

Contribution **P111**

Mean-field modeling of the creep deformation response of alloy 1.4959 (800H) addressing precipitate kinetics

C. Rojas-Ulloa, F. Chen, J. T. Tchuindjang, O. Dedry, T. Nguyen-Minh, A. Mertens, A. Vendramini, A. Di Giovanni, V. Tuninetti, L. Duchêne, A.M. Habraken

Project funded by:



FRIA grants B1 4000 – 8987
B2 4002 – 1907



European Project HORIZON-
CL4-2022-RESILIENCE-01-19



Introduction context & motivation

Numerical model development & contributions

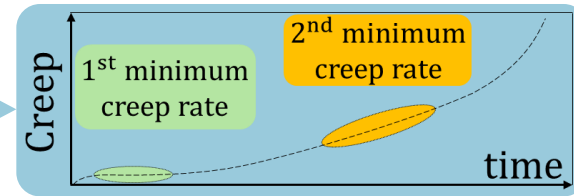
Results model validation

Outlook conclusions & prospects

Why Mean-Field Creep?

To model the **non-classical** behaviour of 800H

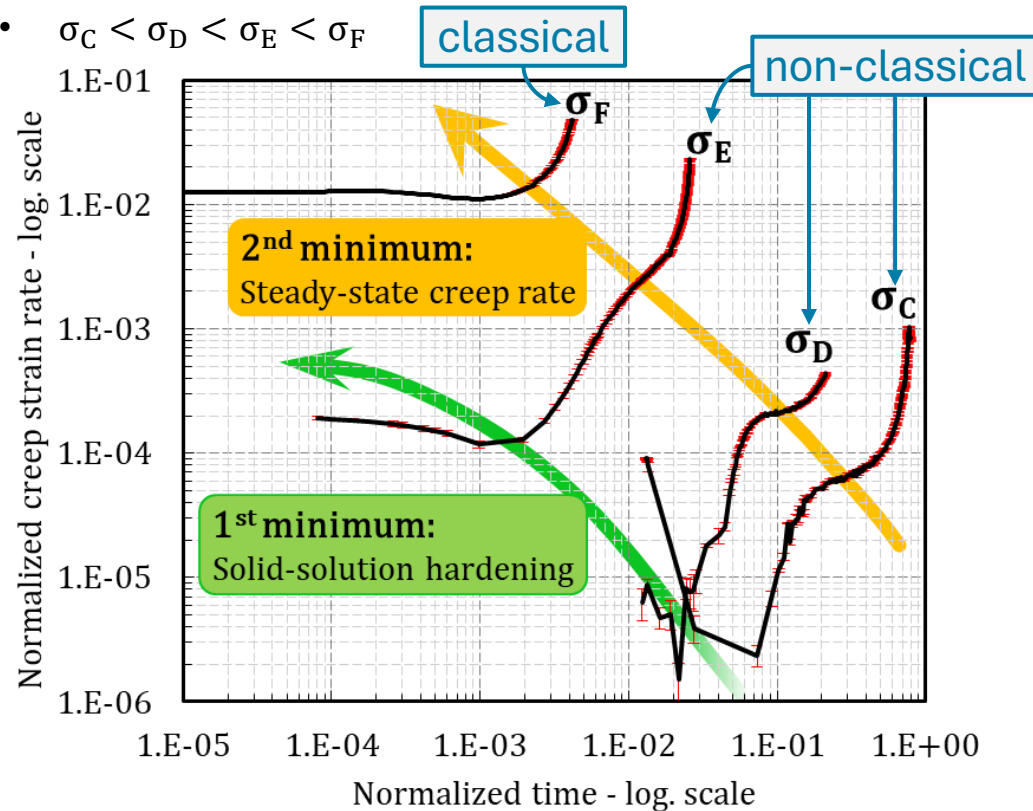
two-minimum creep
strain rate minima*



Experimental normalized creep curves w/st.Dev. (ULiège)

- Low stresses & a single high temperature (\$\$\$!!)

$$\sigma_C < \sigma_D < \sigma_E < \sigma_F$$



my PhD. Project in a nutshell

Objective: Service life assessment of 800H in industry

Challenge: Creep deformation $\rightleftharpoons$ Microstructure evolution

Finite element modelling of creep, using LAGAMINE**

- New viscoplastic model
- Parameter identification & validation

Experimental creep curves

complemented with

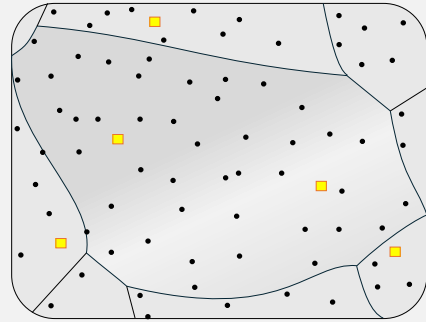
Virtual creep curves

Mean-Field Creep (MFC) model

* Also studied in 2.25Cr-1Mo (K. Maruyama, MSEA, 1997) [1]
18Cr9Ni-3Cu-Nb-N T. Hatakeyama, MSEA, 2022) [2]

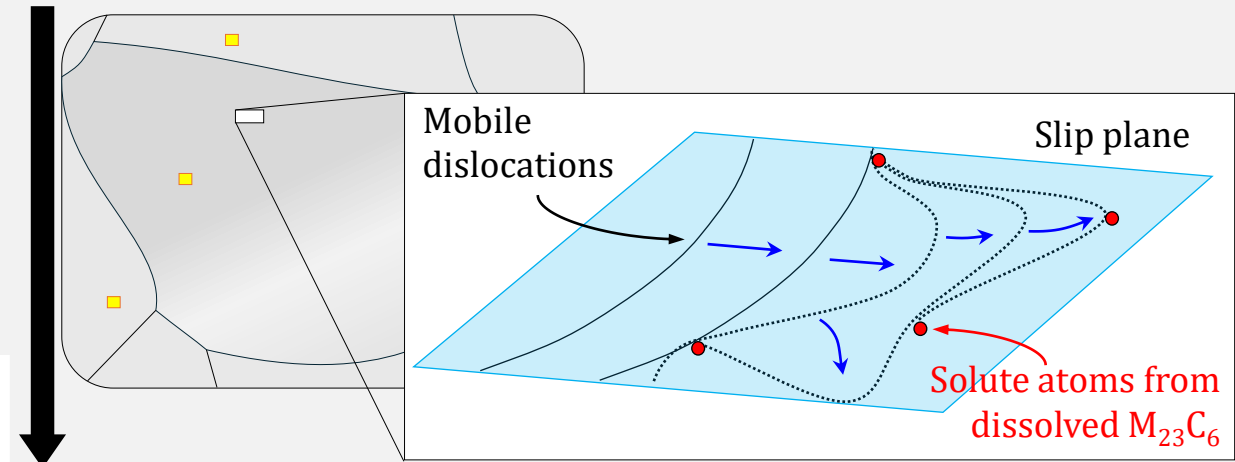
** in-house FE code developed in MSM team, ULiège [3]

Initial microstructure



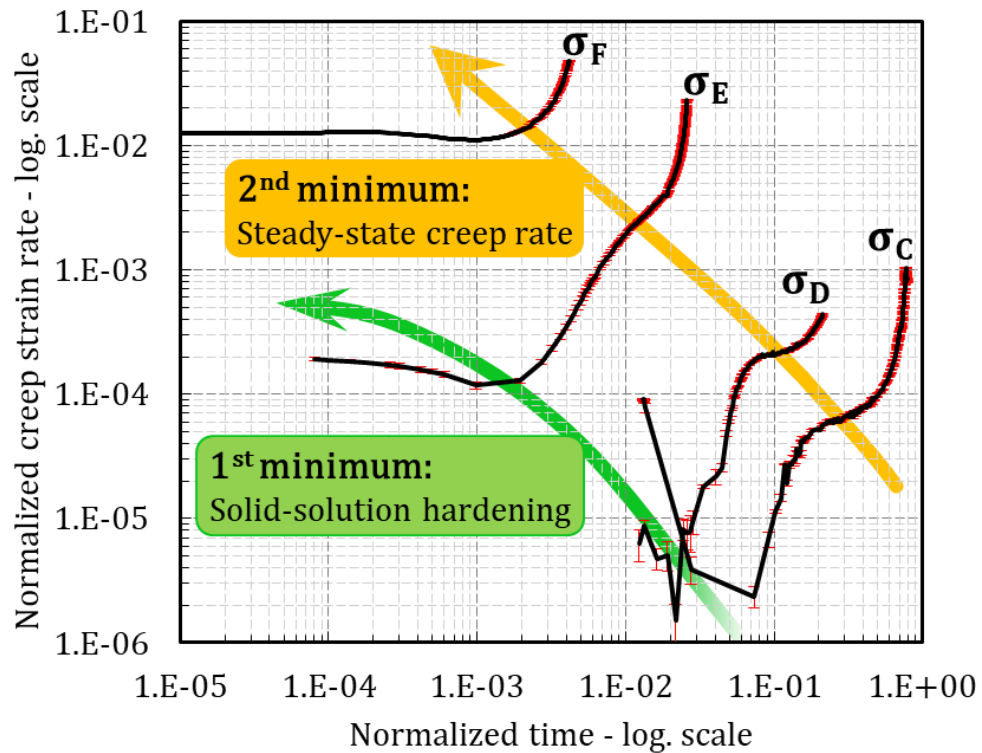
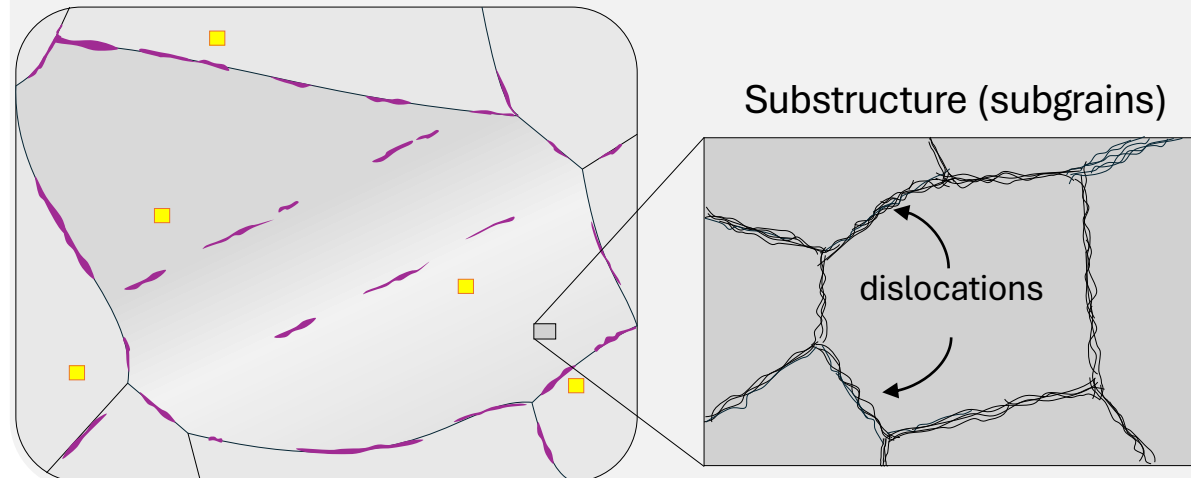
- Coarse austenite
- Annealing twins
- Precipitates:
 - Ti(C,N) carbonitrides
 - Intragranular $M_{23}C_6$

