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Integrated Physical-Constitutive Computational Framework for Plastic Deformation Modeling

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Motivation

- Framework for the simulation of macroscopic stress-strain relations within a wide temperature and strain rate range
- Combination of constitutive creep relations and physically-based microstructure evolution
- Time dependent stress relaxation
- Construction of deformation maps

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The model

Overview

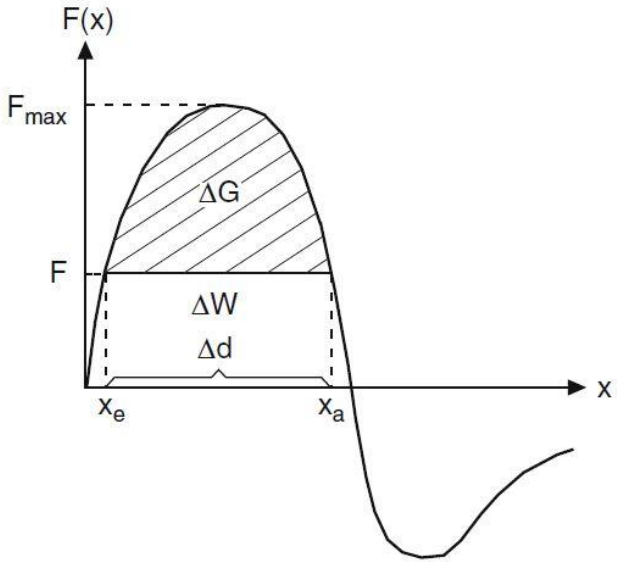
	Creep	State parameter evolution
Low-temperature plasticity	Dislocation glide*	Dislocation density evolution – Extended Kocks-Mecking model
Power-law creep	LT – creep* HT – creep* Harper-Dorn	
Diffusional flow	Coble – creep Nabarro-Herring	
	Grain boundary sliding	*Mechanical threshold concept $\hat{\tau}$

Thermal activation of dislocation movement

Effect of temperature and strain rate on stress needed to pass the obstacle

- $$\tau_{\mathrm{th}} = \hat{\tau} \cdot \exp\left(-\frac{kT}{\Delta F} \ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)\right)$$

$\hat{\tau}$ … mechanical threshold
ΔF … total energy
ΔG … Gibbs free energy
$\dot{\varepsilon}_0$ … critical strain rate



Power law creep

$$\dot{\varepsilon} = \frac{A \cdot D \cdot G \cdot b}{k_B \cdot T} \cdot \left(\frac{\sigma_s}{G}\right)^n$$

