Integrated Physical-Constitutive Computational Framework for Plastic Deformation Modeling

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Euromat, September 13th, 2021
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
The model
# Overview

| Creep | State parameter evolution |
|-------|---------------------------|
| Low-temperature plasticity | Dislocation density evolution |
| Power-law creep | – Extended Kocks-Mecking model |
| Diffusional flow | |
| Dislocation glide* | |
| LT – creep* | |
| HT – creep* | |
| Harper-Dorn | |
| 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

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

- \( \hat{\tau} \) … mechanical threshold
- \( \Delta F \) … total energy
- \( \Delta G \) … Gibbs free energy
- \( \dot{\varepsilon}_0 \) … critical strain rate
Power law creep

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

Lattice diffusion controlled
\[ n_{HT} = 4.4 \]
\[ Q_{tr} = 127.2 \text{ kJ/mol} \] → HT - creep

Core diffusion controlled
\[ n_{LT} = 6.4 \]
\[ Q_C = 83.2 \text{ kJ/mol} \] → LT - creep

\( D_{eff} \ldots \) 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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\[
\log(\dot{\varepsilon}) = n \log(\sigma)
\]

- \(n = 3-7\): Power-law creep
- \(n = 1\): Diffusional creep

\[
\sigma_{NH} = \frac{k_B T [K] d^2}{42 \cdot b^3 \cdot D_v} \cdot \dot{\varepsilon}
\]

\[
\sigma_C = \frac{k_B T [K] d^3}{42 \cdot b^3 \cdot \pi \cdot \delta \cdot D_b} \cdot \dot{\varepsilon}
\]

- \(\sigma_{NH}\): Nabarro – Herring Creep
- \(\sigma_C\): Coble – Creep

\(d\) … grain diameter
\(D_v\) … lattice diffusion coefficient
\(\delta\) … grain boundary thickness
\(D_b\) … boundary diffusion coefficient
Connection of creep mechanisms

\[
\left( \frac{1}{\sigma_{\text{ges}}} \right)^{n_c} = \left( \frac{1}{\sigma_G} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{LT}}} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{HT}}} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{NH}}} \right)^{n_c} + \left( \frac{1}{\sigma_C} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{GBS-GB}}} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{GBS-L}}} \right)^{n_c} + \left( \frac{1}{\sigma_{\text{HD}}} \right)^{n_c}
\]
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

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

\[
\sigma = \alpha GbM \sqrt{\rho}
\]
\[ \left( \frac{1}{\sigma_{\text{dyn}}} \right)^{n_c} = \left( \frac{1}{\sigma_{\text{LT}}} \right)^{n_c} + \cdots + \left( \frac{1}{\sigma_{\text{HD}}} \right)^{n_c} \]
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
Conclusion
Summary

• Combination of constitutive creep mechanisms and physically based microstructure evolution models

• Summation rule

• Stress relaxation

• Deformation maps