1st minimum: solid-solution hardening (SSH)



2nd minimum: steady-state creep rate + aging

Intergranular $M_{23}C_6$ precipitation



* After C. Rojas-Ulloa, JMS, 2026 [4]

Non-linear equation system*, based on dislocation density (ρ)

creep strain rate - - - - - $\dot{\epsilon} = \frac{b\rho_m v_{\text{eff}}}{m_T(1 - D_c)}$

mean mobile dislocation density rate - - - - -
$$\dot{\rho}_m = \underbrace{v_g \rho_m (\rho_m^{1/2} + \rho_s^{1/2})}_{\text{Frank-Read source}} + \underbrace{v_g \left(\frac{\beta \rho_s R_{\text{DW}}}{h_{\text{DW}}^2} - \frac{\rho_m}{2R_{\text{DW}}} \right)}_{\text{Production \& pile-up at DW}} + \underbrace{v_g \left(\frac{\rho_s}{2r_i} - \frac{\rho_m}{\lambda_{\text{eq}}} \right) + v_c \left(\frac{\rho_s}{\lambda_{\text{eq}}} + \frac{\rho_s f_v b}{r_i} \right)}_{\text{PD interaction}}$$

$$- \underbrace{v_g \left(\frac{\rho_m}{h_{\text{DN}}} \right)}_{\text{DD interaction}} - \underbrace{v_g \delta_{\text{anh}} \rho_m^2 + \rho_m \rho_s}_{\text{Dynamic \& static recovery}} - v_c \delta \rho_m^{3/2}$$

mean static dislocation density rate - - - - -
$$\dot{\rho}_s = \underbrace{v_g \frac{\rho_m}{2R_{\text{DW}}} - v_c \frac{\rho_s}{h_{\text{DW}}}}_{\text{Production \& pile-up at DW}} + \underbrace{v_g \left(\frac{\rho_m}{\lambda_{\text{eq}}} - \frac{\rho_s}{2r_i} \right) - v_c \left(\frac{\rho_s}{\lambda_{\text{eq}}} + \frac{\rho_s f_v b}{r_i} \right)}_{\text{PD interaction}}$$

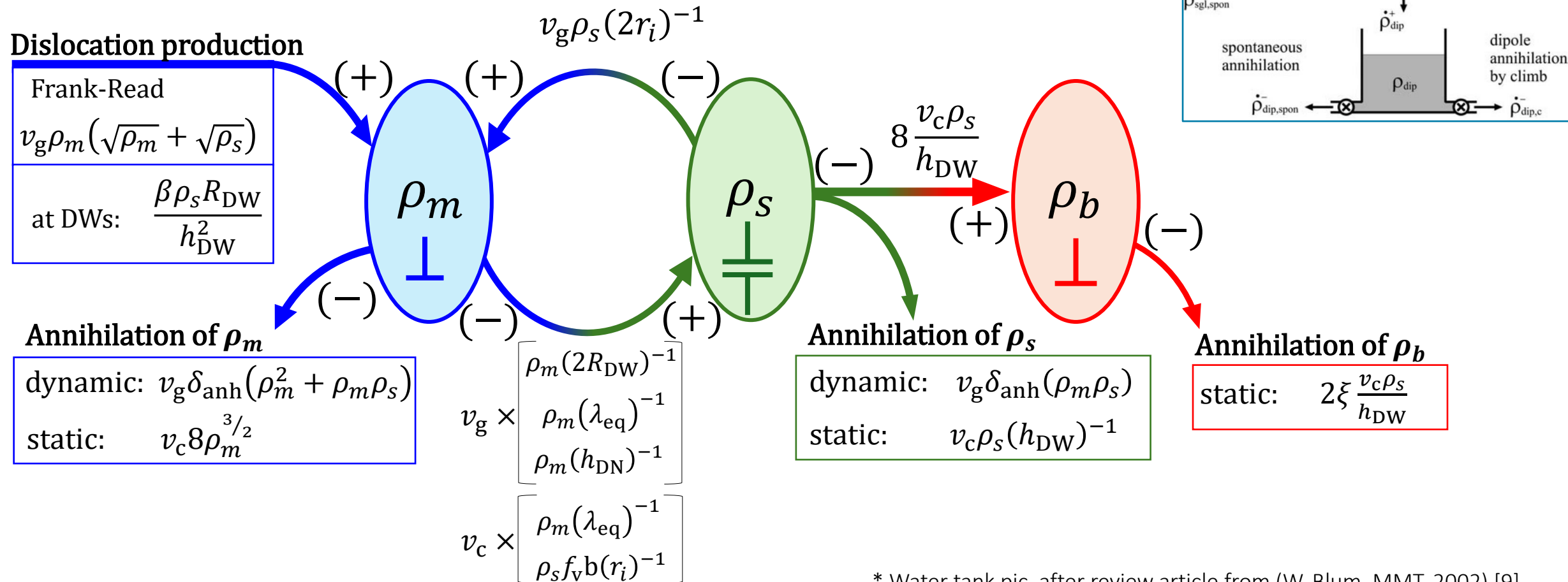
$$+ \underbrace{v_g \frac{\rho_m}{h_{\text{DN}}}}_{\text{DD interaction}} - \underbrace{v_g \delta_{\text{anh}} \rho_m \rho_s}_{\text{Dynamic recovery}}$$

mean boundary dislocation density rate - - - - -
$$\dot{\rho}_b = \underbrace{v_c \left[8(1 - 2\xi) \frac{\rho_s}{h_{\text{DW}}} \right]}_{\text{pile-up \& annihilation at DW}}$$

* a combination of scientific contributions:

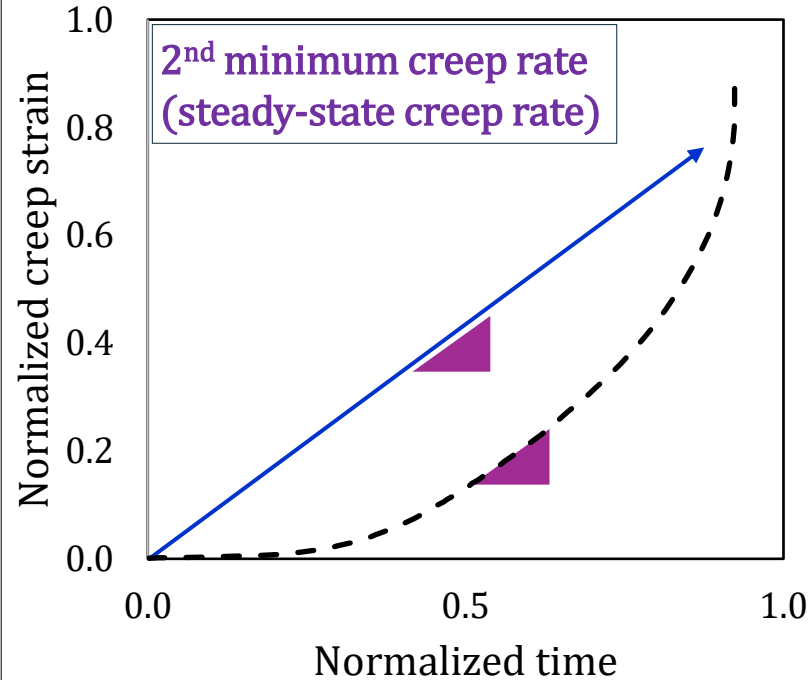
- (N.M. Ghoniem, Res Mech.,1990) [5]
- (S.D. Yadav, MSEA, 2016) [6]
- (F. Riedlsperger, 2020, 2023) [7,8]

Non-linear equation system = classic predator-prey system
or
classic water tank problem from ODE*

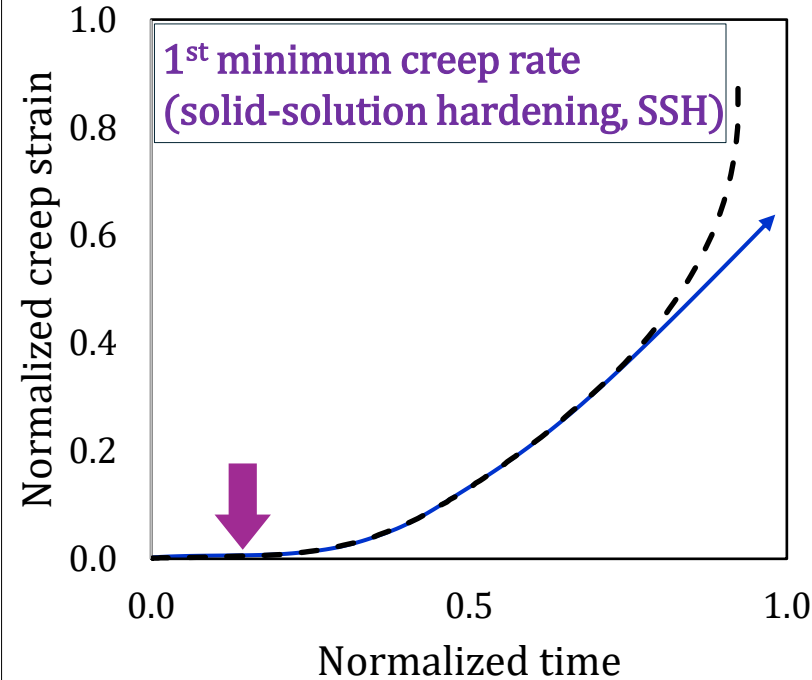


* Water tank pic. after review article from (W. Blum, MMT, 2002) [9]

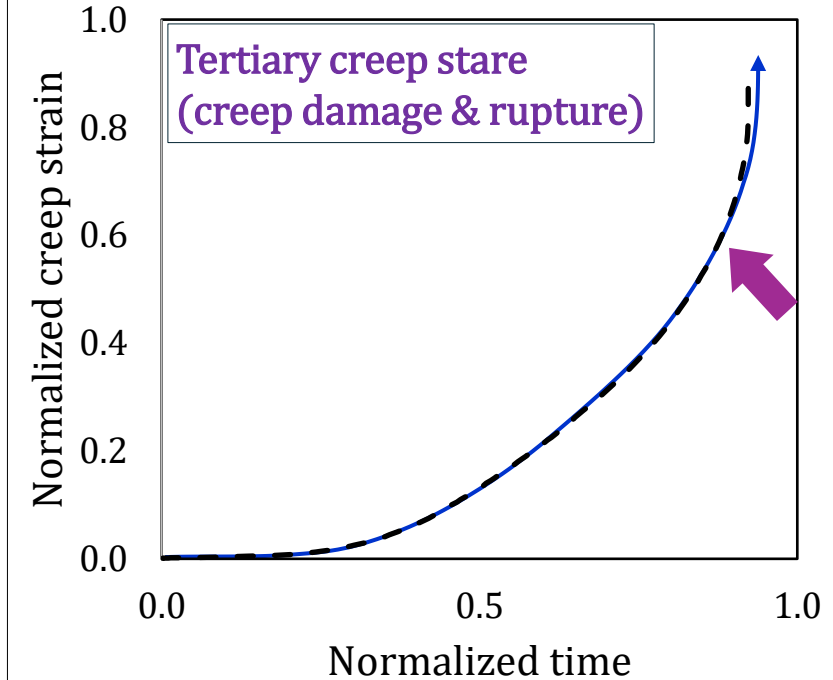
1. Prediction of the steady-state creep rate level



2. Prediction of the solid-solution creep strain hardening



3. Prediction of loss of load carrying capacity, damage & fracture



Here is where our two main contributions stem from...

