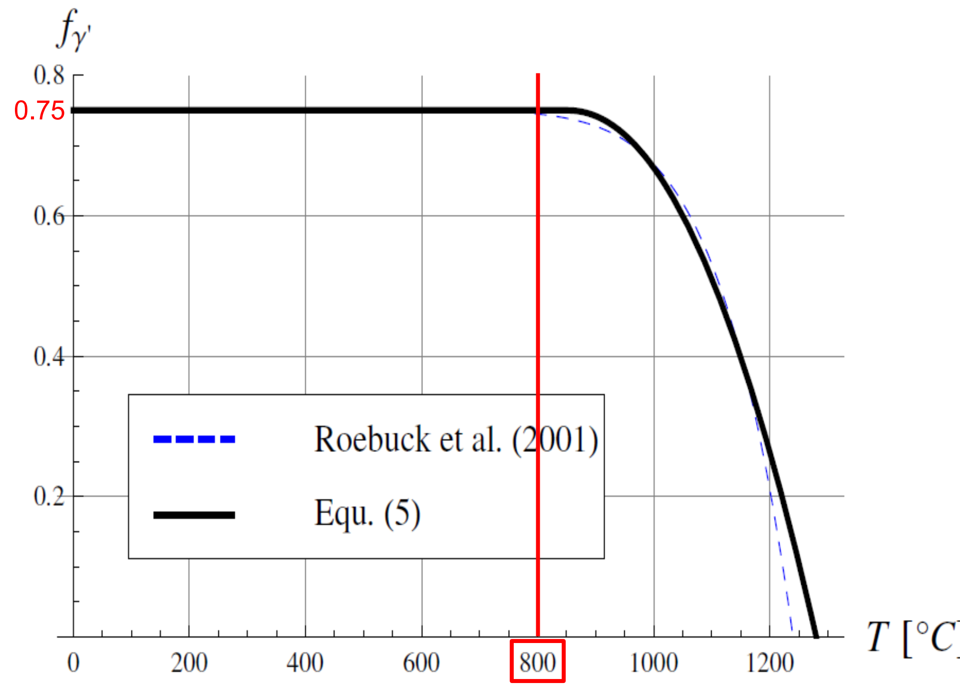
Microstructural model

Ni-base single crystal superalloys





Representative volume element



B. Fedelich et al. superalloys2012: 12th international symposium on superalloys.

Intermediate temperature (RT-800˚c):

$f^x + f^y + f^z + f^p = 1$

$f^p = 75\%$

$f^x = f^y = f^z \cong 8.3\%$

Finite element model

- **Elastic behavior**

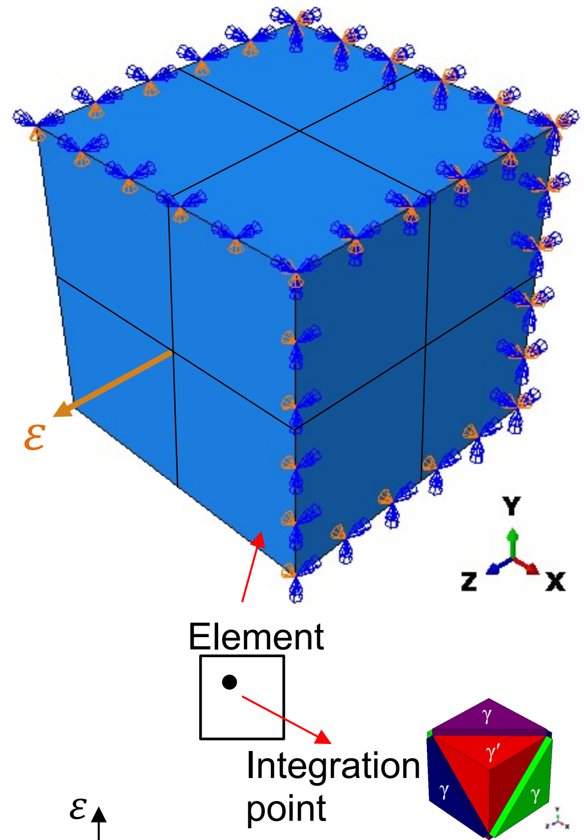
  Elasticity is described by the temperature-dependent anisotropic elastic constants

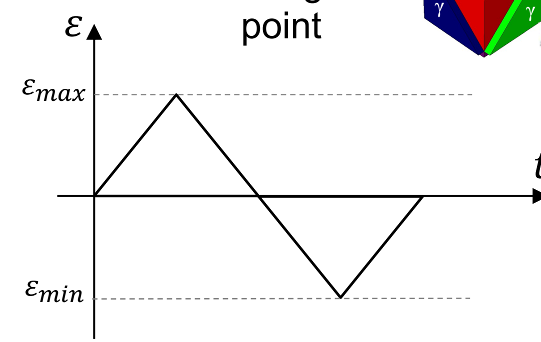
- **Plastic behavior**

  Flow rule for plastic deformation

Gamma (γ) Gamma prime (γ′) Cube slip

Phenomenological constitutive model





$$R = \frac{\varepsilon_{max}}{\varepsilon_{min}} - 1$$

Constitutive law

Flow rule for ⟨110⟩{111} slip in γ matrix channel

$$\dot{\gamma}_{\alpha}^{110} = \dot{\gamma}_{0}^{110} \cdot \exp\left(-\frac{Q^{110}}{RT}\right) \cdot \left|\frac{\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}}{\hat{\tau}_{\alpha}^{\mathrm{slip}} + \tau^{\mathrm{oro}} - \hat{\tau}^{\mathrm{soft}}}\right|^{p_1} \cdot \mathrm{sign}\left(\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}\right)$$

Thermal effect

Movement of dislocations

Dislocation climb along γ / γ′

Flow rule for ⟨112⟩{111} slip in γ′ precipitate

$$\dot{\gamma}_{\alpha}^{112} = \dot{\gamma}_{0}^{112} \cdot \exp\left(-\frac{Q^{112}}{RT}\right) \cdot \left|\frac{\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}}{\hat{\tau}_{\alpha}^{\mathrm{slip}} - \hat{\tau}_{\alpha}^{\mathrm{m}} + \hat{\tau}_{\alpha}^{\mathrm{kw}}}\right|^{p_1} \cdot \mathrm{sign}\left(\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}\right)$$

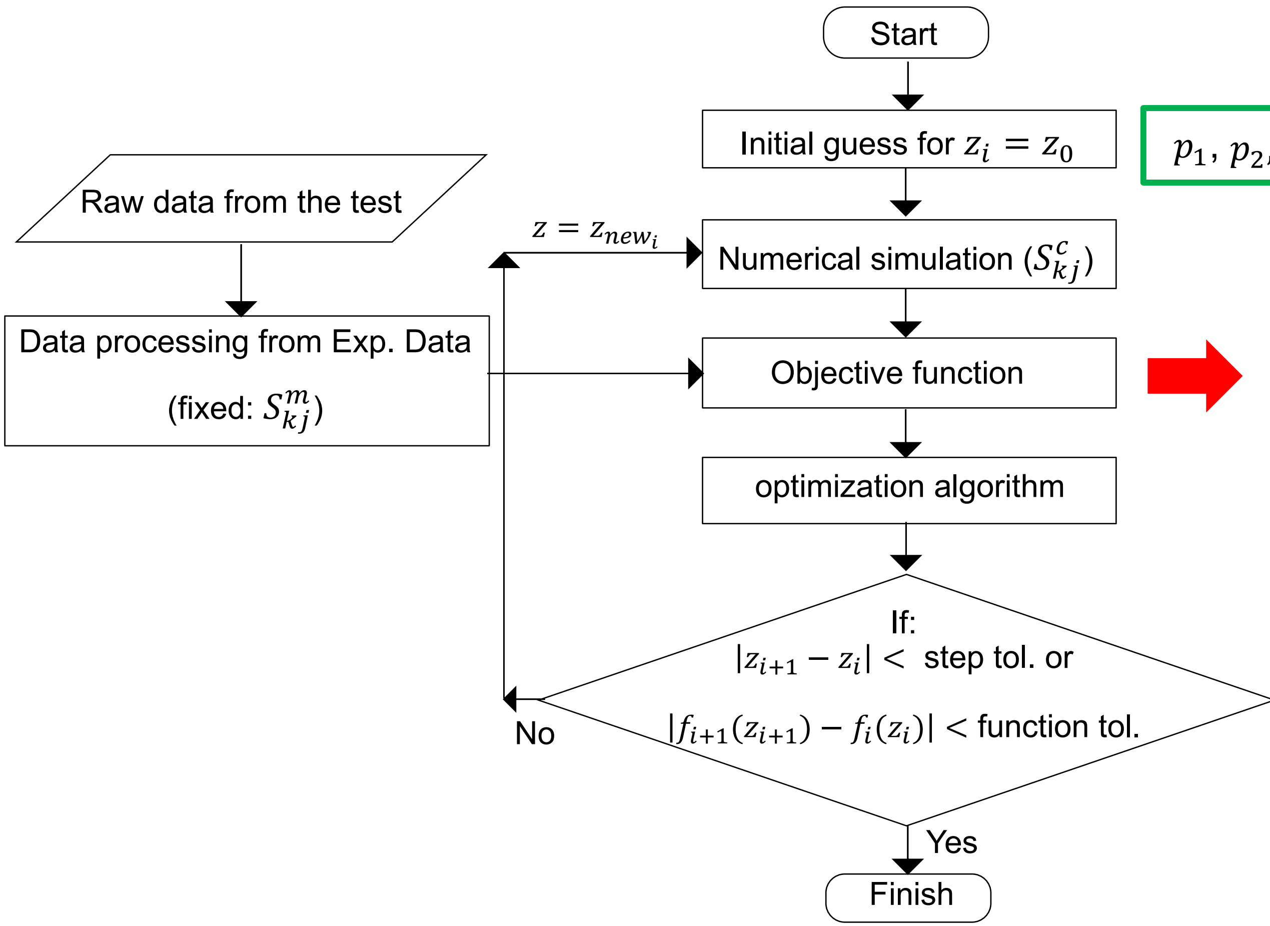
Nucleation of dislocation ribbons for γ′ shearing