<u>Lattice diffusion controlled</u>

n_{HT} = 4.4 → HT - creep

Q_{tr}= 127.2 kJ/mol

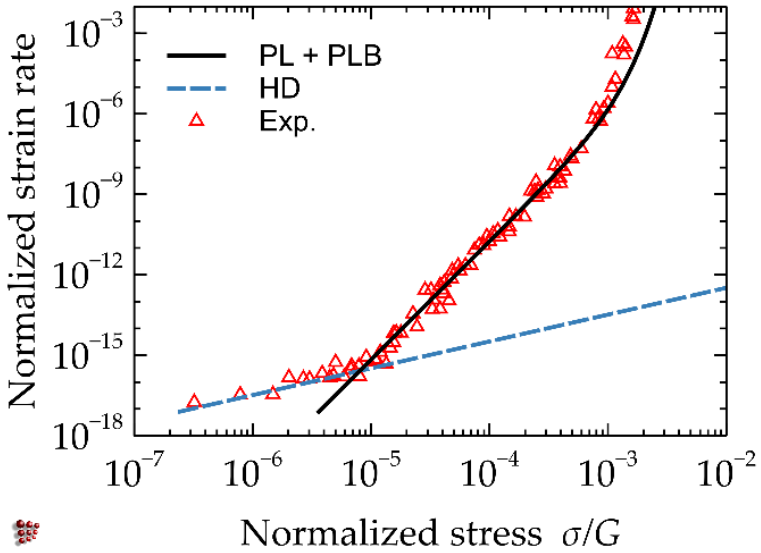
<u>Core diffusion controlled</u>

n_{LT} = 6.4 → LT - creep

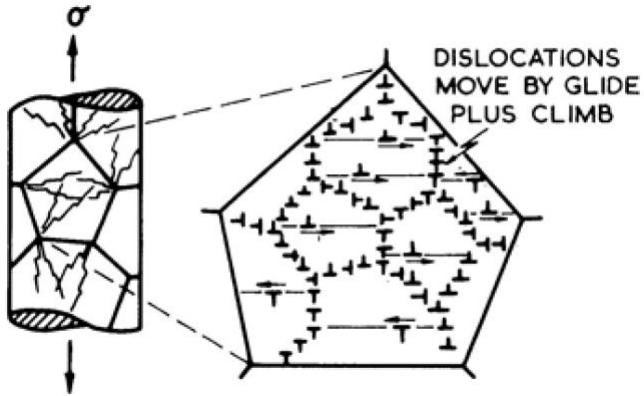
Q_C = 83.2 kJ/mol

D_{eff}… effective diffusion coefficient
includes trapping of vacancies at solute atoms, excess vacancies and pipe diffusion enhancement

Power law breakdown

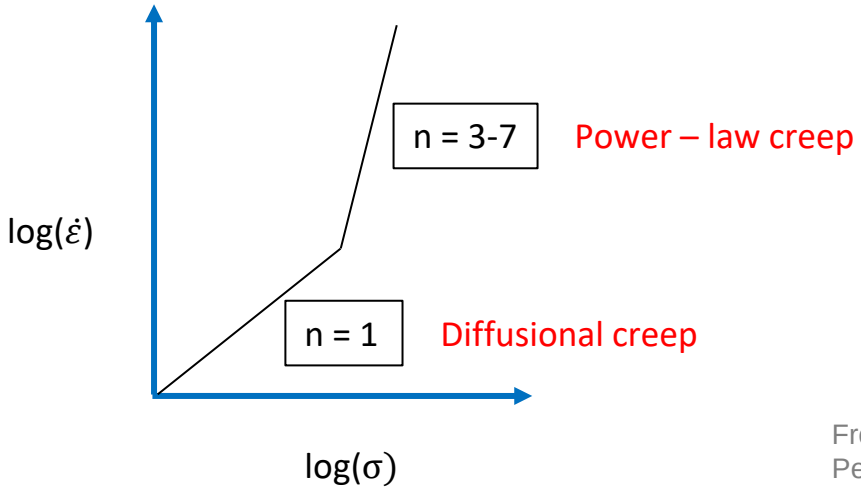


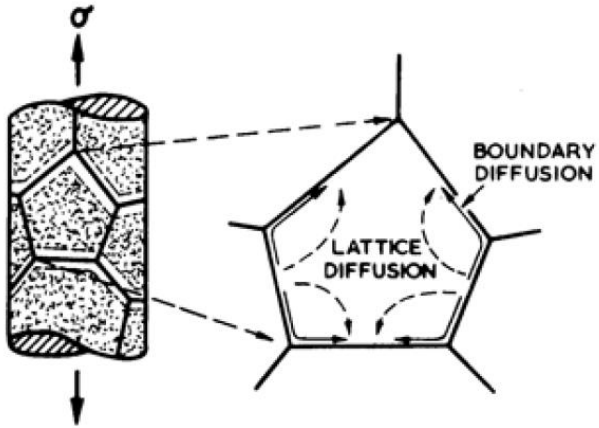
$$\dot{\varepsilon}_i = \frac{A_i \cdot D_i \cdot G \cdot b}{k_B \cdot T} \cdot \left[\sinh\left(\alpha' \frac{\sigma_S}{G}\right)\right]^{n_i}$$



Frost, H., Ashby, M., 1982. Deformation-mechanism maps, 1st ed. Pergamon Press, Oxford.