Modification of the apparent representative volume (V_r)

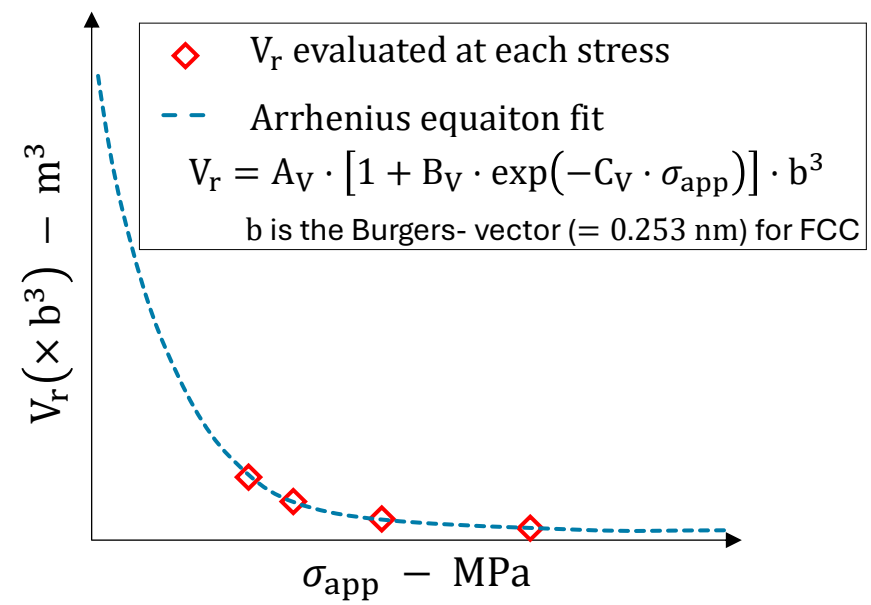
➤ The mean glide velocity of

dislocations is defined as: $v_G = k_G \exp\left(\frac{-Q_G}{k_B T}\right) \exp\left[\frac{-(\sigma_{int})V_r}{k_B T}\right] 2 \sinh\left(\frac{\sigma_{app} V_r}{k_B T}\right)$ with:

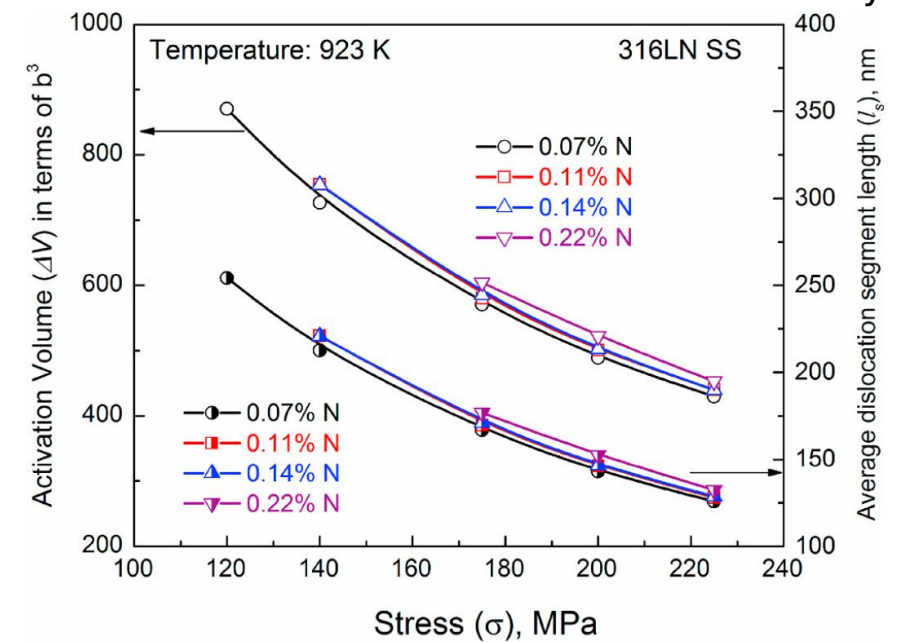
k_G	Glide pre-exp. constant	Fitting param.
Q_G	Glide activation energy	Fitting param.
k_B	Boltzmann constant	$1.38 \times 10^{-23} \text{ J K}^{-1}$
T	Temperature (K)	Variable
σ_{int}	Internal stress	Variable
σ_{app}	Applied (true) stress	Variable

➤ For a single temperature & multiple stresses in 800H, no unique V_r was found!

❖ V_r follows an Arrhenius-like stress dependency!



Similar behaviour found for 316N stainless steel by *



* after (C. Parveen, MSEA, 2021) [10]

Step 2: Prediction of the SSH creep rate peak



SSH incorporated within the internal stress equation

$$v_{G,C} = (...) \exp \left[\frac{-\sigma_{\text{int}} V_r}{k_B T} \right] 2 \sinh \left(\frac{\sigma_{\text{app}} V_r}{k_B T} \right)$$

→ Taylor stress: $\sigma_{\text{tay}} = \alpha m_T G b \sqrt{\rho_m}$

$$\sigma_{\text{int}} = \sigma_{\text{tay}} + \sigma_{\text{ss}}$$

Solid-solution hardening stress: $\sigma_{\text{ss}} = f_{\text{ss}}(\sigma_{\text{app}}, T) \cdot (\chi_i)^{2/3}$

• power for FCC materials

• solute atom concentration, $i = \text{Cr}$

physical function:

$$f_{\text{ss}} = f_{\text{ss}0} \cdot \exp \left[\frac{-1}{C_1} \frac{k_B T}{\Delta E_b} \ln \left| \frac{\dot{\epsilon}}{\dot{\epsilon}_0} \right| \right]$$

- Used to predict SSH in HEAs by *
- cool trick to adapt to creep:

$$\ln \left| \frac{\dot{\epsilon}}{\dot{\epsilon}_0} \right| = m \cdot \ln \left| \frac{\sigma_y(T)}{\sigma_{\text{app}}} \right|$$

• Pre-exponential function:

$$f_{\text{ss}0} = \frac{1}{\sqrt{2}} m_T G (v_{\text{eq}})^{3/4}$$

• Energy barrier function:

$$\Delta E_b = \Phi m_T G b^3 \left(\frac{w}{b} \right)^{3/2} \sqrt{\frac{\sigma_{\text{app}}}{m_T G}}$$

$$\Phi(T) = \phi_1 \exp \left(-\phi_2 / RT \right)$$

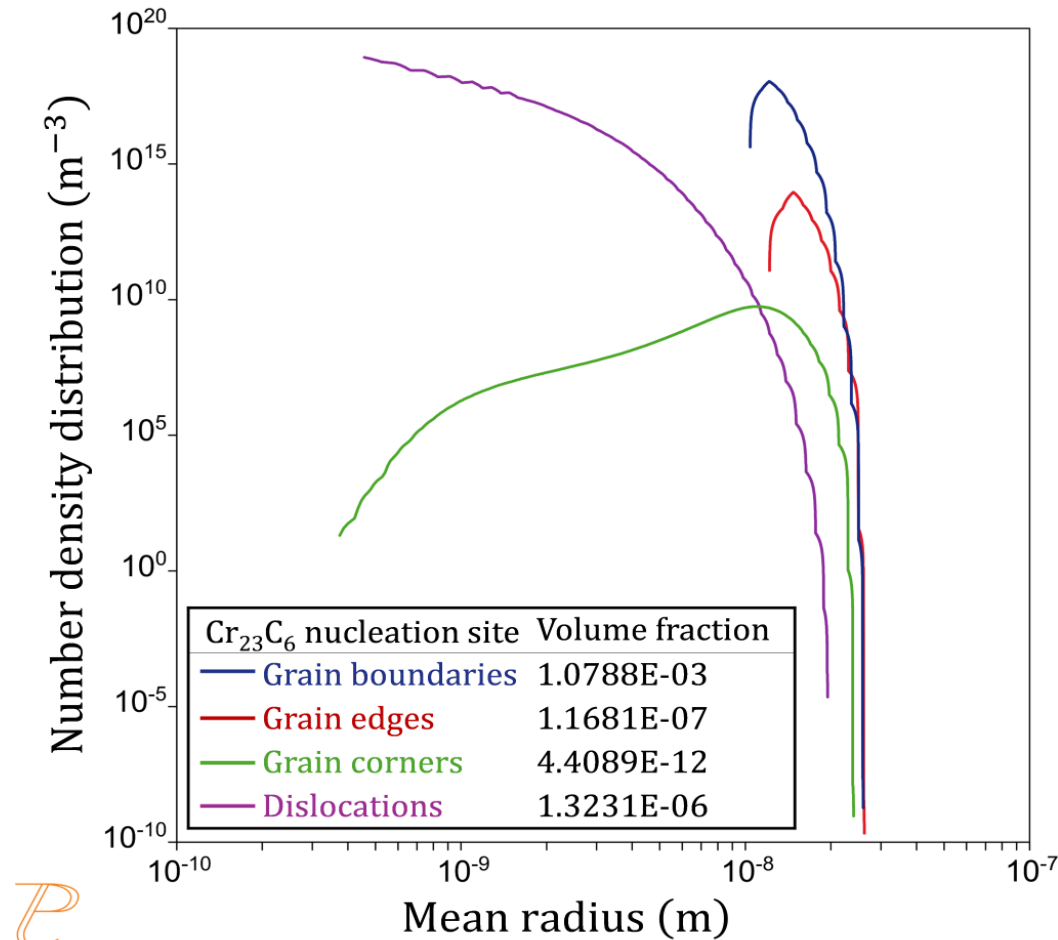
with:

m_T	Taylor factor	3.06
G	Shear modulus	known [4]
C_1	Material constant	Fitting param.
σ_y	Yield stress	known [4]
v_{eq}	Equiv. atom misfit	See [11]
$\frac{w}{b}$	Aver. travel dist. ratio	≈ 0.17 ([11])
$\phi_{1,2}$	Material constants	Fitting params.
R	Gas constant	$8.314 \text{ Jmol}^{-1}\text{K}^{-1}$