Kear-Wilsdorf-locks screw dislocation

Flow rule for cube slip in ⟨110⟩{100} slip systems for both γ matrix and γ′ precipitate

$$\dot{\gamma}_{\alpha}^{\mathrm{Cube}} = \dot{\gamma}_{0}^{\mathrm{Cube}} \cdot \exp\left(-\frac{Q^{\mathrm{Cube}}}{RT}\right) \cdot \left|\frac{\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}}{\hat{\tau}_{\alpha}^{\mathrm{slip}}}\right|^{p_1} \cdot \mathrm{sign}\left(\tau_{\alpha} + \tau_{\alpha}^{\mathrm{INT}}\right)$$

Inverse analysis



$p_1, p_2, \hat{\tau}_0^{slip}(m), \hat{\tau}_0^{slip}(c), \delta, s_1, s_2$

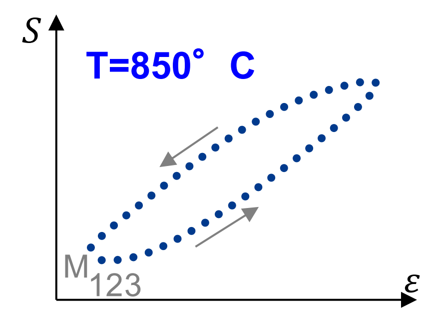
$$f(z) = \sum_{j=1}^{N} \sum_{k=1}^{M} \left(\frac{S^m_{kj} - S^c_{kj}(z)}{S^m_{j,max}} \right)^2$$

$$df(z_i) = \frac{f(z_i + \Delta z_i) - f(z_i)}{\Delta z_i}$$

$\Delta z_i = 5\% \, z_i$

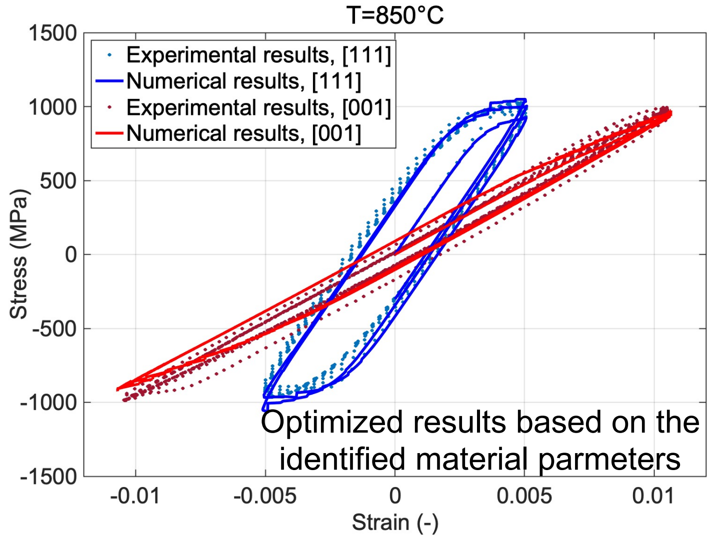
S^c_{kj}: **computational results**

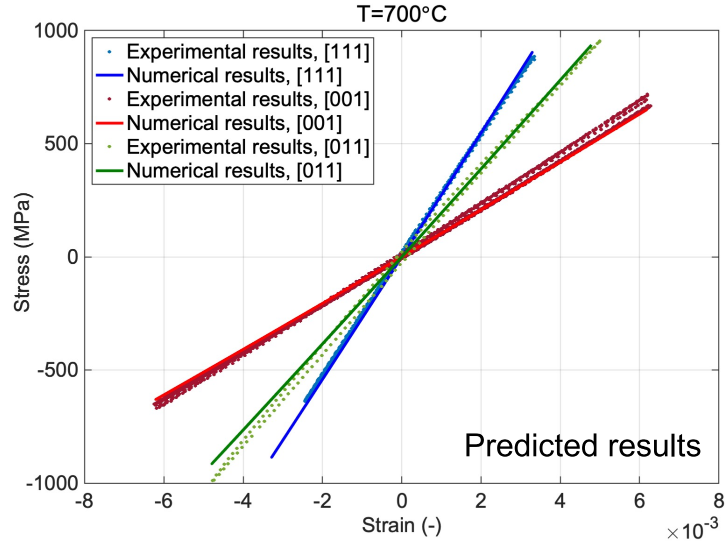
S^m_{kj}: **measured results from** exp.

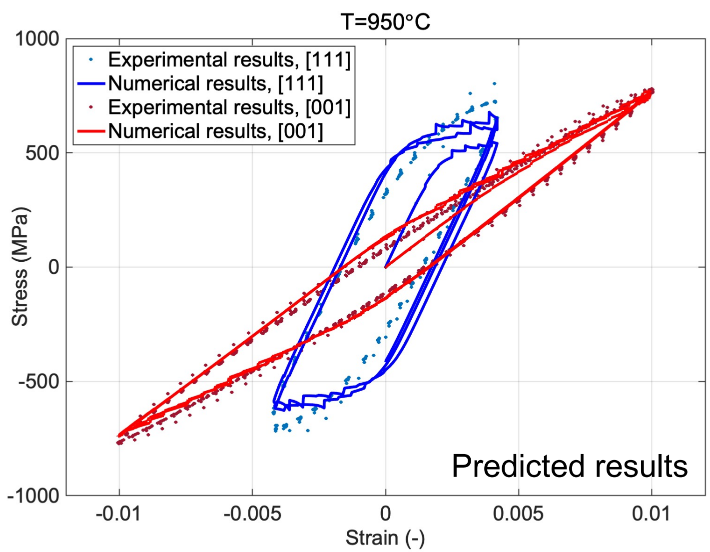


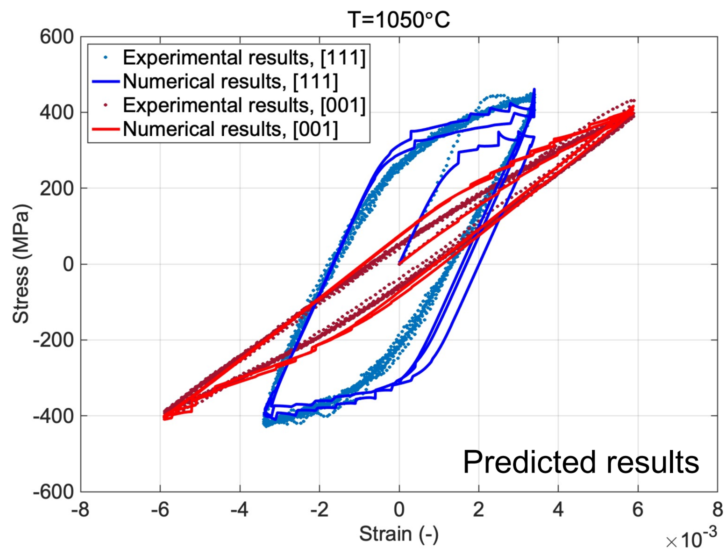
N =2: [001] & [111]

Optimized & predicted results









Experimental data from Fedelich et al. (2012)

Summary

- Accurate modelling of internal stress captures back stress (kinematic hardening)
- The isothermal low cycle fatigue behavior prediction at different temperatures and loading directions using inverse analysis
- Scalebridging approach (microstructural model) allows prediction of fatigue at various temperatures

Source:
Shamardani and Hartmaier, International Journal of Fatigue 151 (2021) 106363

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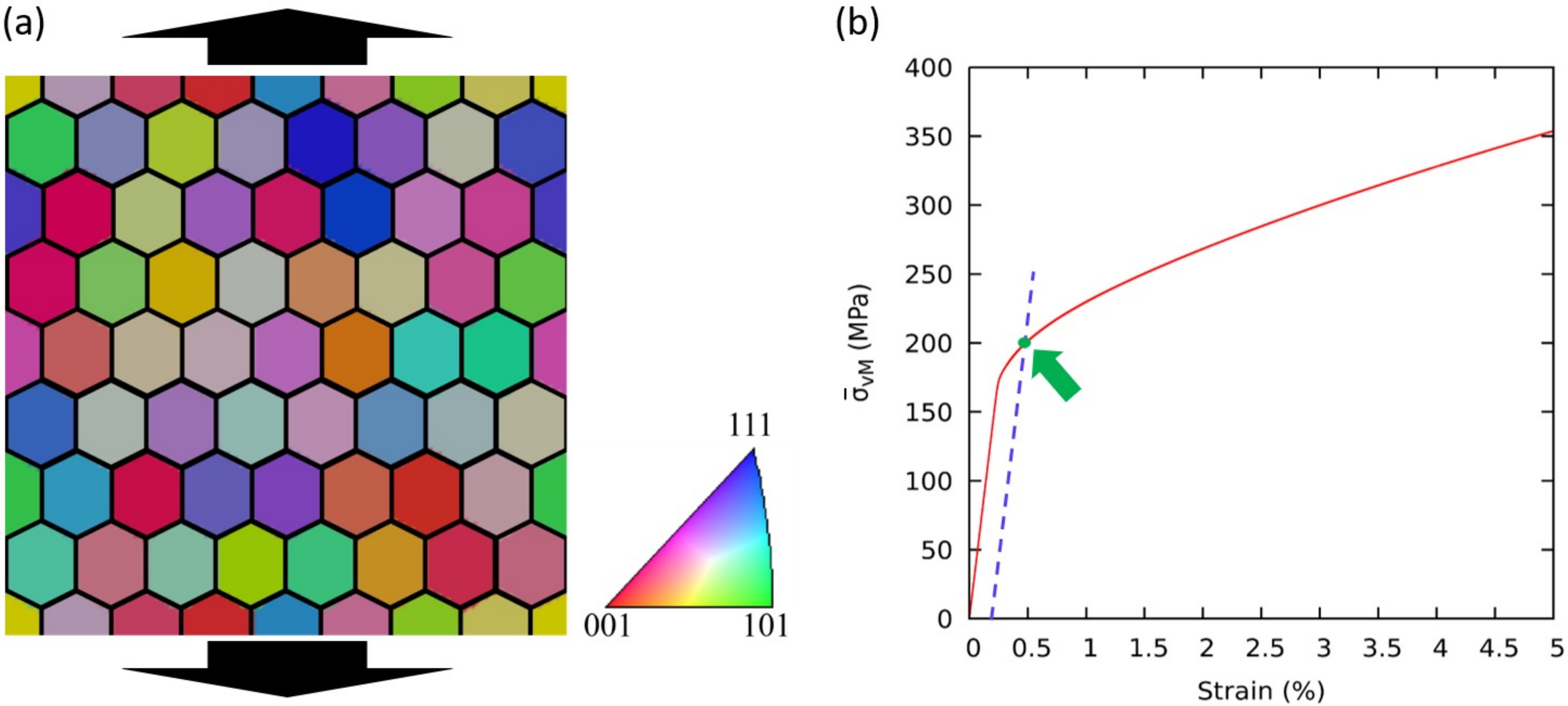
Dislocation-density based CP + Phasefield solver