Diffusional Flow





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Diffusional creep

Nabarro – Herring Creep: $\sigma_{\mathrm{NH}} = \frac{\mathrm{k_B} \cdot T\,[\mathrm{K}] \cdot d^2}{42 \cdot b^3 \cdot D_{\mathrm{v}}} * \dot{\varepsilon}$

Coble – Creep: $\sigma_{\mathrm{C}} = \frac{\mathrm{k_B} \cdot T\,[\mathrm{K}] \cdot d^3}{42 \cdot b^3 \cdot \pi \cdot \delta \cdot D_{\mathrm{b}}} * \dot{\varepsilon}$

d … grain diameter
D_v …lattice diffusion coefficient
δ … grain boundary thickness
D_b …boundary diffusion coefficient

Connection of creep mechanisms

$$\left(\frac{1}{\sigma_{\mathrm{ges}}}\right)^{n_{\mathrm{c}}} = \left(\frac{1}{\sigma_{\mathrm{G}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{LT}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{HT}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{NH}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{C}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{GBS-GB}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{GBS-L}}}\right)^{n_{\mathrm{c}}} + \left(\frac{1}{\sigma_{\mathrm{HD}}}\right)^{n_{\mathrm{c}}}$$

State parameter evolution

- Kocks-Mecking model – athermal contribution
  - Dislocation generation (A-term), dynamic recovery (B-term) and static recovery (C-term)
  - A, B and C are calibrated by obtained flow curves

$$\frac{\partial \rho}{\partial \varepsilon} = \frac{M}{b \cdot A}\sqrt{\rho} - 2BM\frac{d_{crit}}{b}\rho - 2CD_d\frac{Gb^3}{\dot{\varepsilon}kT}(\rho^2 - \rho_{equ}^2)$$