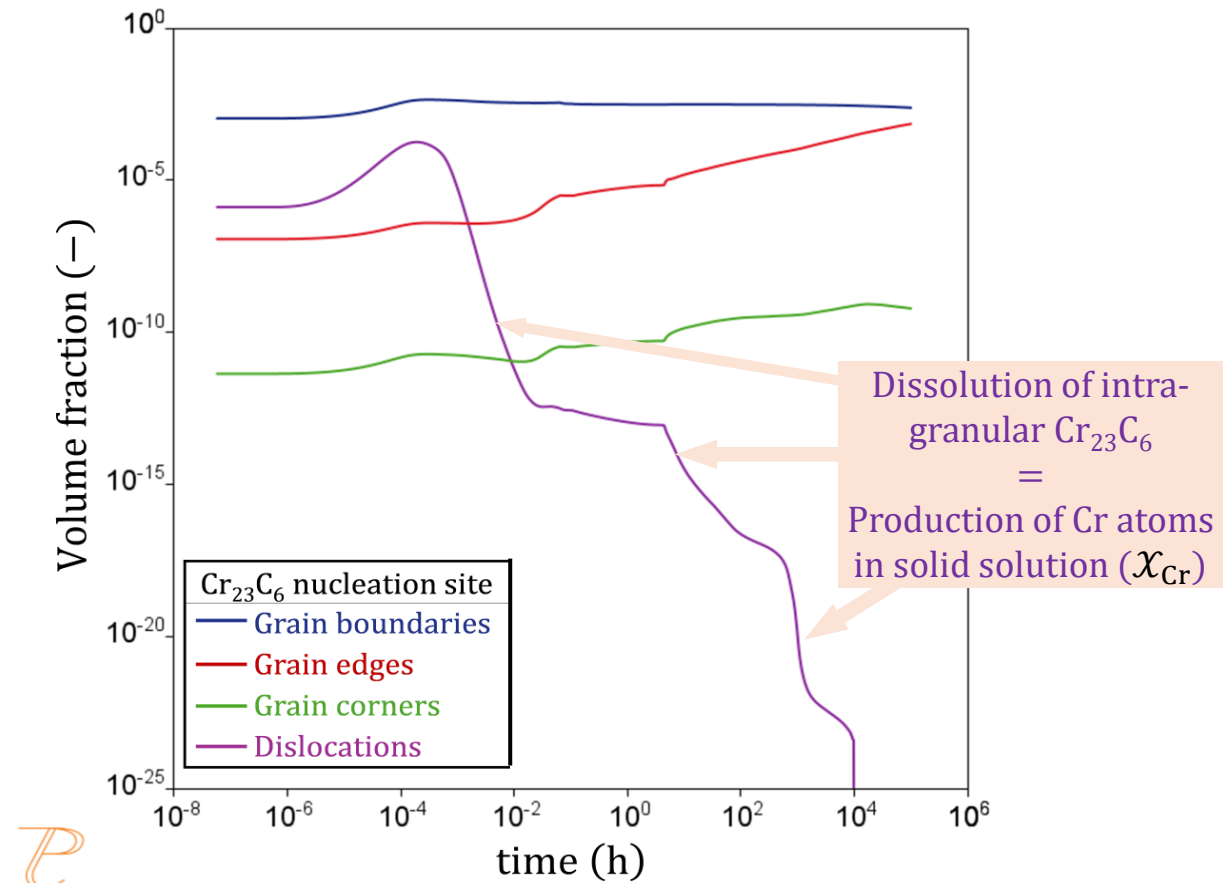
* (I. Toda-Caraballo et al., Acta Mat., 2019) [11]

Ex-situ simulations were conducted for 800H alloy

Number density distribution of Cr_{23}C_6 before creep
(after solution annealing + water quenching)



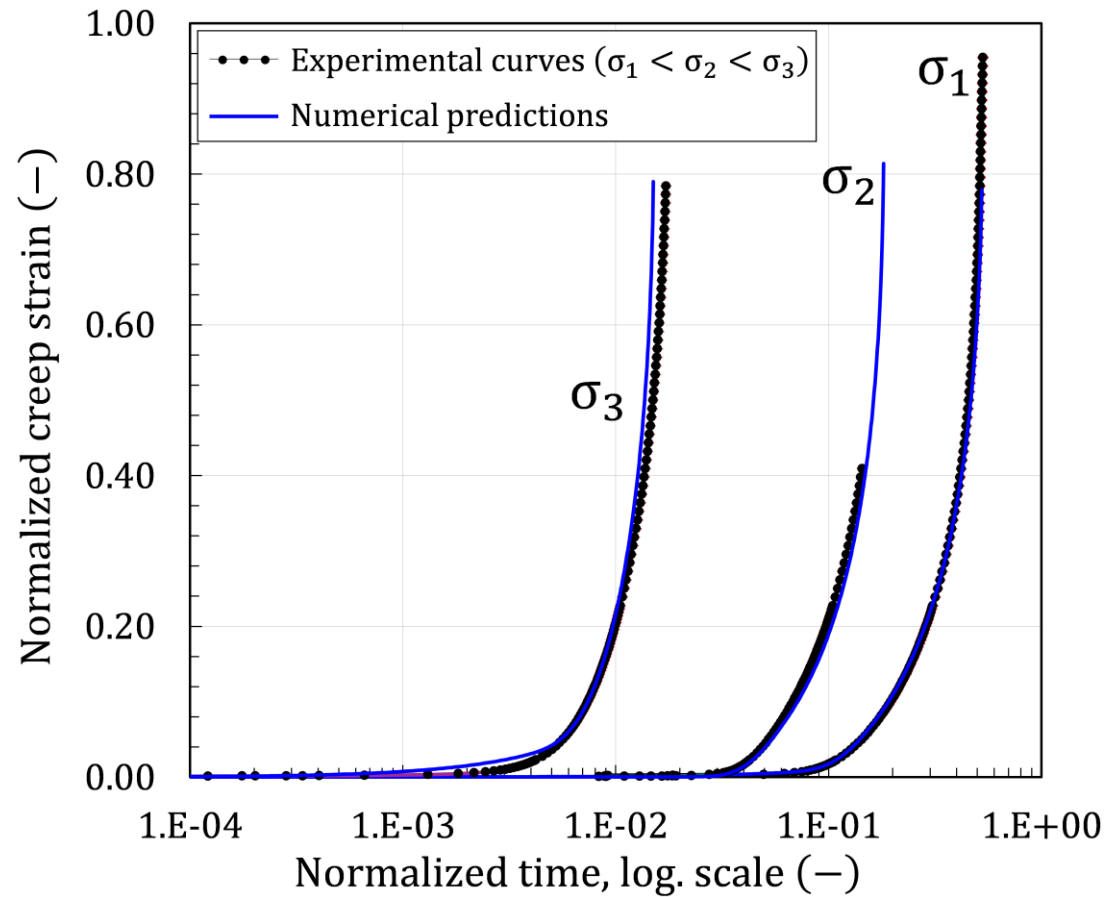
Volume fraction of C during creep (aging)
thermo-kinetic simulation at 1000°C



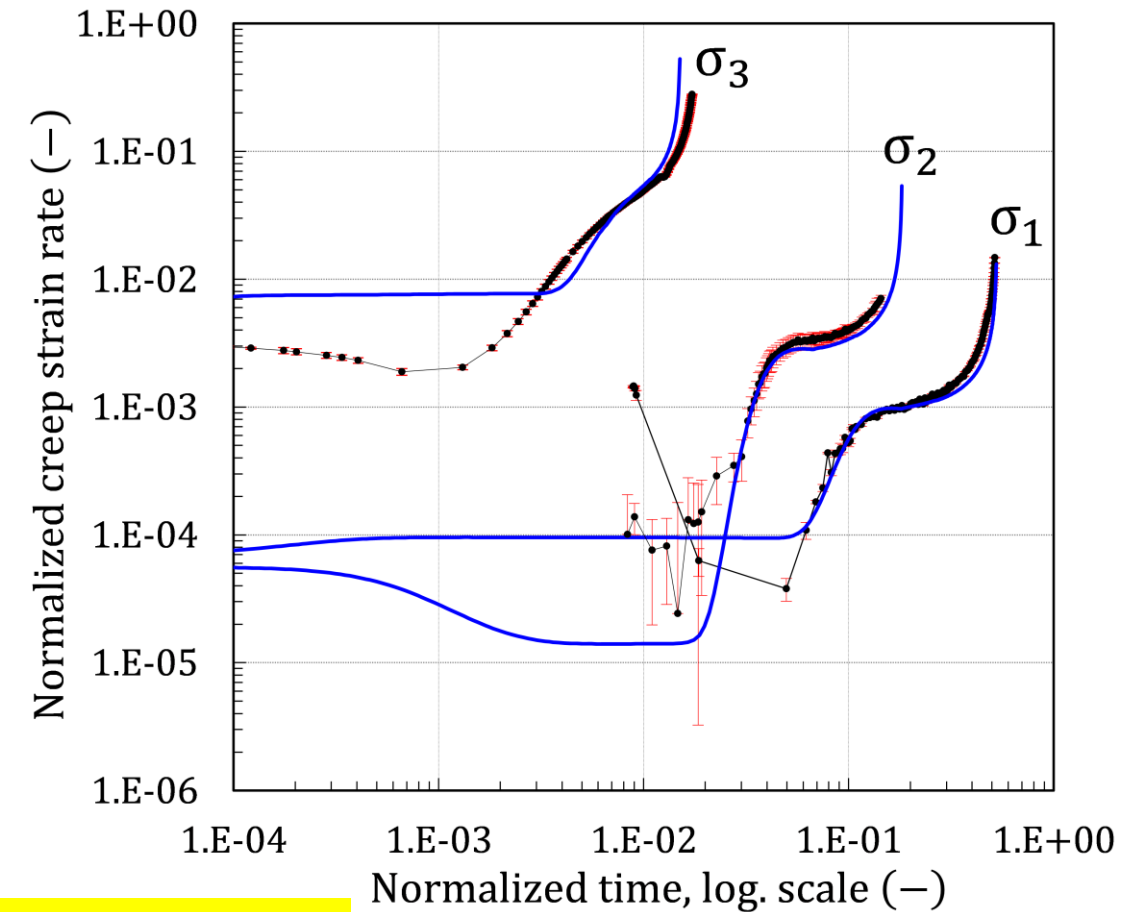
* After C. Rojas-Ulloa, JMS, 2026 [4]