Dislocation-density based CP model

Flow rule (Orowan law):

$$\dot{\gamma}^{\mathrm{s}} = \rho^{\mathrm{s}}_{\mathrm{total}} \mathrm{b} \nu^{\mathrm{s}}$$

Dislocation mobility:

$$\nu^{\mathrm{s}} = \nu_0 \left| \frac{\tau^{\mathrm{s}}}{\tau^{\mathrm{s}}_{\mathrm{c}}} \right|^{\frac{1}{\mathrm{m}}}$$

Strain hardening (Taylor law):

$$\tau^{\mathrm{s}}_{\mathrm{c}} = \tau_0 + \mathrm{c}_1 \mathrm{G} \mathrm{b} \sqrt{\rho^{\mathrm{s}}_{\mathrm{total}}}$$

Nonlocal dislocation density-based CP model

Consideration of statistically stored dislocation denisties (SSD) and geometrically necessary dislocation densities (GND)

$$\rho^{s}_{\text{total}} = \rho^{s}_{\text{SSD}} + \rho^{s}_{\text{GND}}$$

Nye tensor evolution (strain gradient/rotation of strain tensor)

$$\dot{\mathbf{\Lambda}} = \left(-e_{jkl}\dot{\varepsilon}^{p}_{il,k}\right)^{T}\mathbf{e}_i \otimes \mathbf{e}_j,$$

GND evolution based on Nye tensor

$$\dot{\rho}^{\alpha}_{g} = \dot{\rho}^{\alpha}_{g(e)} + \dot{\rho}^{\alpha}_{g(s)} = \frac{1}{b}\left(|\mathbf{d}^{\alpha}\dot{\mathbf{\Lambda}}\mathbf{l}^{\alpha}| + |\mathbf{d}^{\alpha}\dot{\mathbf{\Lambda}}\mathbf{d}^{\alpha}|\right)$$

SSD evolution (Kocks-Mecking law)

$$\dot{\rho}^{\alpha}_{s} = \left(c_1\sqrt{\rho^{\alpha}_{s} + \rho^{\alpha}_{g}} - c_2\rho^{\alpha}_{s}\right)\dot{\gamma}^{\alpha}$$

Phenomenological nonlocal crystal plasticity model

$$F = F_e F_p$$

$$\dot{F}_p = L_p F_p$$

empirical CP model

$$L_p = \sum_{\alpha=1}^{N_S} \dot{\gamma}_\alpha \tilde{M}_\alpha$$

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left| \frac{\tau_\alpha + \tau_\alpha^{GNDk}}{\hat{\tau}_\alpha + \hat{\tau}_\alpha^{GNDi}} \right|^{p_1} sign\left(\tau_\alpha + \tau_\alpha^{GNDk}\right)$$

$$\dot{\hat{\tau}}_\alpha = \sum_{\beta=1}^{N_S} h_0 \chi_{\alpha\beta} \left(1 - \frac{\hat{\tau}_\alpha}{\hat{\tau}^f}\right)^{p_2} \left|\dot{\gamma}_\beta\right|$$

non-local terms (higher order strain gradients)

$$\tau_\alpha^{GNDk} = \tilde{S}^{GND} \cdot \tilde{M}_\alpha$$

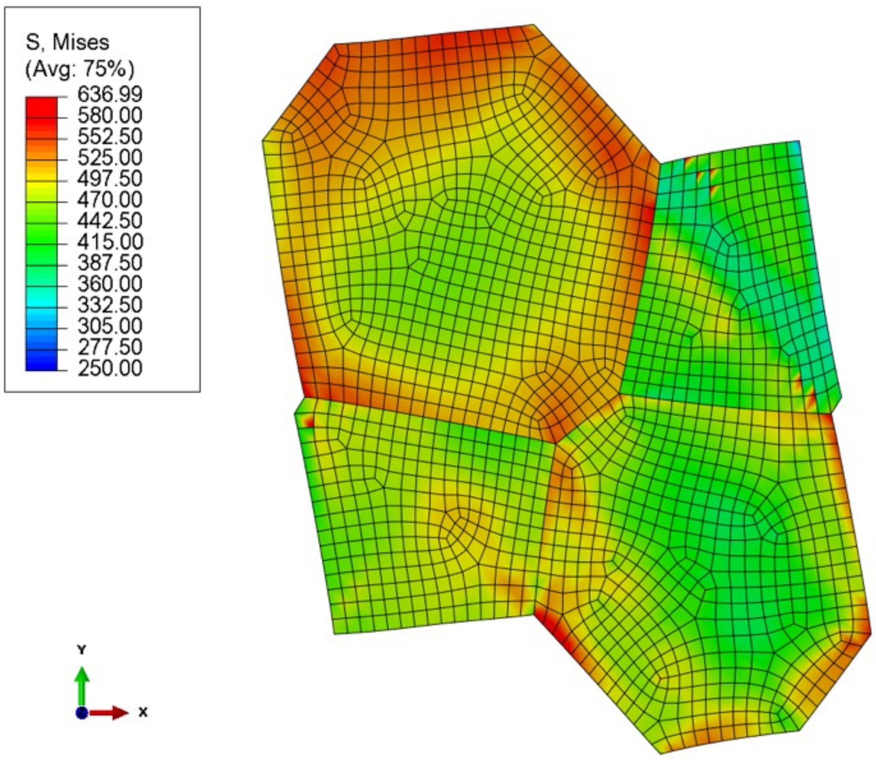
$$\tilde{S}^{GND} = F_p S^{GND} F_p^T$$

$$S^{GND} \propto L^3 \cdot \frac{\partial^2 F_p}{\partial x^2}$$

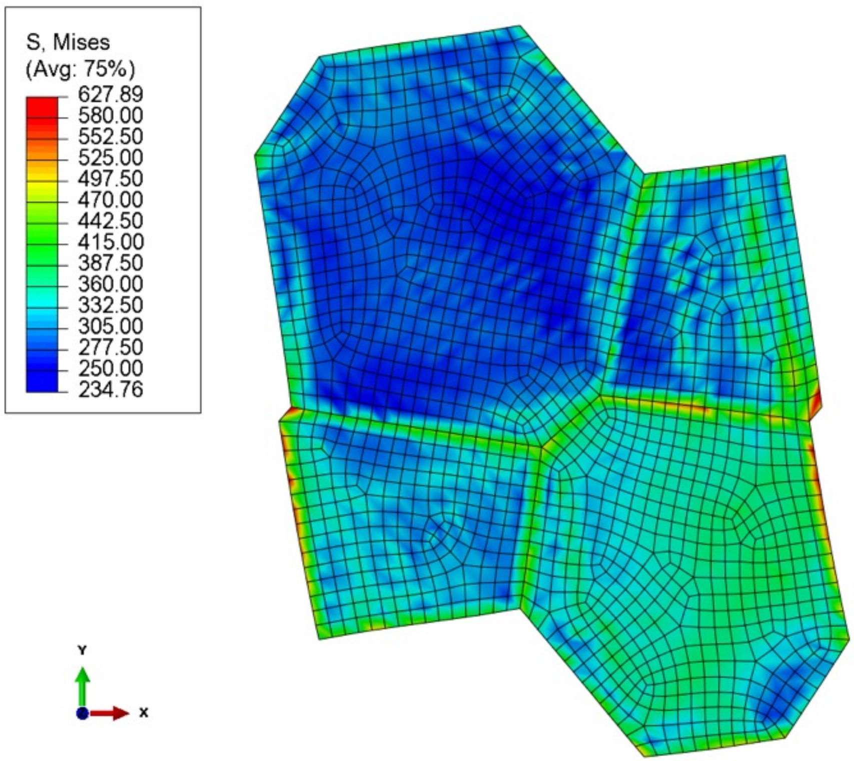
$$\hat{\tau}_\alpha^{GNDi} \propto \left| \frac{\partial F_p}{\partial x} \right|$$