$$\sigma = \alpha GbM\sqrt{\rho}$$

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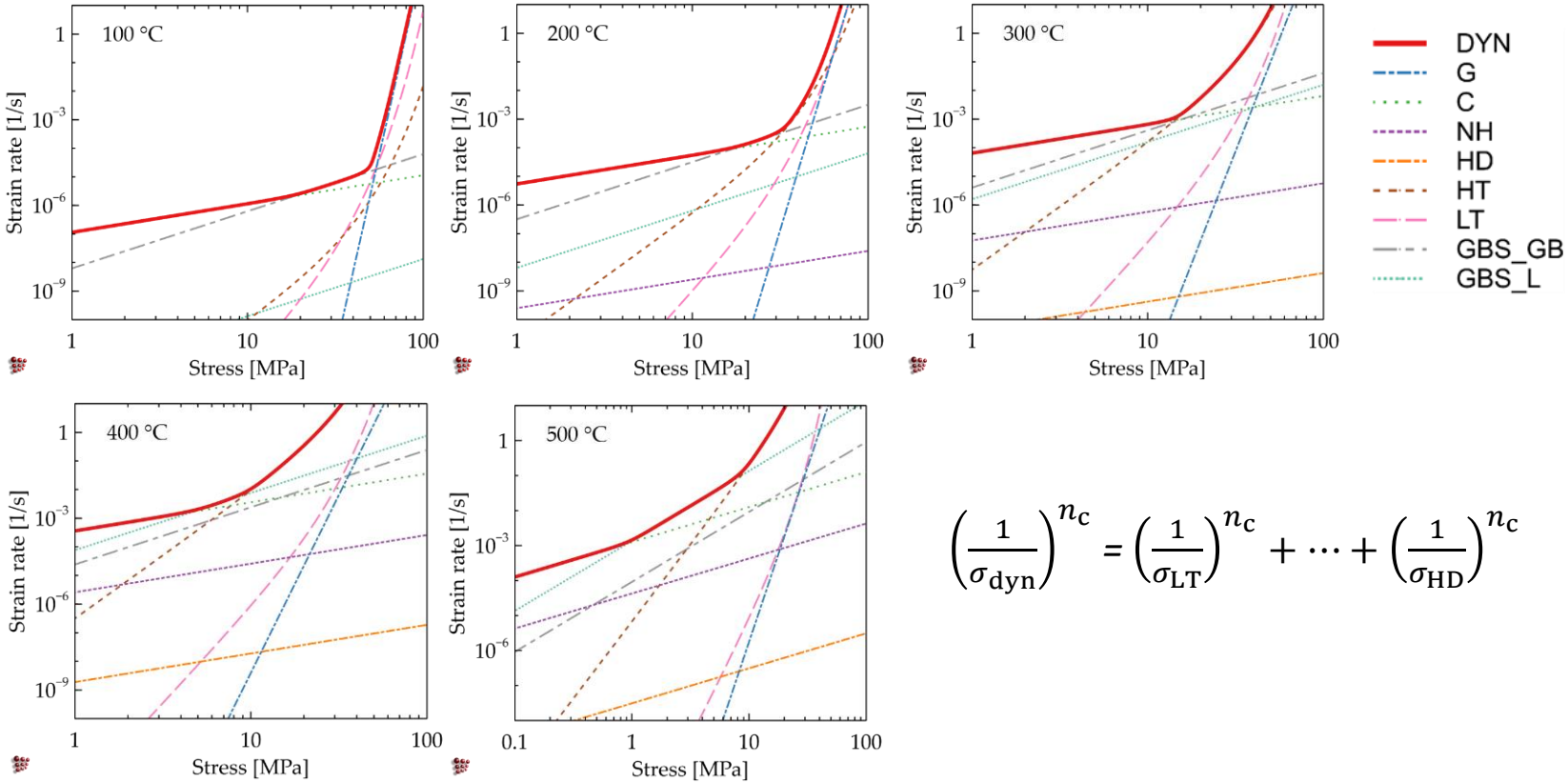
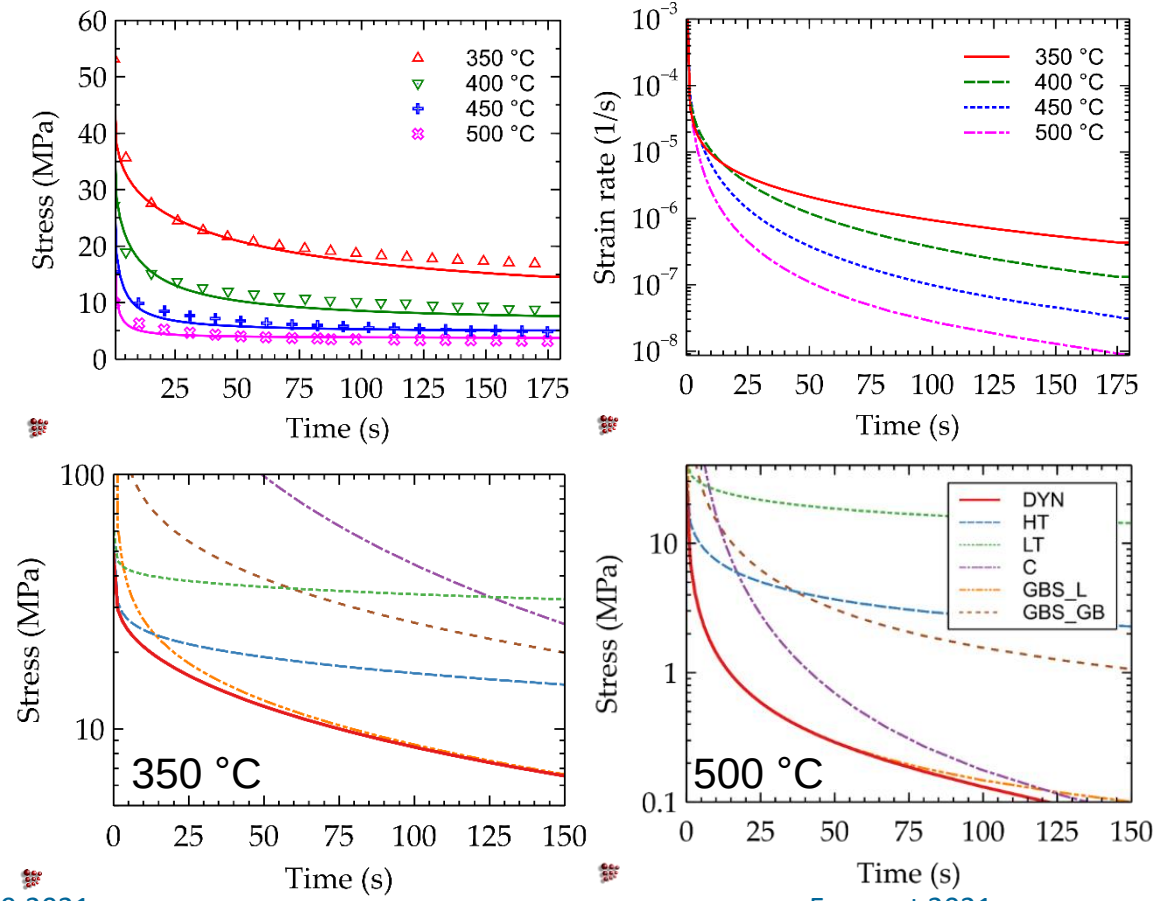
Simulation



$$\left(\frac{1}{\sigma_{\mathrm{dyn}}}\right)^{n_c} = \left(\frac{1}{\sigma_{\mathrm{LT}}}\right)^{n_c} + \cdots + \left(\frac{1}{\sigma_{\mathrm{HD}}}\right)^{n_c}$$