Low stress

Normalized creep **strain** vs. time curves (ULiège)
(Single temperature & multiple (low) stress levels)



Normalized creep **strain rate** vs. time curves (ULiège)
(Single temperature & multiple (low) stress levels)

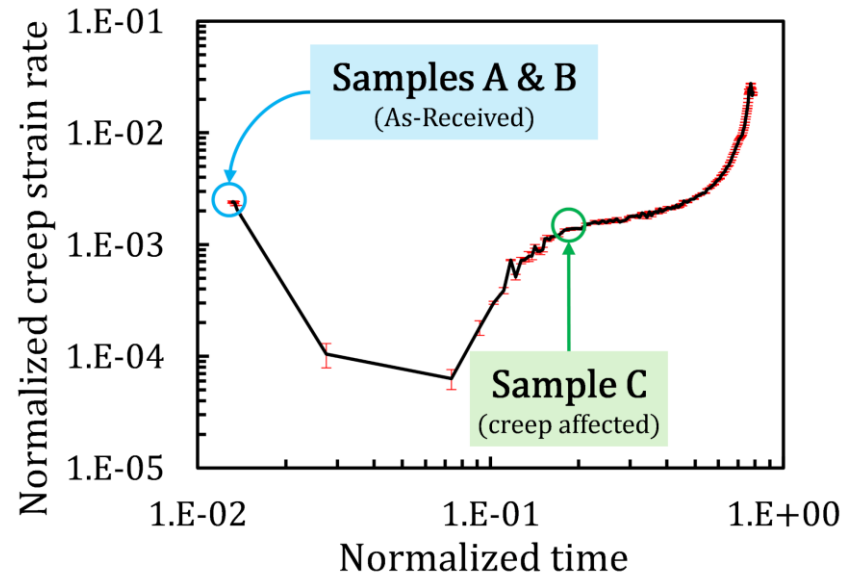


❖ Let us analyse the evolution of the mobile dislocation density (ρ_m) in test σ_1

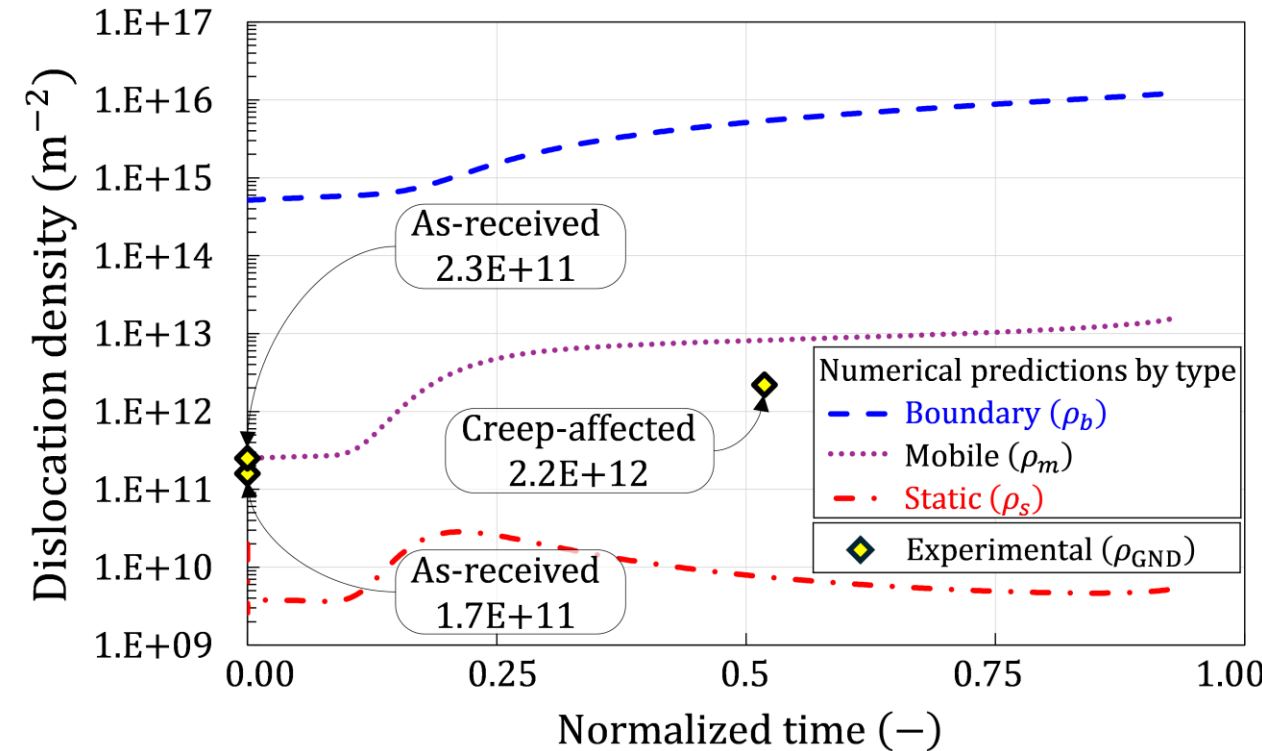
* After C. Rojas-Ulloa, JMS, 2026 [4]

Low stress

Experimental geometrically necessary dislocations measurements performed with EBSD



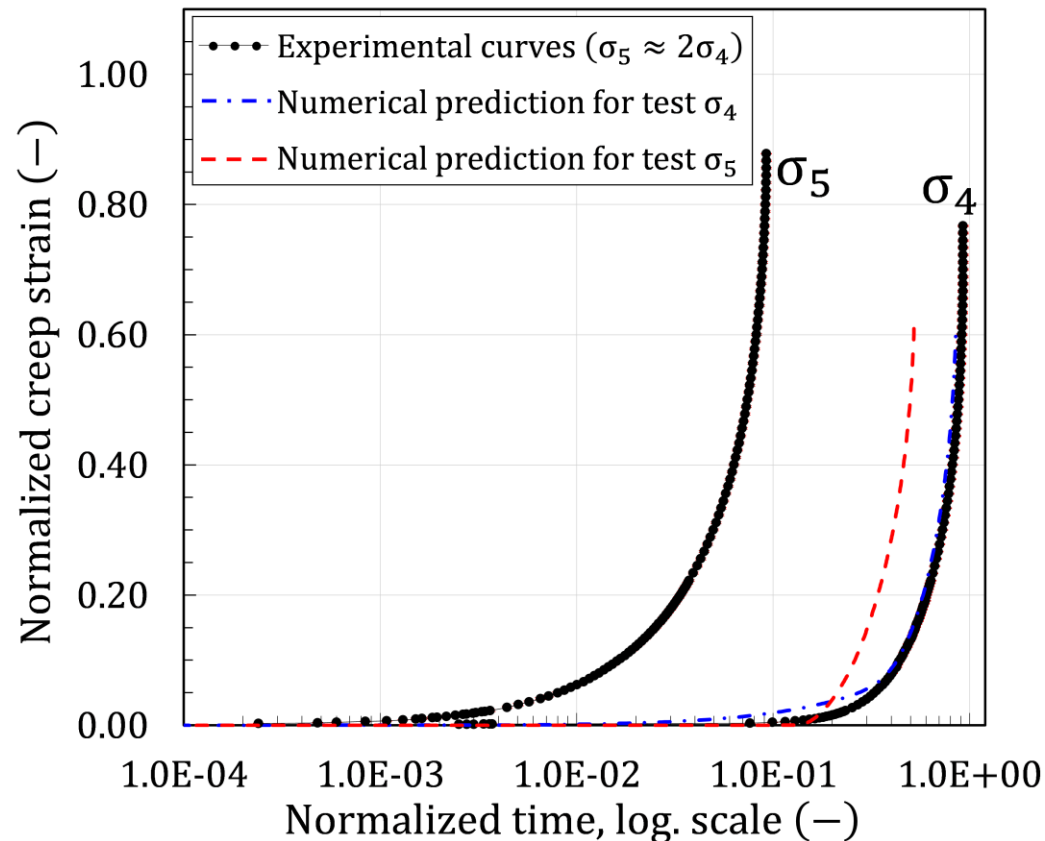
Mean dislocation densities predicted by MFC compared to experimental measurements for a single creep test



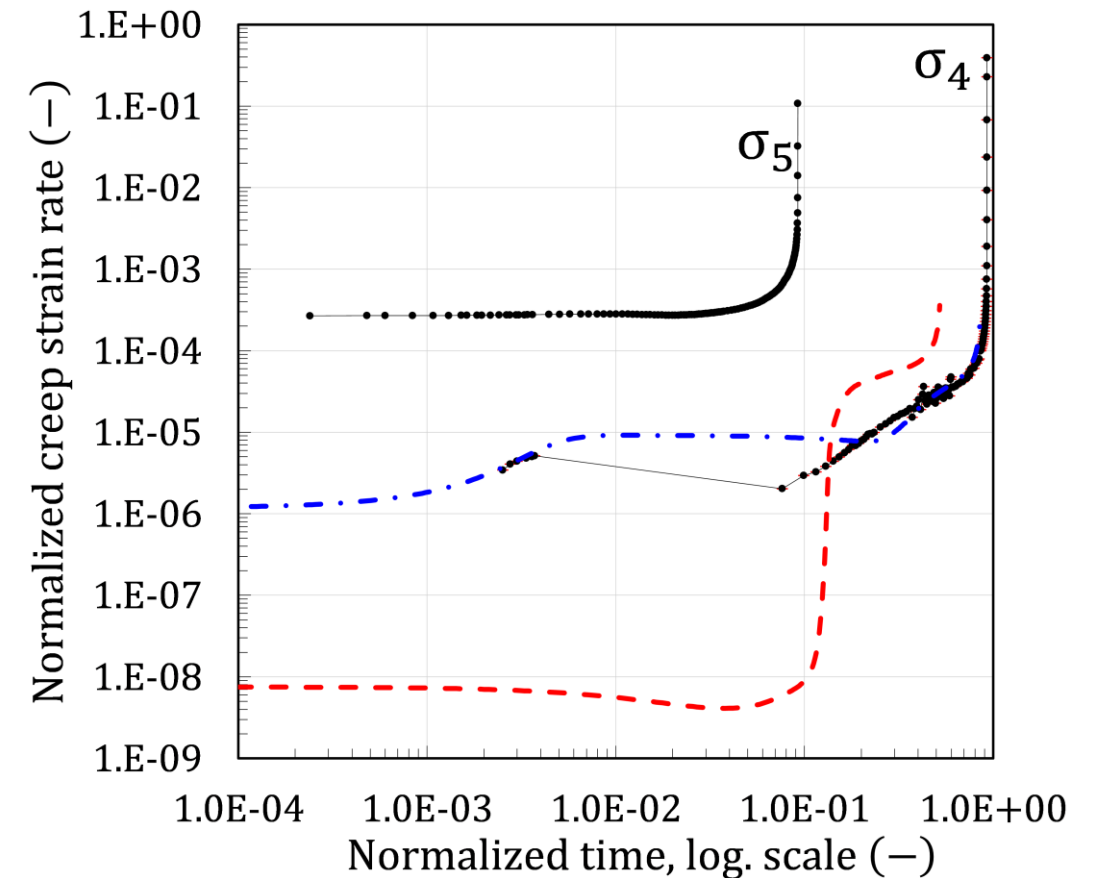
* After C. Rojas-Ulloa, JMS, 2026 [4]