Source: Ma, Hartmaier, Philosophical Magazine 2013

Phenomenological Nonlocal crystal plasticity model

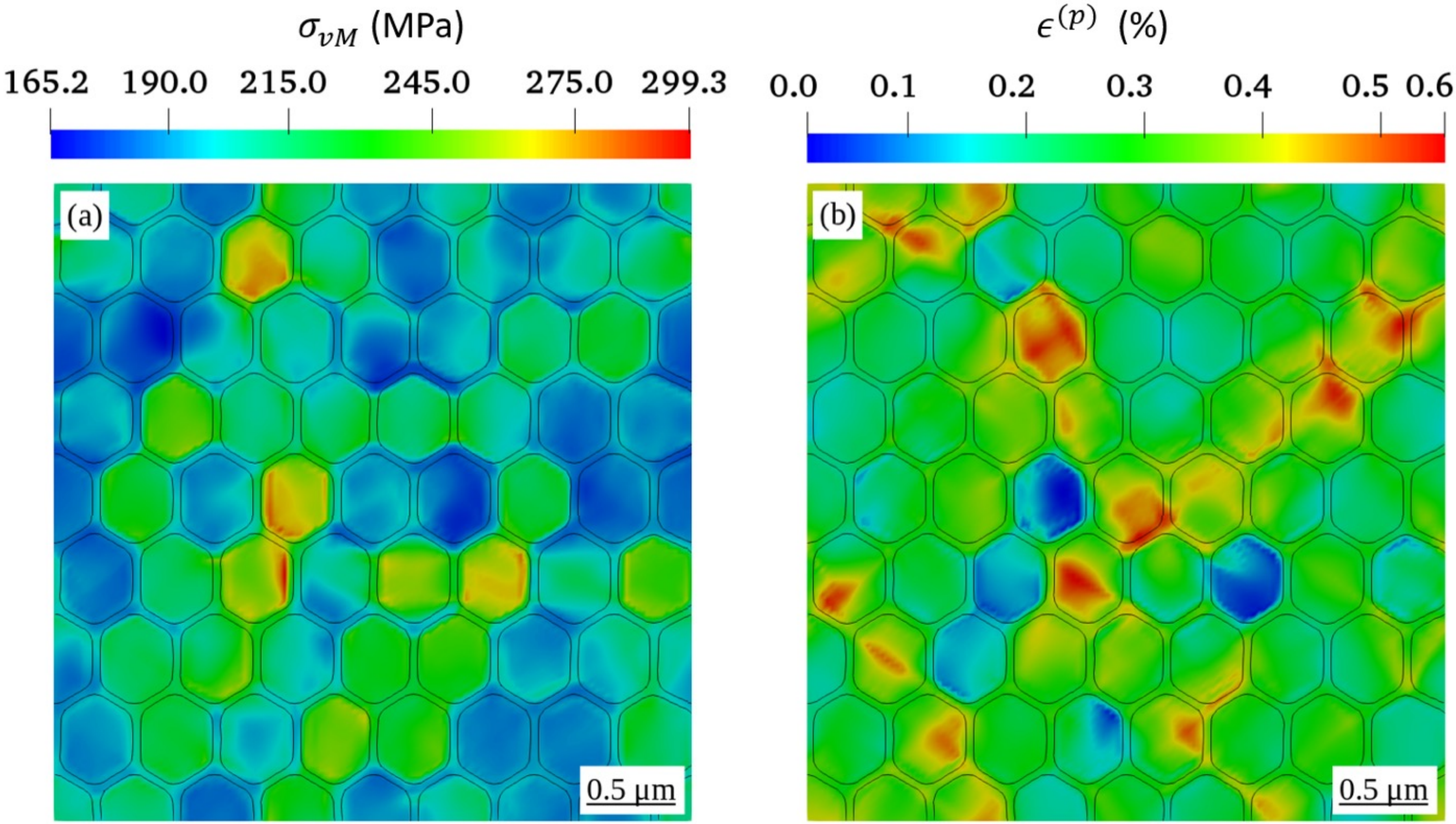


local

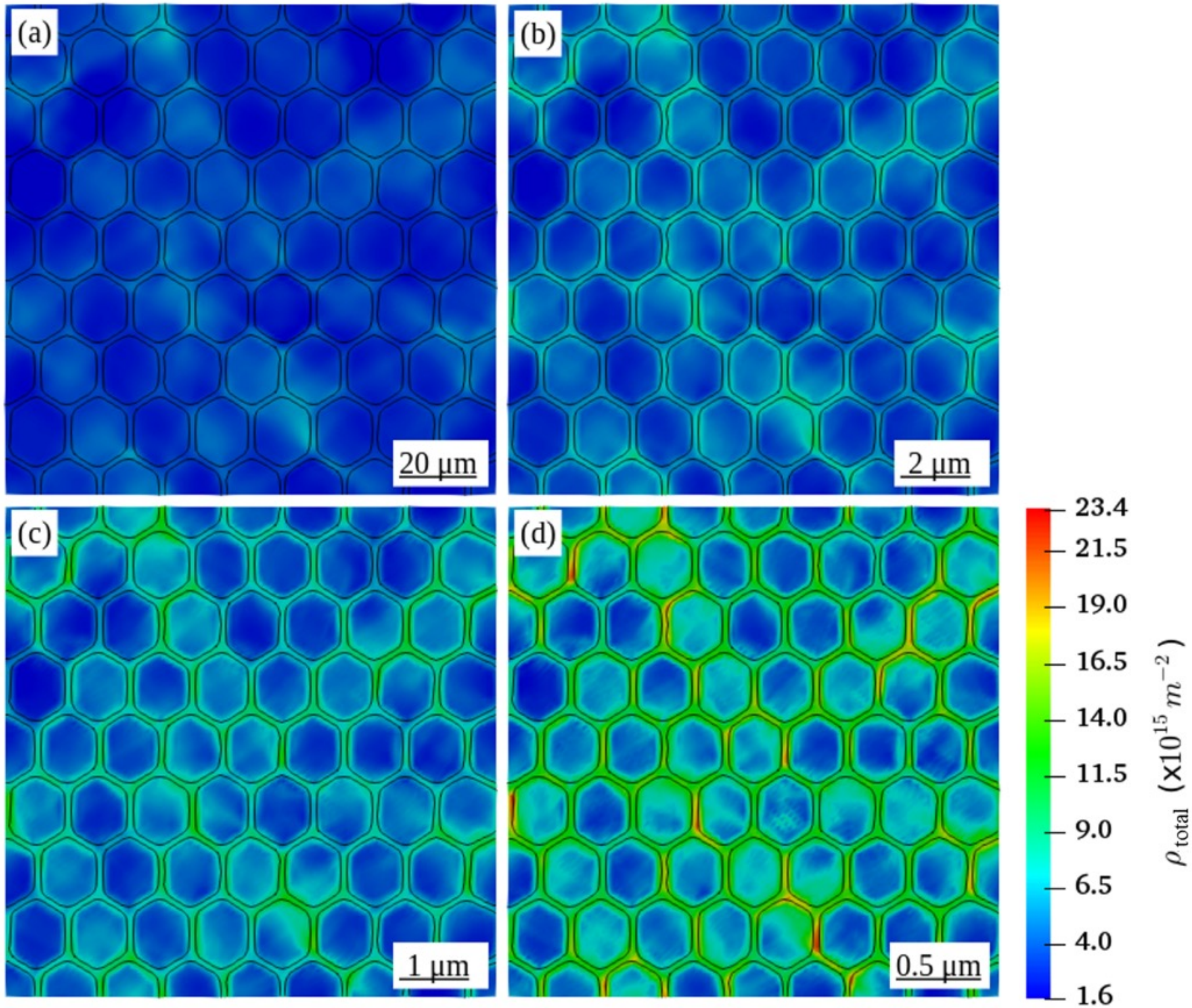


nonlocal

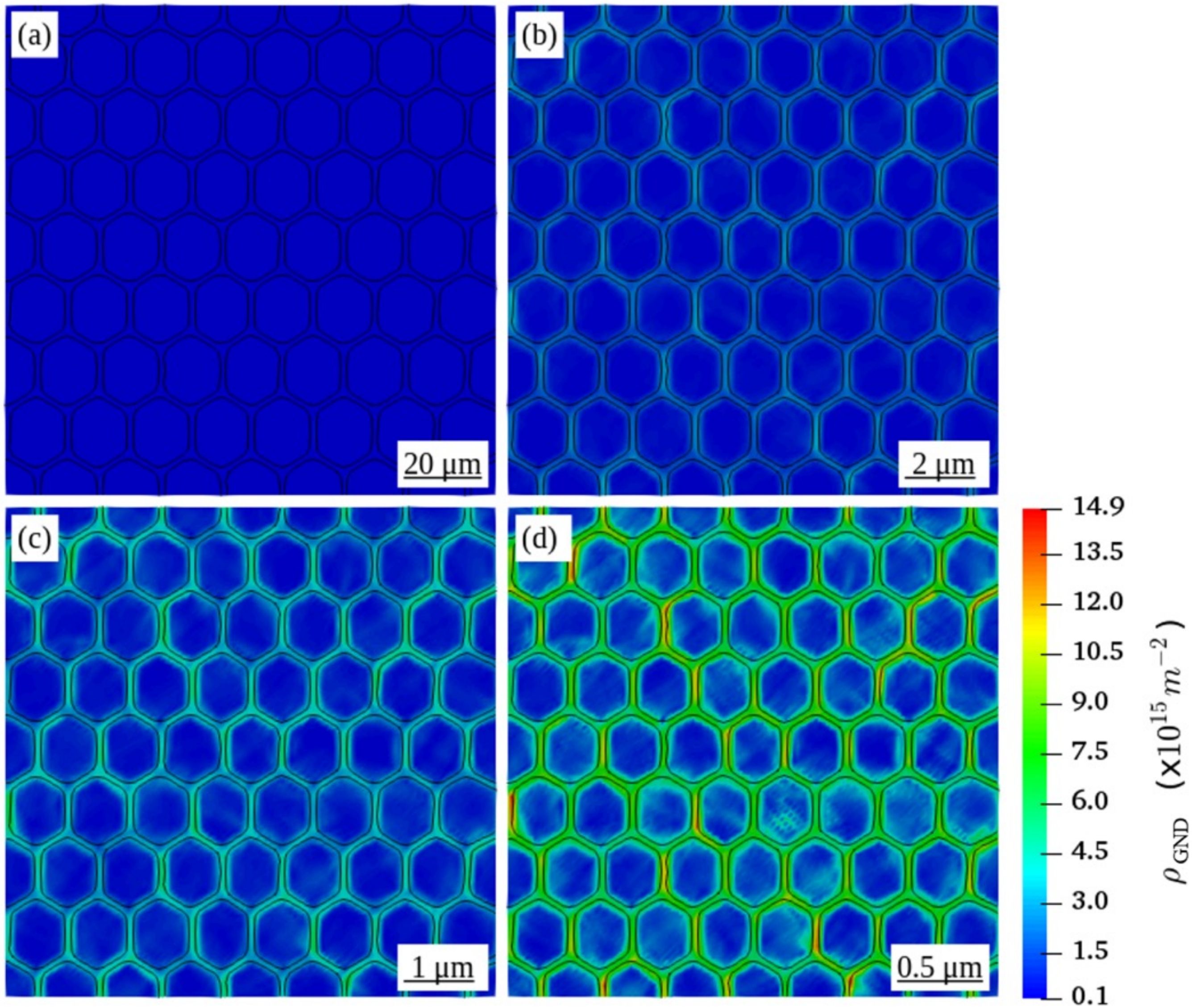
Dislocation-based CP model: deformation pattern