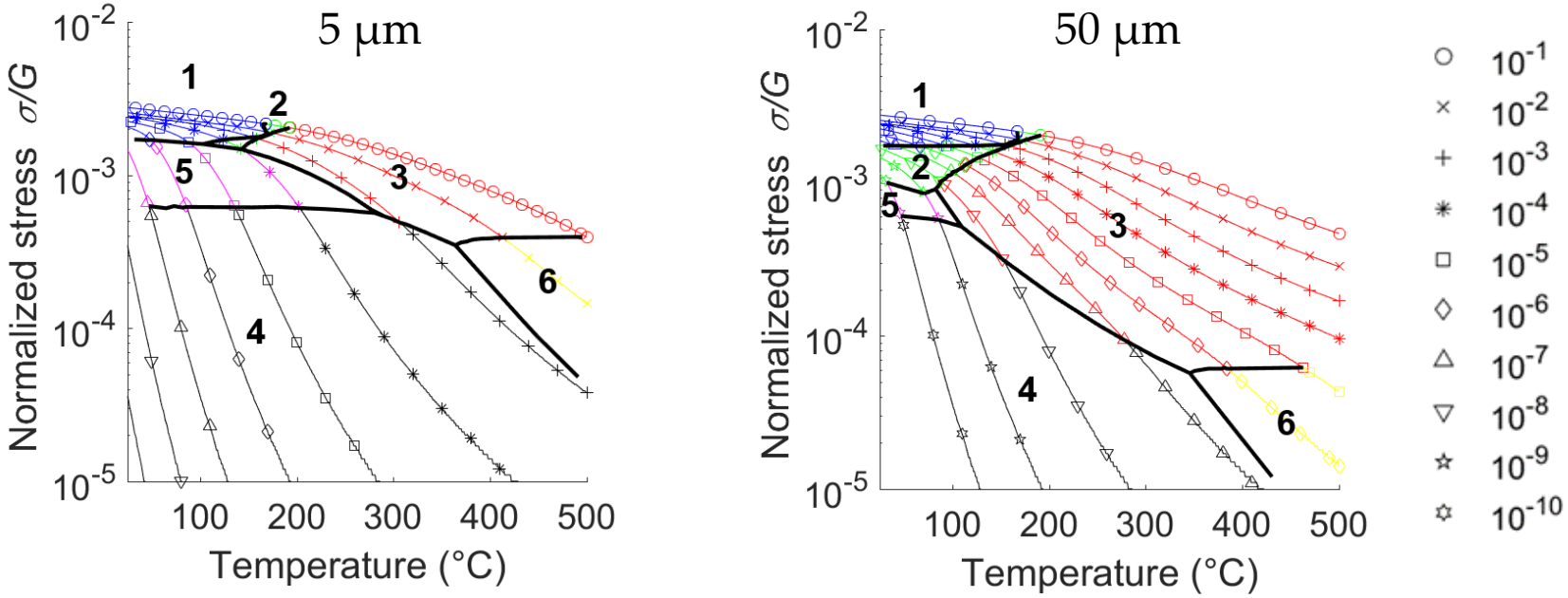
Relaxation



$$\dot{\sigma} = E \cdot \dot{\varepsilon}$$

$$\sigma_{t+\Delta t} = \sigma_t - \dot{\sigma} \cdot \Delta t$$

Deformation maps



1: Dislocation glide 2: LT creep 3: HT creep 4: Coble creep

5: D_{gb}-controlled GBS 6: D_l-controlled GBS

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Conclusion

Summary

- Combination of constitutive creep mechanisms and physically based microstructure evolution models
- Summation rule
- Stress relaxation
- Deformation maps