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Mathematical framework for a semi-physical model for the prediction of creep life of Fe-Ni-Cr alloys addressing solid-solution hardening

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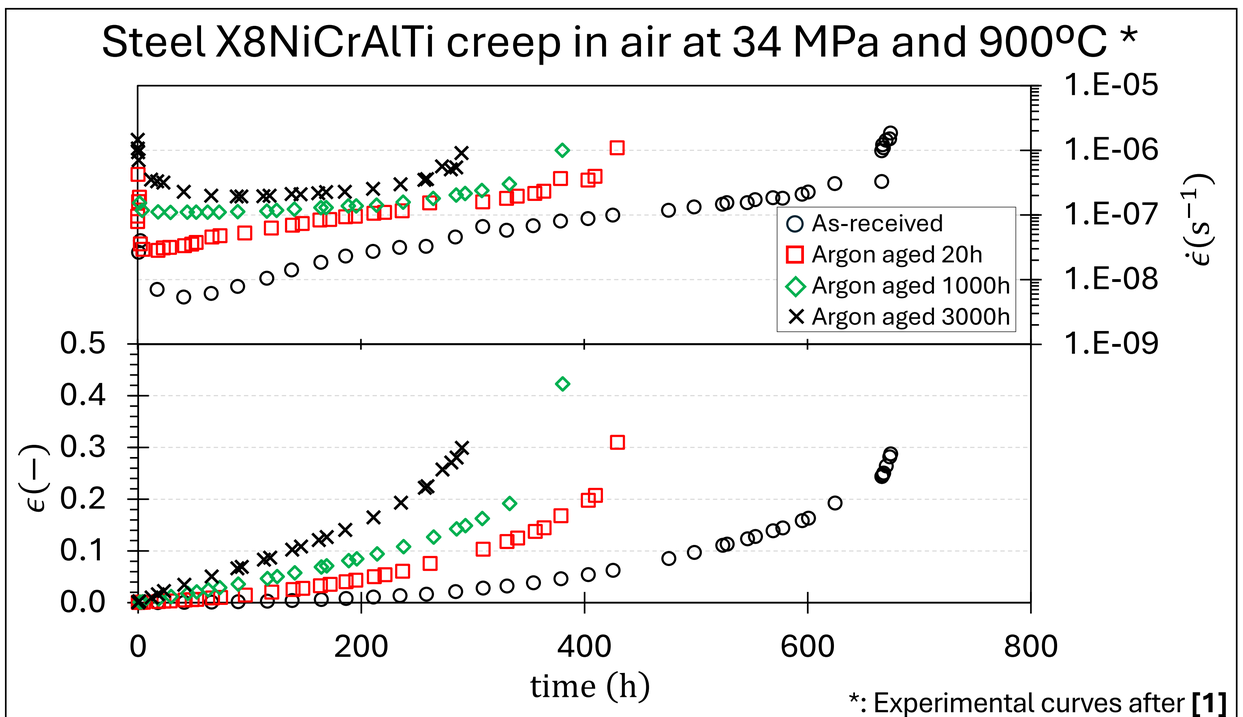
Motivation

Accurate prediction of creep deformation and creep life requires suitable numerical models capable of addressing complex creep deformation responses.



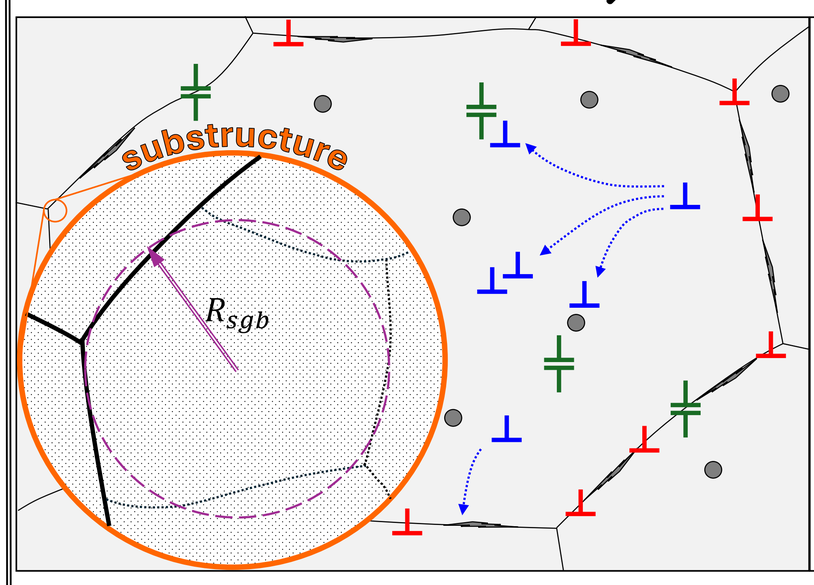
*: Experimental curves after **[1]**

As received (○)
- Non-stable microstructure ➔ Non-classical creep response

Argon aged at 900ºC (□ <◇ <×)
- Progressively more stable microstructure ➔ towards classical creep response

To this end, the effect and evolution of microstructural features influencing the creep behavior of alloys must be considered.