Total dislocation density

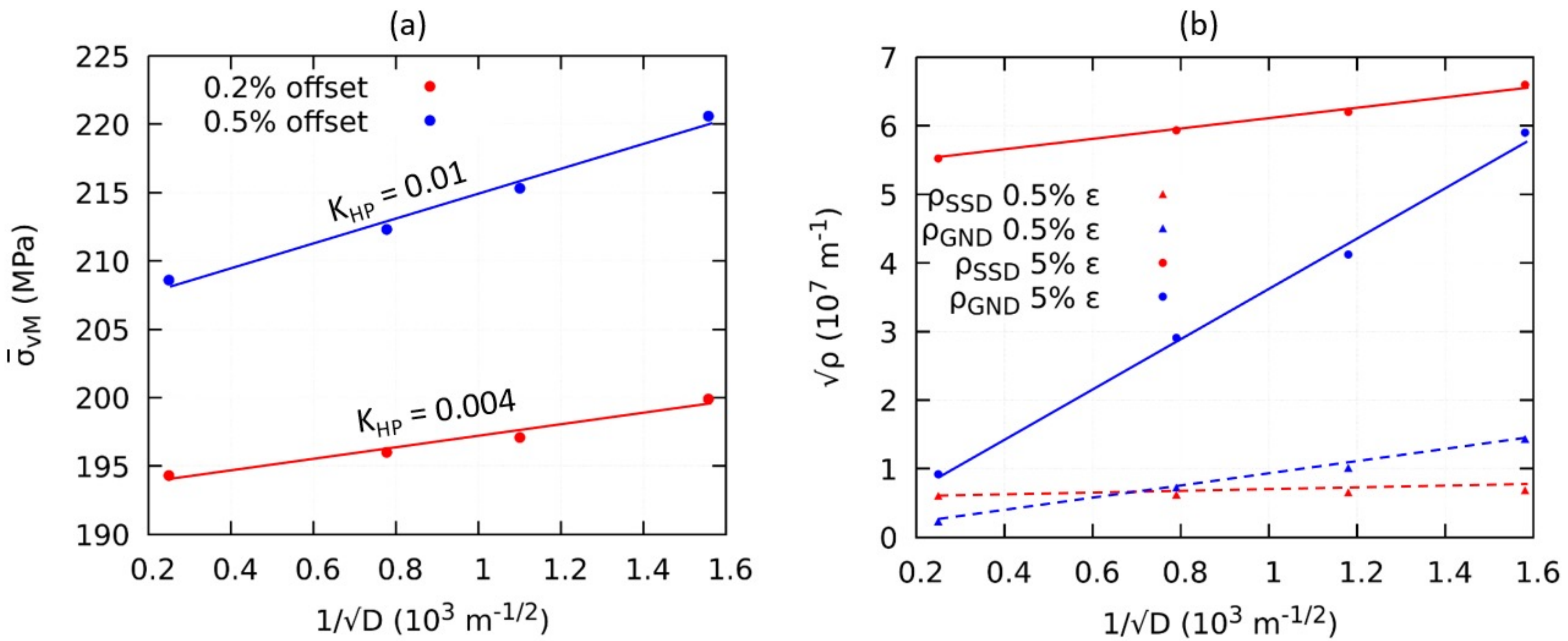


GND density



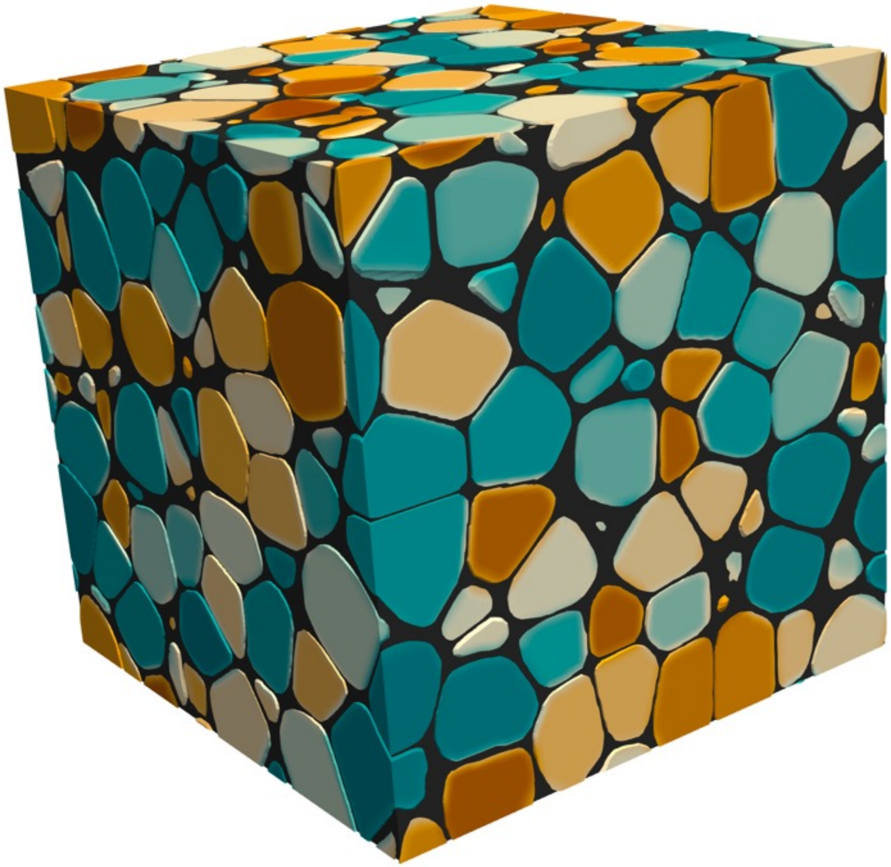
(a)
20 μm
(b)
2 μm
(c)
1 μm
(d)
0.5 μm
14.9
13.5
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.1
ρ_{GND} $(\times 10^{15} m^{-2})$

Prediction of Hall-Petch coefficient



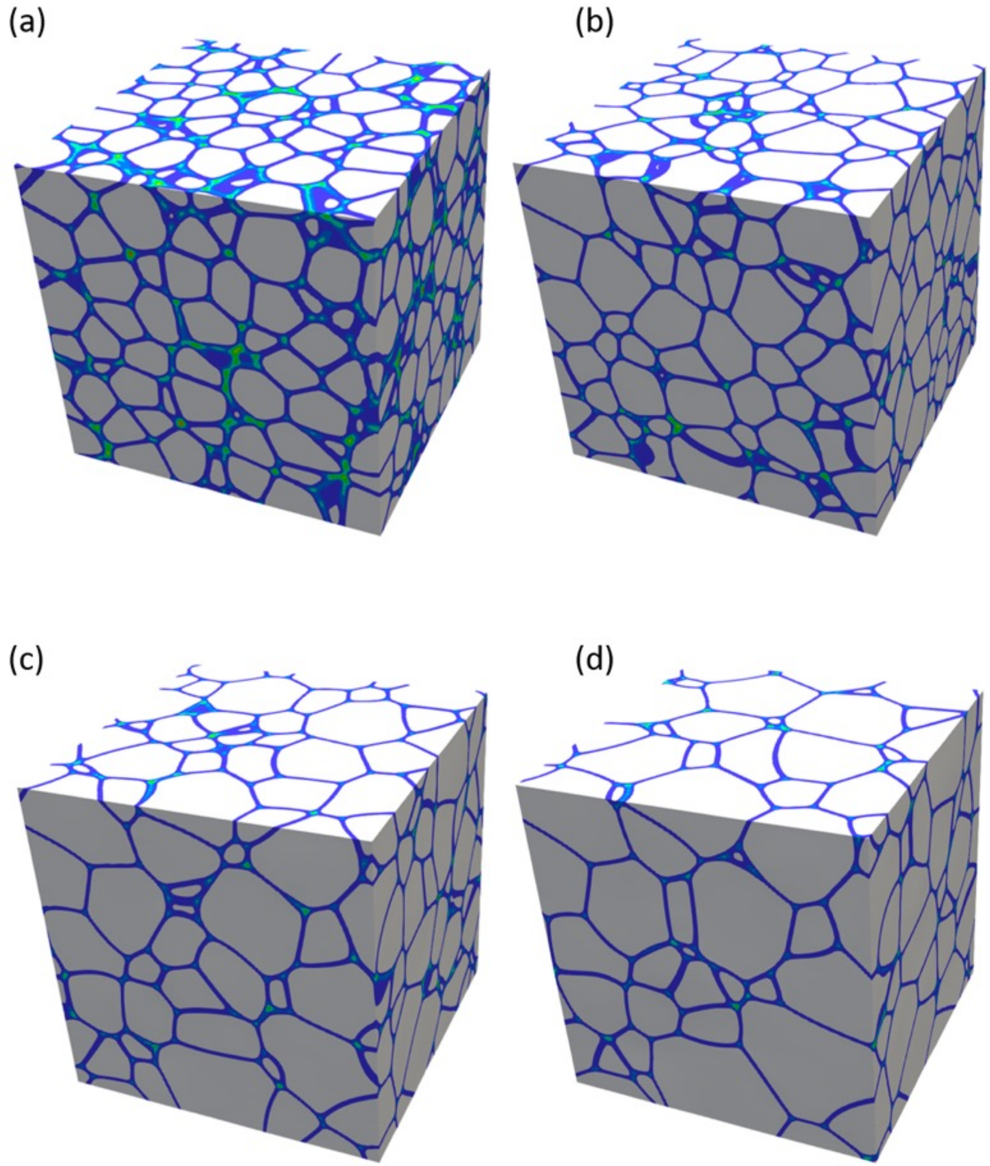
- ➢ Correct trend in fine grain strengthening, but quantitatively too small
- ➢ Initial conditions (pre-deformation, residual stresses) not considered