High stress

Normalized creep **strain** vs. time curves (ULiège)
(Single temperature, with low & high stress levels)



Normalized creep **strain rate** vs. time curves (ULiège)
(Single temperature, with low & high stress levels)

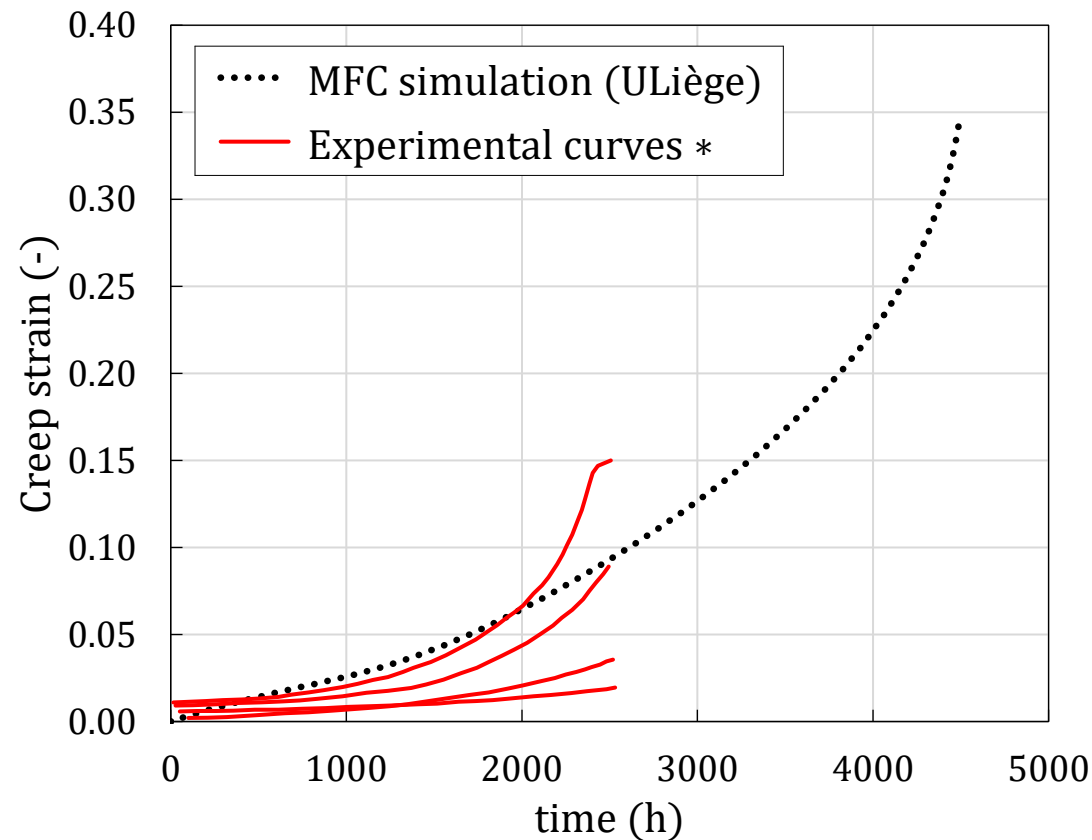


❖ Test conducted at σ_5 is found beyond the limits of our **MFC** model

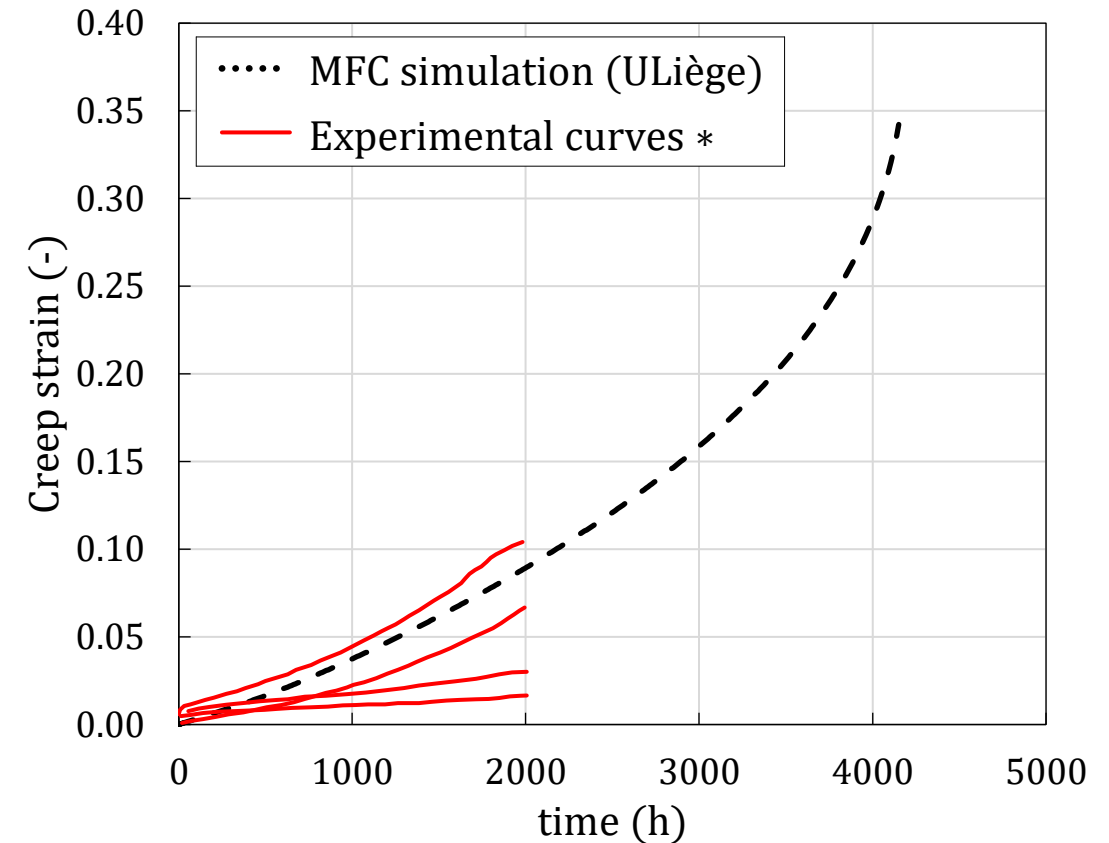
* After C. Rojas-Ulloa, JMS, 2026 [4]

Aging effect

Creep strain vs. time curves (literature*)
as-received material



Creep strain vs. time curves (literature*)
Argon-aged material (800hours at 1000°C)