Creep deformation ⇆ Microstructure evolution



Microstructural features

Dislocation types
- ⊥ **m**obile (ρ_m)
- ⫫ **s**tatic (or dipole) (ρ_s)
- ⊥ **b**oundary (ρ_b)

Precipitates
- Intragranular
- Intergranular

mean subgrain radius (R_{sgb})

solute atoms ( )

A common physical framework: The **Orowan equation**

$$\dot{\epsilon} = \frac{\rho_m \cdot b \cdot v}{m_T}$$

- $\dot{\epsilon}$: Creep strain rate (s^{-1})
- ρ_m: Mobile dislocation density (m^{-2})
- b: Burgers vector (m)
- v: Velocity (ms^{-1})
- m_T: Taylor factor (−)

Engineering approach

Semi-physical equations ⇆ Empirical phenomena

[2]: relation between steady-state creep rate ($\dot{\epsilon}_{ss}$) & mobile dislocation density:

Derivation of ϵ_{ss}- ρ_m relation:

$$\int d\epsilon_{ss} = \int \frac{\rho_m b v}{m_T} dt \longrightarrow \epsilon_{ss} = \frac{\rho_m b}{m_T} \cdot \frac{C_L}{\sqrt{\rho_m}} \longrightarrow \frac{d\rho_m}{d\epsilon_{ss}} = \frac{2m_T}{bC_L} \rho_m^{1/2}$$

(Work hardening)

Generalization for ϵ and extension for dynamic & static recovery:

$$\frac{d\rho_m}{d\epsilon} = \frac{2m_T}{bC_L} \rho_m^{1/2} - \omega\rho_m - \frac{2\tau_L v_C}{b\sigma} \rho_m^2 \dot{\epsilon}^{-1}$$

Analytical resolution for $\dot{\epsilon}_{ss}$:

$$\dot{\epsilon}_{ss} = \frac{\tau_L C_L}{\sigma} v_c \frac{(\sigma - \sigma_i)^3}{(\alpha m_T G b)^3}$$

- $\dot{\epsilon} = \dot{\epsilon}_{ss}$
- $\dot{\rho}_m = 0$
- no dynamic recovery
- Taylor equation dislocation stress (σ_d) $\sigma_d = \alpha m_T G b \sqrt{\rho_m} = \sigma - \sigma_i$

❖ **New physical phenomena** included as internal-stresses (σ_i):

$\sigma_i = \sigma_{GBPS} + \sigma_{SSH} + \sigma_{PH} + \cdots$
- σ_{PH}: *precipitate hardening*
- σ_{SSH}: *solid-solution hardening*
- σ_{GBPS}: *grain boundary precipitate strengthening*

Semi-physical approach

Semi-physical equations ⇆ Physical phenomena

mean field model, HT-9 **[3]**, improved for steel P91 **[4]**, and Ni-based alloy **[5]**.

$$\dot{\epsilon} = \rho_m b v_e m_T^{-1}$$

$$\dot{\rho}_m = v_e \left[\rho_m^{3/2} + \frac{\beta \rho_s R_{sgb}}{h^2} - \frac{\rho_m}{2R_{sb}} + f_m^{PH}(\rho_m, \rho_s, PK) - \delta_a(\rho_m^2 - \rho_m\rho_s) \right] - 8\rho_m^{3/2} v_C$$

(f_m^{PH}: *precipitate hardening terms* (see **[5]**))

$$\dot{\rho}_s = v_e \left[\frac{1}{2R_{sgb}} + f_s^{PH}(\rho_m, \rho_s, PK) - \delta_a \rho_m \rho_s \right] + 8\rho_m^{3/2} v_C$$

$$\dot{\rho}_b = 8(1 - 2\zeta) \frac{\rho_s}{h_b} v_C - \frac{\rho_b}{R_{sgb}} f_{sgb}^{growth}(\rho_i, PK)$$

$$\dot{R}_{sgb} = f_{sgb}^{growth}(\rho_i, PK) - f_{sgb}^{nucleation}$$

PK = particle {· mean diameter; kinetics {· number density}

[4,5] effective velocity v_e from glide (v_G) & climb (v_C):

$$v_e^{-1} = \left(v_G^{-1} + f_{PK} \cdot v_C^{-1} \right)$$

$$v_G = k_1 \exp\left(-Q_{self}/K_B T\right) \exp\left[-(\sigma_d + \sigma_i)V_r/K_B T\right] 2\sinh\left(\sigma V_r/K_B T\right)$$

$$v_C = \{f_{pipe} + f_{lattice}\} \exp\left[-(\sigma_d + \sigma_i)\Omega/K_B T\right] 2\sinh\left(\sigma\Omega/K_B T\right)$$