Microstructure evolution

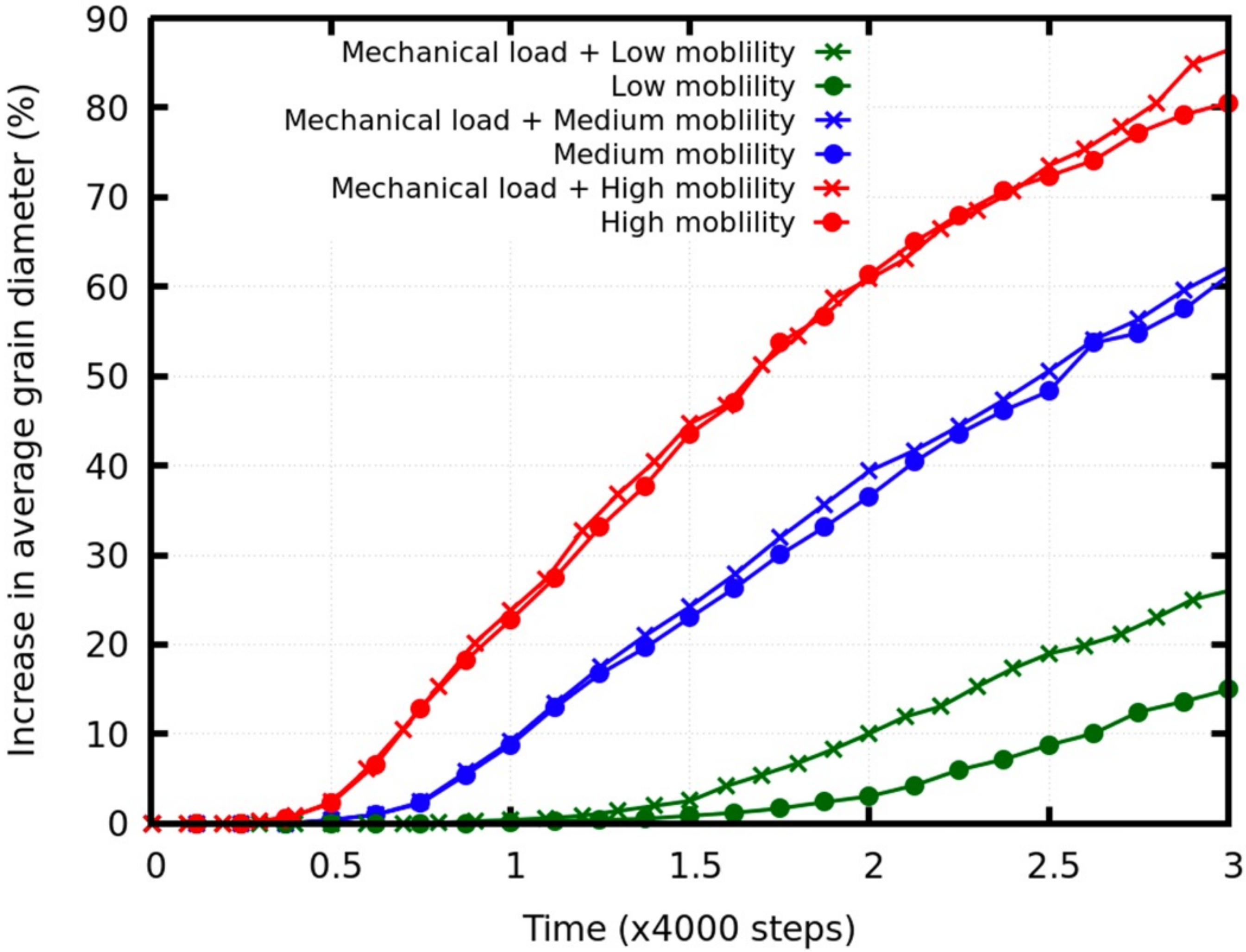


What is the influence of plastic strain on grain growth?

Microstructure evolution



Microstructure evolution



Summary

Dislocation-based strain-gradient plasticity model

- predicts Hall-Petch relation qualitatively correctly, but
  - Magnitude of Hall-Petch coefficient too low compared to experimental values
  - Grain boundary strengthening at onset of plasticity not captured
  - Necessity to consider residual stresses, pre-deformation, initial GNDs
- Influence of plastic strain on grain growth is small in this model

Source:
Amin et al., Materials 12 (2019) 2977

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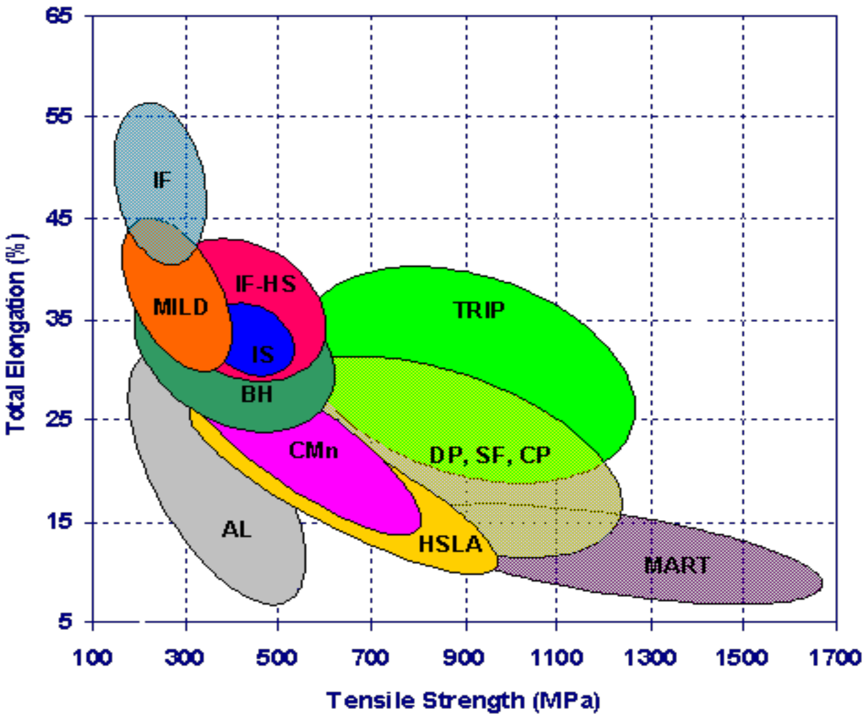
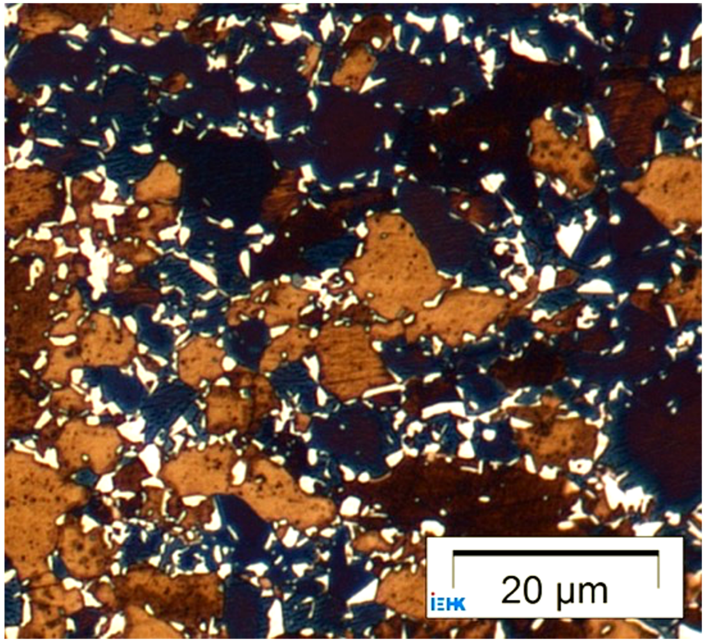
TRIP-TRansformation Induced Plasticity



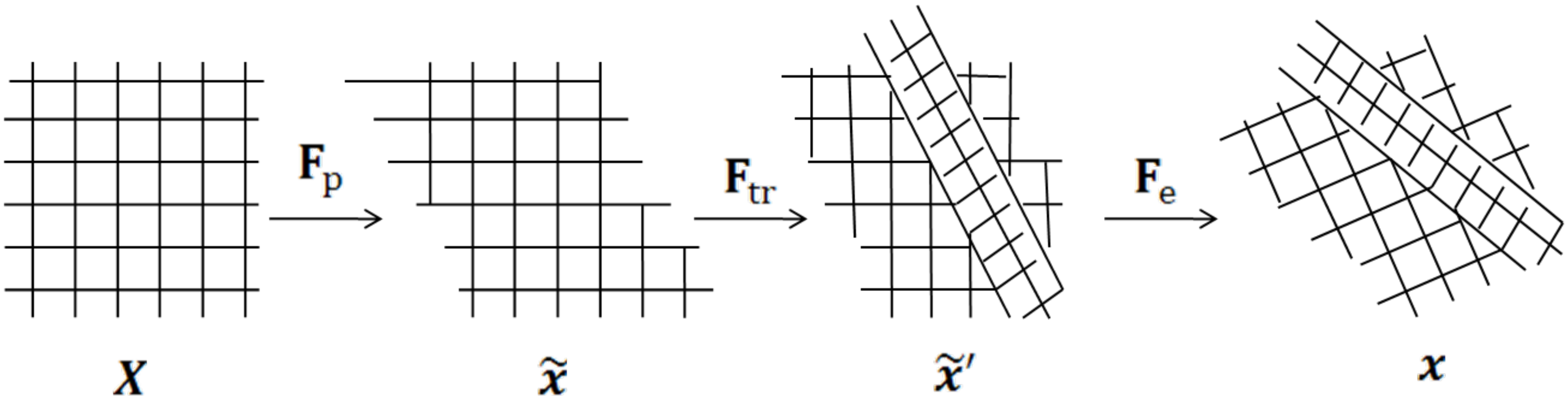


http://www.uss.com/corp/auto/tech/index.asp

Transformation induced plasticity causes

- good deformability at
- high strength

Constitutive model for TRIP



$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \widetilde{\mathbf{x}}'} \frac{\partial \widetilde{\mathbf{x}}'}{\partial \widetilde{\mathbf{x}}} \frac{\partial \widetilde{\mathbf{x}}}{\partial \mathbf{X}} = \mathbf{F}_\mathrm{e} \mathbf{F}_\mathrm{t} \mathbf{F}_\mathrm{p}$$

Multiplicative decomposition of deformations by elasticity, plasticity and phase transformation

Constitutive model for TRIP

Deformation velocity gradient

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$$

$$\mathbf{F}(t + \Delta t) = (\mathbf{I} + \mathbf{L}\Delta t)\mathbf{F}(t)$$

Plastic deformation

$$\mathbf{L}_p = \sum_{\alpha=1}^{N_S} \dot{\gamma}_\alpha \mathbf{M}_\alpha$$

$$\mathbf{M}_\alpha = \mathbf{m}_\alpha \otimes \mathbf{n}_\alpha$$

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left| \frac{\tau_\alpha}{\tau_\alpha^c} \right|^n \mathrm{sign}(\tau_\alpha)$$

Transformation

rate of volume fraction

$$\mathbf{L}_{tr} = \sum_{I=1}^{N_T} \dot{\eta}_I \mathbf{N}_I$$

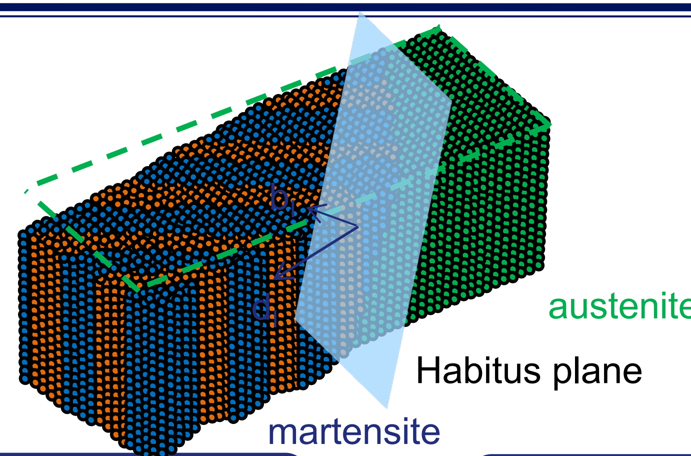
$$\mathbf{N}_I = \mathbf{b}_I \otimes \mathbf{d}_I$$

eigen strain tensor

Martensite transformation

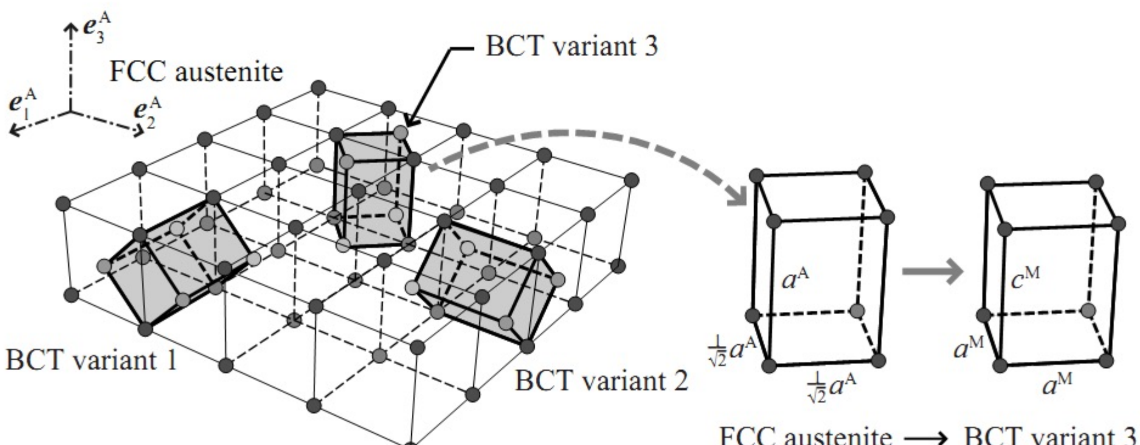
Transformation systems

$$\mathbf{N}_I = \mathbf{b}_I \otimes \mathbf{d}_I$$
$$= \mathbf{R}_I \mathbf{U}_I - \mathbf{I}_I$$



R_I Rotation
U_I Bain strain
d_I Habitus plane normal
b_I shape strain vcktor
N_I Eigenstrain tensor

3 Bain strains ✖ 4 rotations ➡ 12 transformations



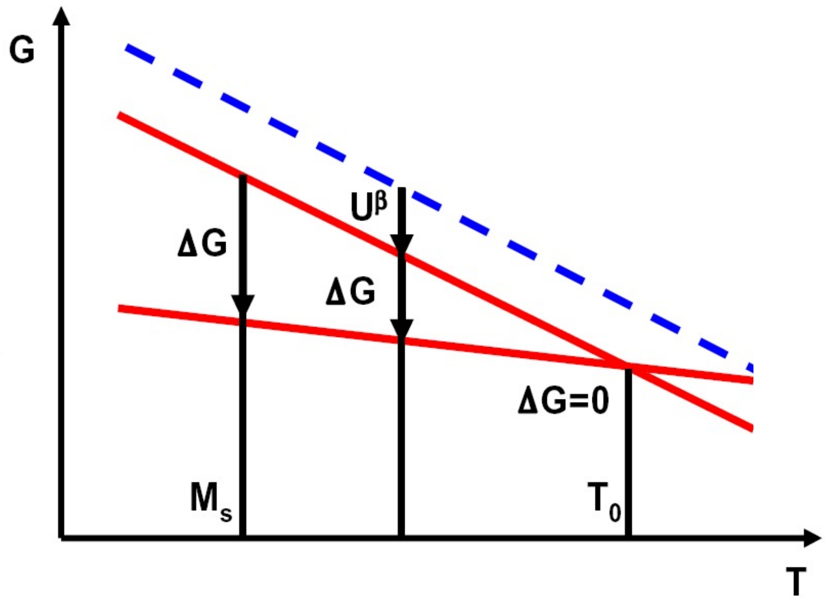
D.D.Tjahjanto; Thesis;2007

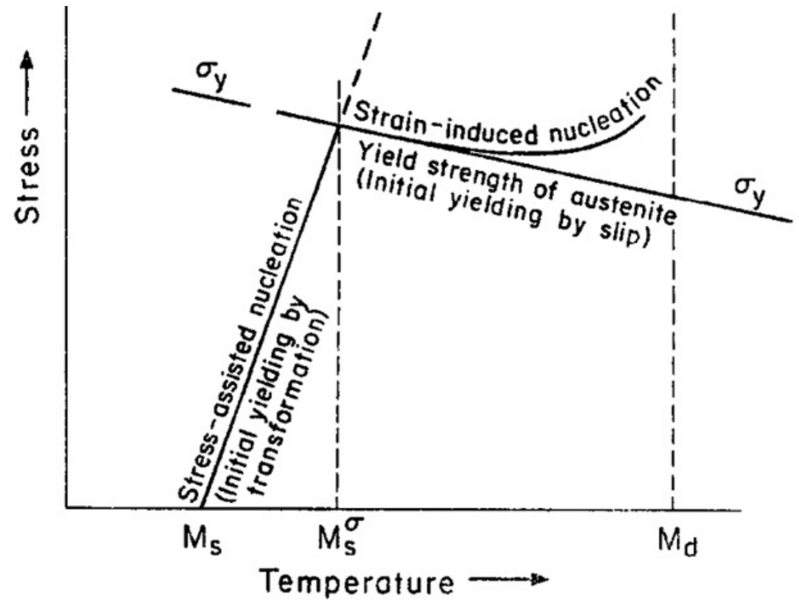
inverse Nishiyama-Wassermann relations

$$[0\,1\,1]_{fcc} \| [1\,1\,1]_{bcc}$$
$$[0\,1\,\bar{1}]_{fcc} \| [2\,\bar{1}\,\bar{1}]_{bcc}$$
$$(\bar{1}\,0\,0)_{fcc} \| (0\,1\,\bar{1})_{bcc}$$

Martensite transformation – volume fraction

Nucleation propability based on Gibbs free energy and on strain energy (applied stress . shape strain vector)



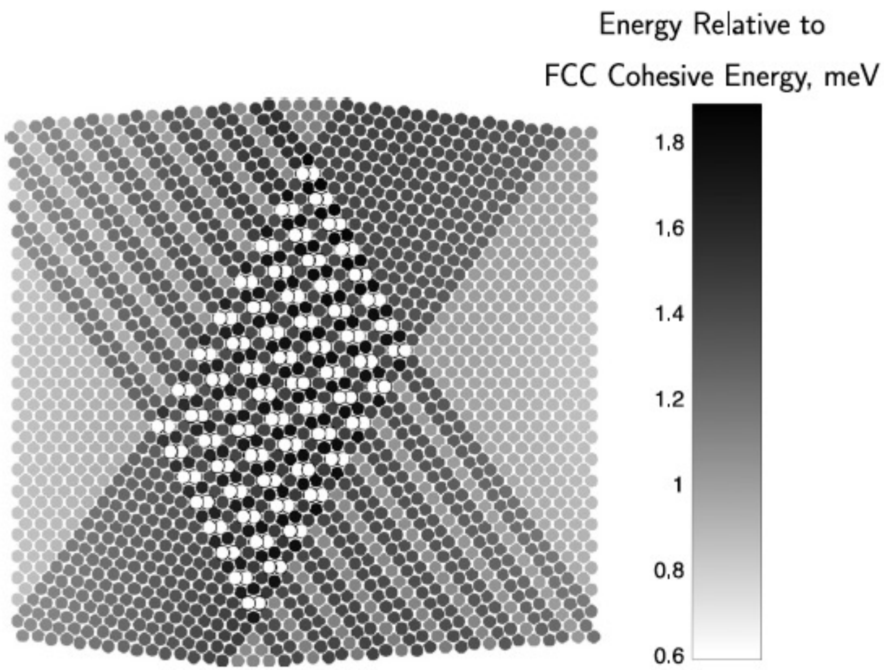


G.B.Olson, M.Cohen; J.Less-Comm.Metals 1972

Martensitic transformation – volume fraction

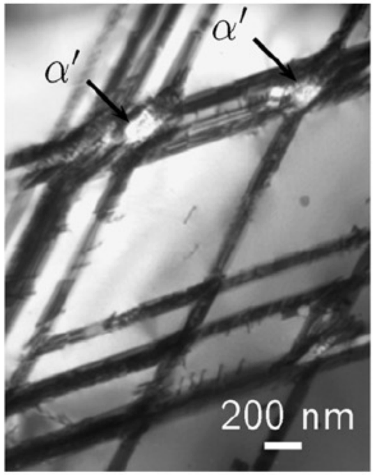
Strain induced martensite nucleation at intersection of shear faults

MD simulation

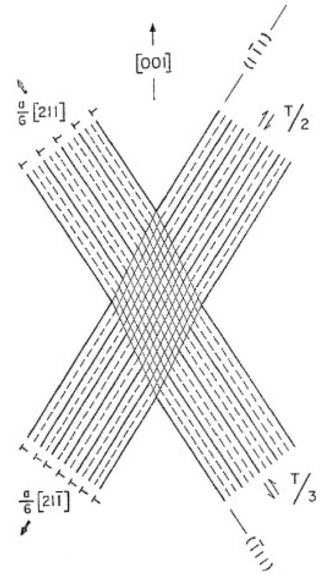


C.W. Sinclair, R.G. Hoagland; Acta Mater.; 2008

experiment



K. Spencer; PhD thesis;2002



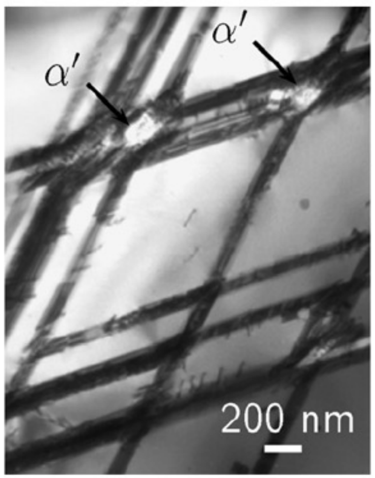
G.B. Olson, M. Cohen; J.Less-Comm.Metals; 1972