❖ **New physical phenomena** included as terms representing physical interactions between dislocations, particles and the substructure

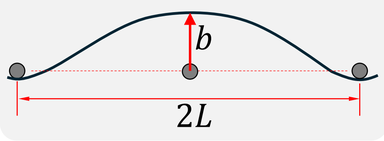
Combination of both approaches to model **solid-solution hardening**

Definition of the critical breakout stress (σ_b) form pinning solute atoms

$$\sigma_b = \frac{W^b}{b^2 L} = W^b \sqrt{\frac{c_i}{b^3}}$$

- c_i: *solute atoms concentration*
- $L = \sqrt{b \cdot c_i}$: *mean solute atoms spacing*

a dislocation line breaks out from solute atoms:



The critical breakout work (W^b) is calculated as **[2]**:

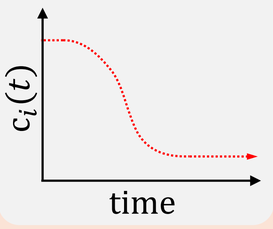
$$W^b = \frac{E}{6\pi(1 - \nu)} \cdot \frac{\Omega_{FCC} - \Omega_i}{C_i^0}$$

- Ω_{FCC}: *atomic volume of FCC structure*
- Ω_i: *atomic volume of solute atoms*
- C_i^0: *initial solute atoms concentration*

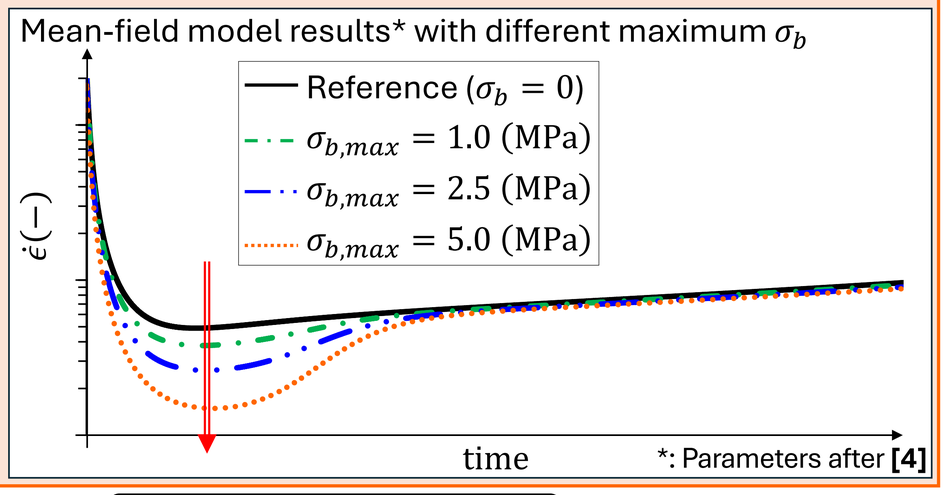
Inclusion of calculated σ_b within the internal stress (σ_i) in v_G and v_C

- Proof of concept:

Approximate $c_i(t)$ during creep test



Mean-field model results* with different maximum σ_b

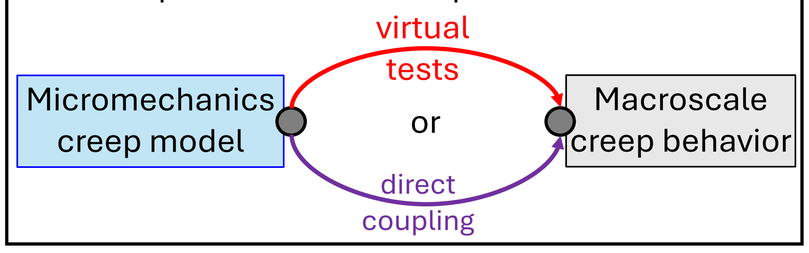


*: Parameters after **[4]**

Prospects

➢ Application and validation of the model:
- Incoloy 800H
- SEW555 alloy (AID4Greenest)
- Ni-superalloys

➢ Develop a multi-scale creep model



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[4]: F. Riedlsperger et al., *Materialia*, 2020.

[5]: F. Riedlsperger et al., *MHT*, 2023.