Martensite transformation

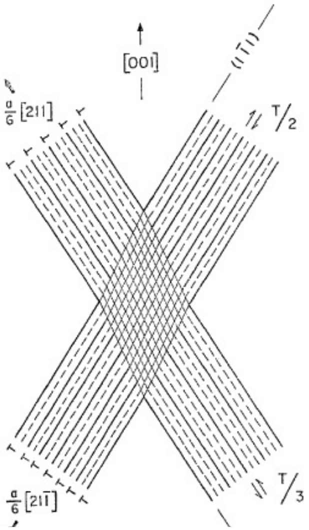
Rate of Martensite volume fraction

$$\dot{\eta}_I = \dot{\eta}_I^{nuc} + \dot{\eta}_I^{gro}$$

strain induced nucleation



K.Spencer; PhD thesis;2002



G.B.Olson, M.Cohen; J.Less-Comm.Metals; 1972

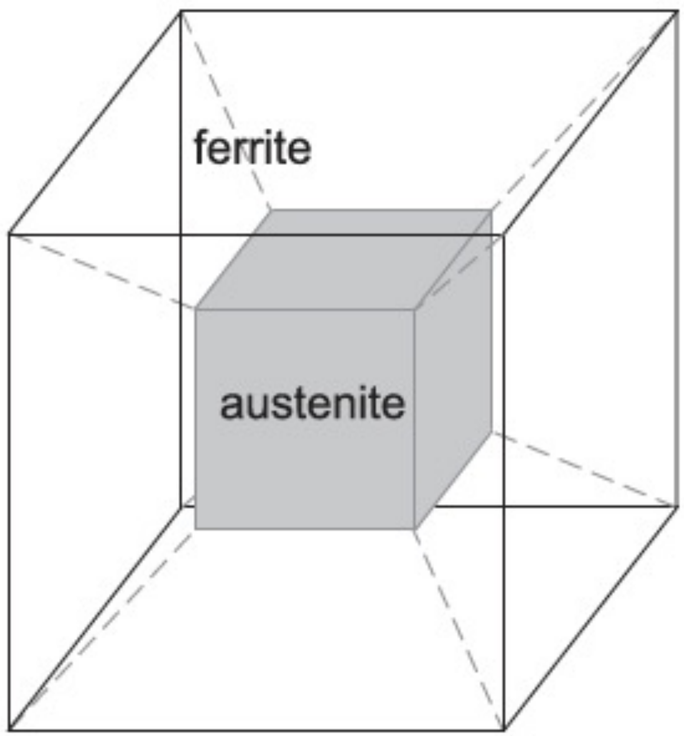
driving force for

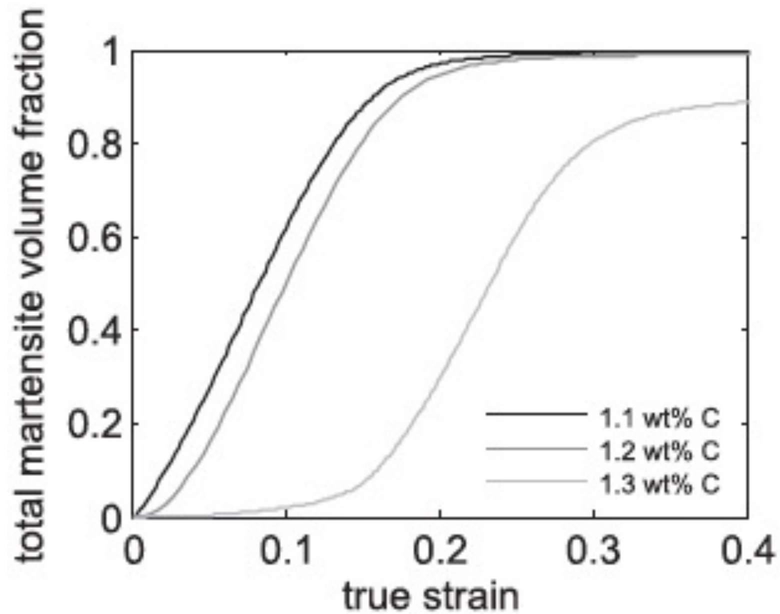
stress assisted growth

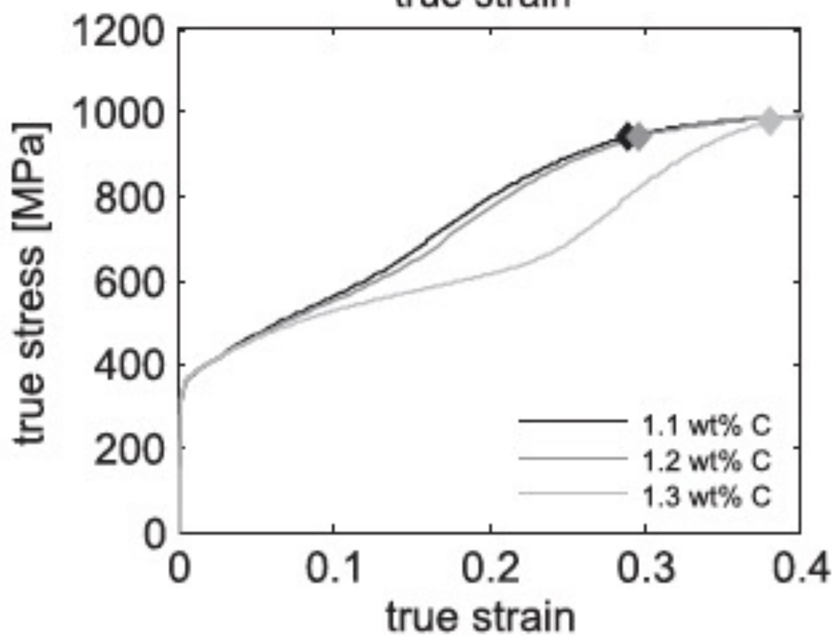
$$\varsigma_I^{gro} = f(\eta_I, \Delta G, \sigma, \ldots)$$

$$\boxed{\dot{\eta}_I = c_3 (1 - \sum_{\beta=1}^{N_T} \eta_\beta)(\varsigma_I^{nuc} + \varsigma_I^{gro})}$$

3D TRIP model







Rate of phase transformation:

$$\dot{\eta}_I = \dot{\eta}_I^{nuc} + \dot{\eta}_I^{gro}$$

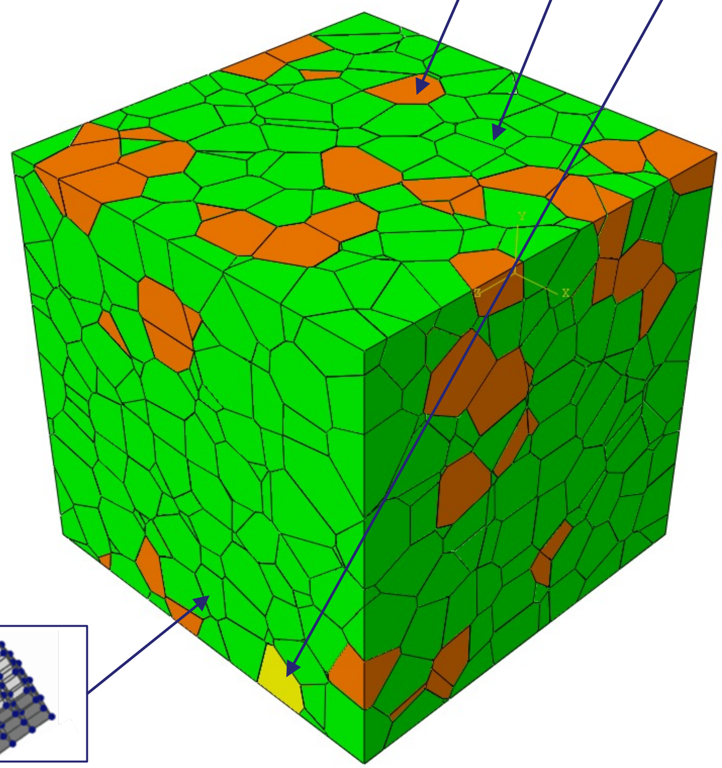
influence of thermodynamic state (temperature and chemical composition taken into account)

Advanced Representative Volume Element

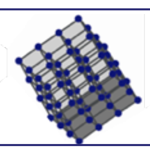
RVE represents experimentally determined volume fractions of phases

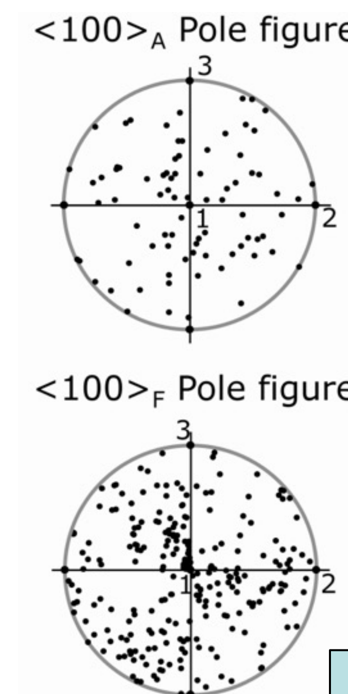
Different crystal structure and flowing behaviour

fcc + bcc + bct



Local crystal orientation





Summary Phase Transformations

- Elementary processes of **phase transformation** can be described by atomistic models
- **Phase field models** yield detailed information on phase boundary motion and transformation kinetics
- **Crystal plasticity-based approach** allows simulation of complex RVE

Source:
Ma and Hartmaier, International Journal of Plasticity 64 (2015) 40

Future Trends in Crystal Plasticity

- Explicit consideration of residual stresses of microstructural features below element size
- Consideration of microstructure evolution
- More realistic descriptions of initial material state, after processing