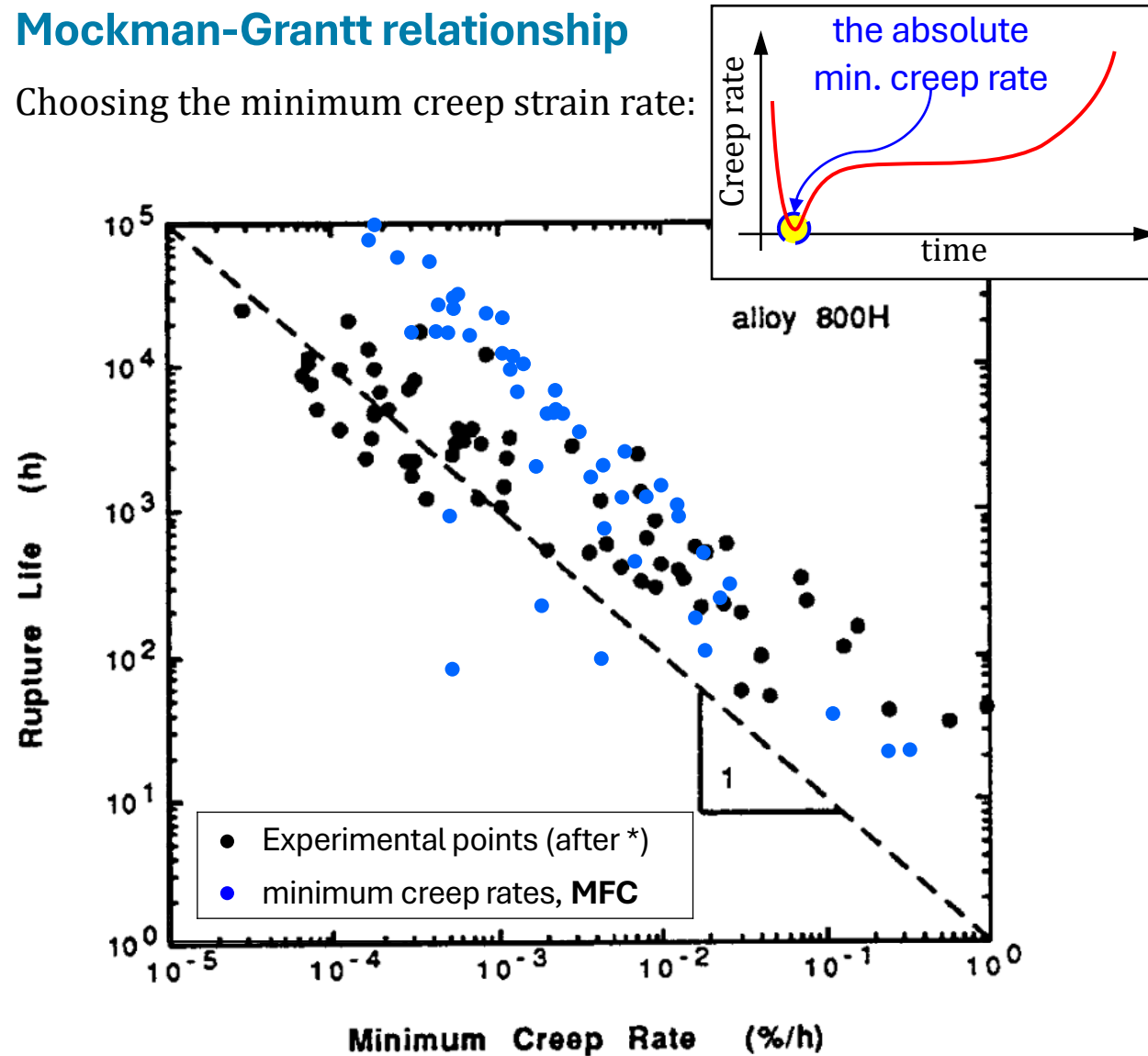


- ❖ Large experimental scattering
- ❖ MFC results within reasonable agreement

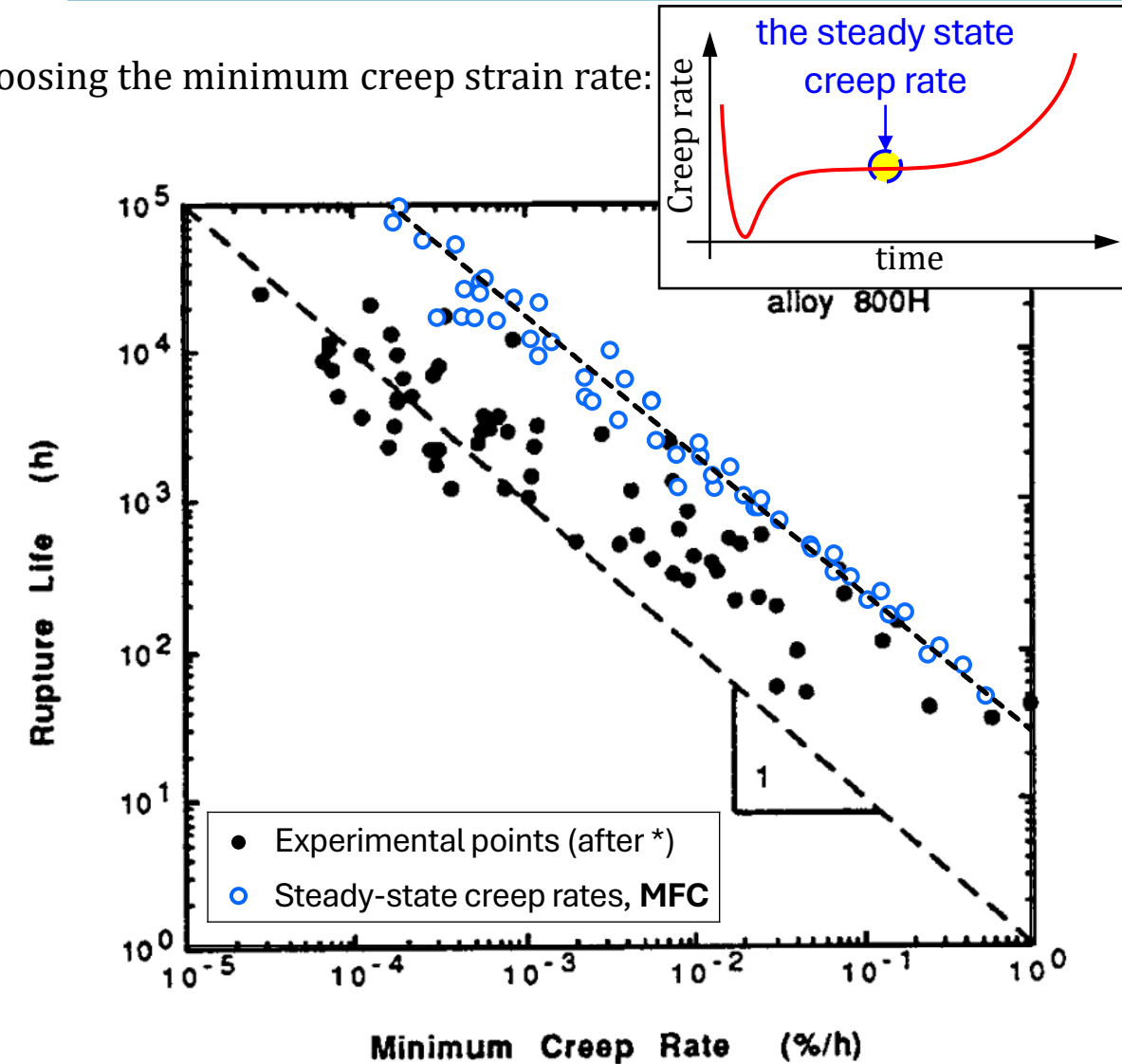
* see (A.M. Young, Journal of Materials Science, 2023) [12]

Mockman-Grantt relationship

Choosing the minimum creep strain rate:



Choosing the minimum creep strain rate:



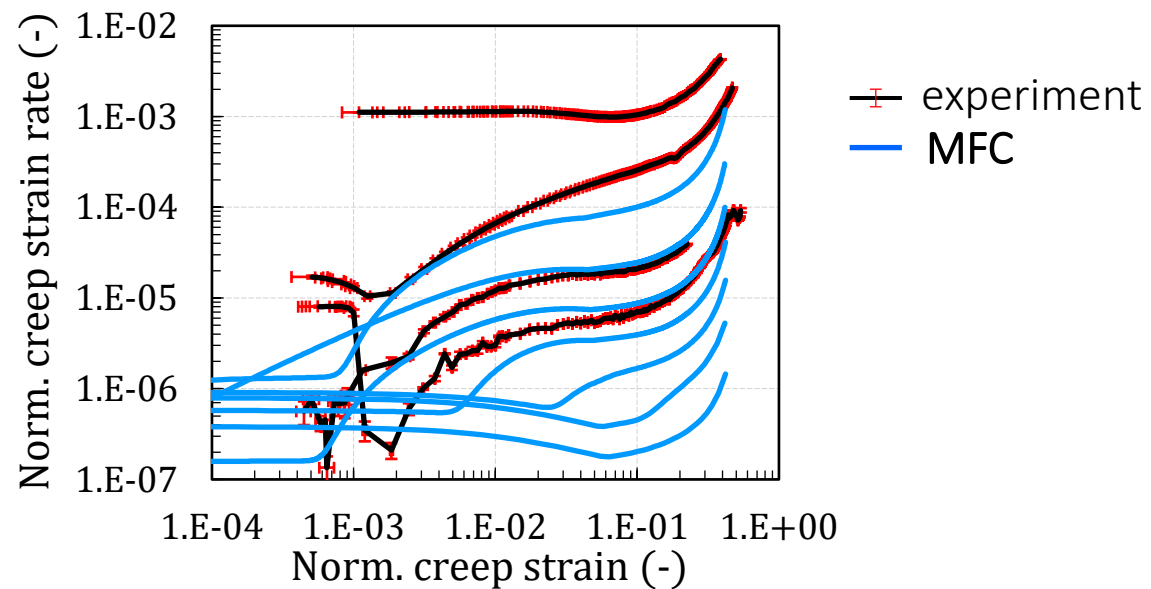
* experimental data points from (R. Swinderman, J. Eng. Gas Turbines Power, 1993) [13]

Mean-field creep model adapted to non-classical creep:

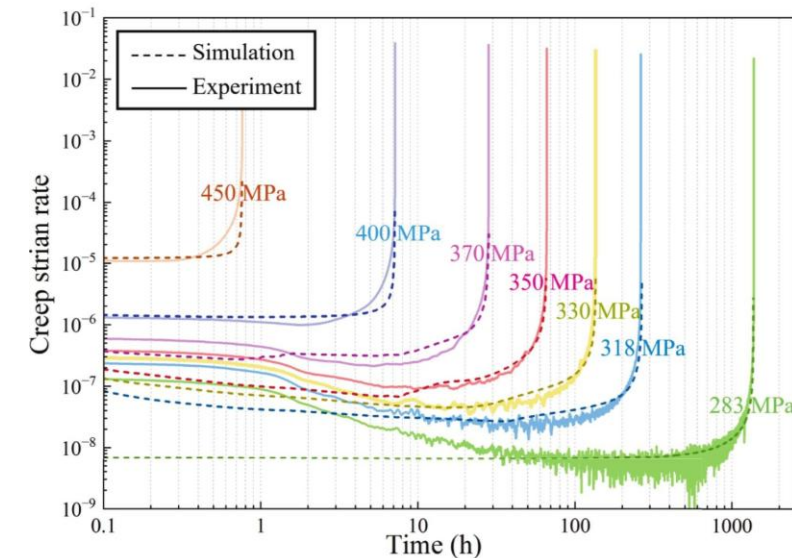
- ✓ Identified & validated with ULiège experiments
- ✓ Results in reasonable agreement with literature
- ✓ Stress-temperature applicability ascertained

Prospects:

- Virtual tests from **MFC** are a good complement to our experimental campaign



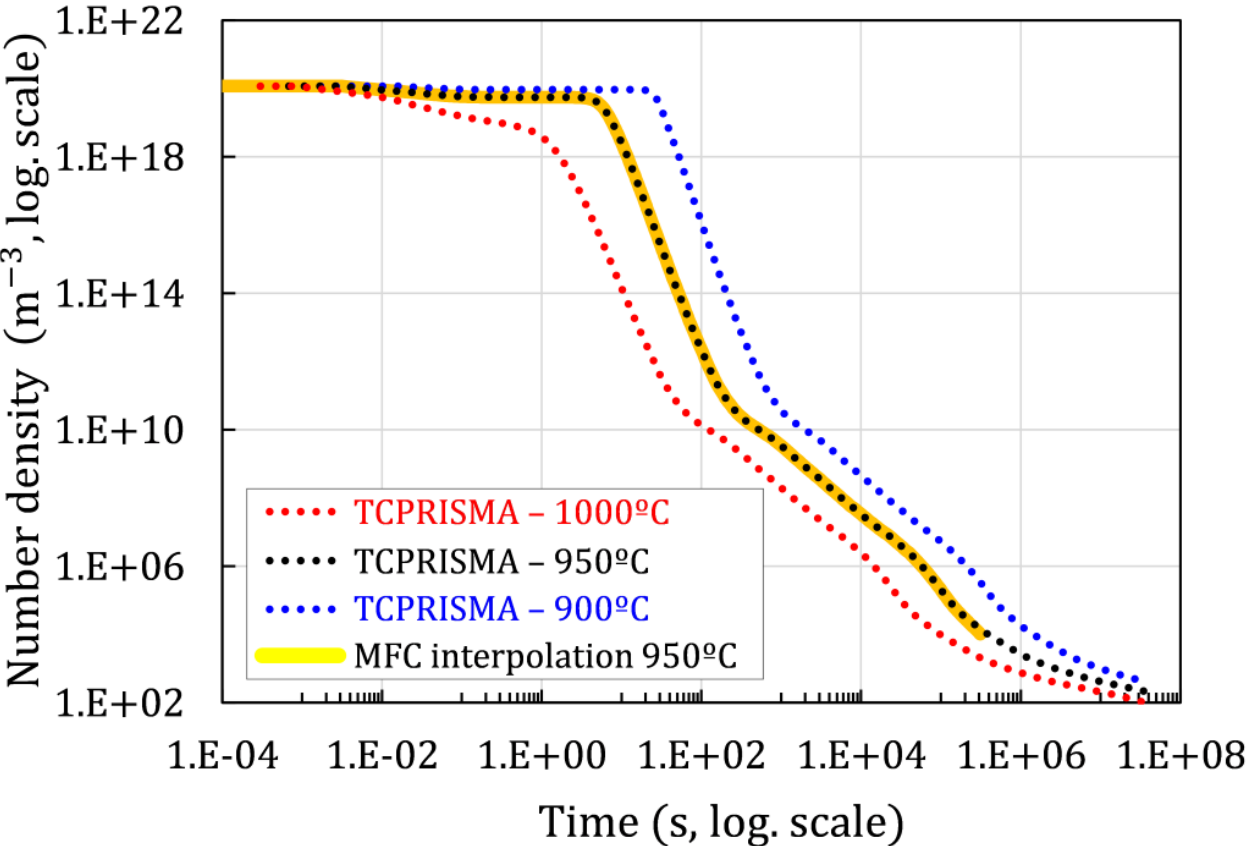
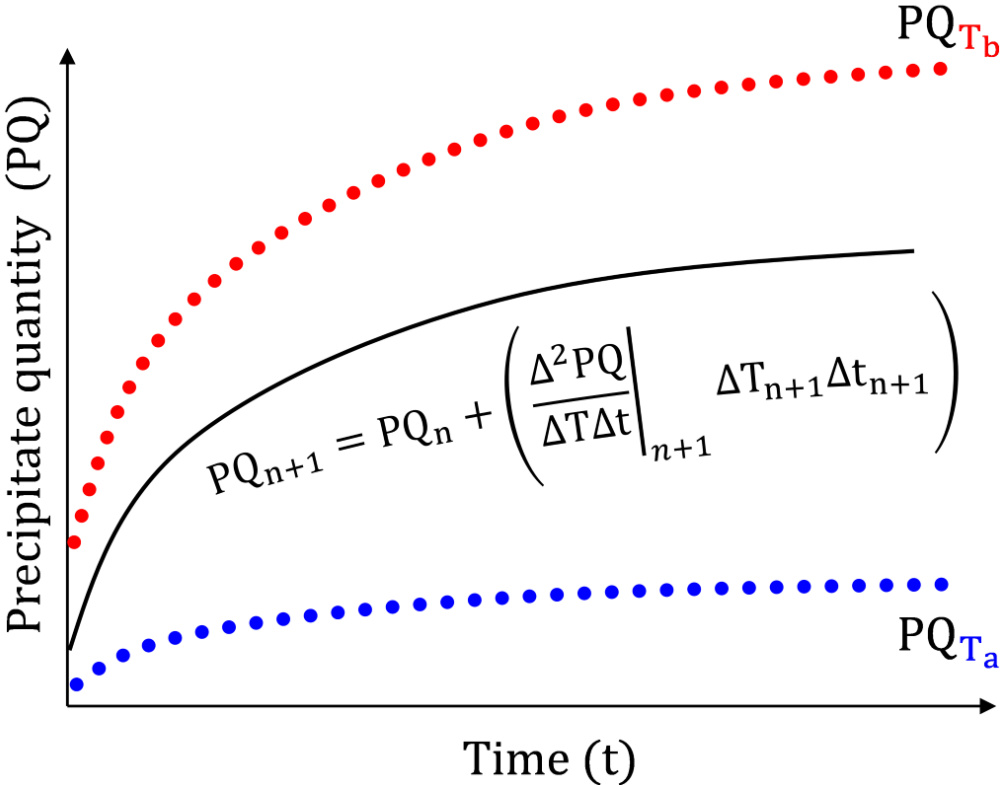
- MFC** model exploitation for other alloys: 30CrMoNiV5—11 alloy (**AID4Greenest** project *)



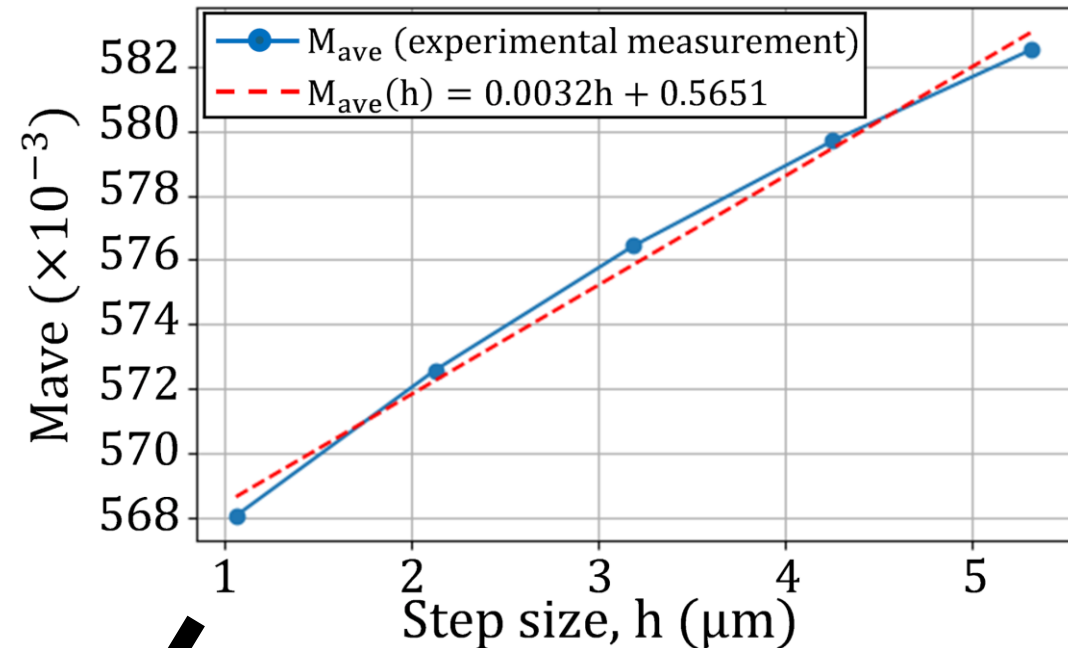
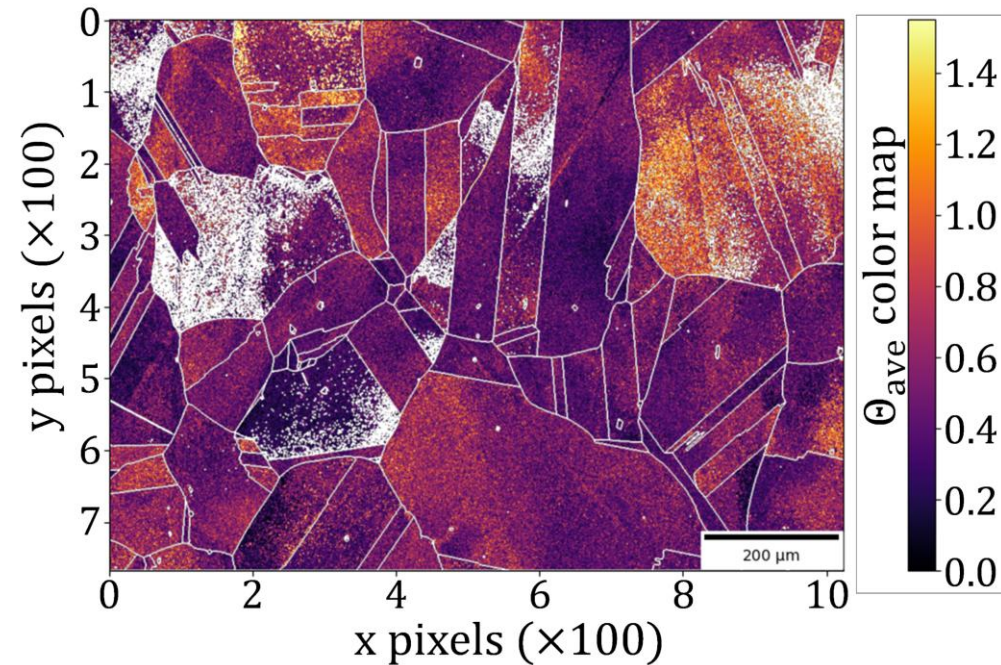
* See (F. Chen, MDA, 2026) [14]



- [1] K. Maruyama et al., *Materials Science and Engineering: A*, Vol. 224(1-2), 1997.
- [2] T. Hatakeyama et al., *Materials Science and Engineering: A*, Vol.831 (2022)
- [3] Lagamine finite element code, visit www.lagamine.uliege.be
- [4] C. Rojas-Ulloa et al., submitted to *Journal of Material Sciences* (Springer), 2nd review in process ☺
- [5] N.M. Ghoniem, J.R. Matthews & R.J. Amodeo, *Res. Mechanica*, Vol.29(1), 1990.
- [6] S.D. Yadav et al., *Materials Science & Engineering: A*, Vol.662, 2016.
- [7] F. Riedlsperger et al., *Materialia*, 2023.
- [8] F. Riedlsperger et al., *Materials at High Temperatures*, 2023.
- [9] W. Blum, P. Eisenlohr & F. Breutinger, *Met. & Material Transactions A*, Vol. 33A, 2002.
- [10] C. Parveen et al., *Materials Science & Engineering: A*, Vol.803, 2021.
- [11] I. Toda-Caraballo et al., *Acta Materialia*, Vol.85, 2015.
- [12] Alice M. Young, M.V. Kral & C.M. Bishop, *Journal of Materials Science*, Vol.58(26), 2023.
- [13] Robert W. Swindeman & Dougleas L. Marriott, *Journal of Engineering for Gas Turbines and Power*, Vol.116(2), 1993.
- [14] Fan Chen, C. Rojas-Ulloa et al., *Materials & Design*, 2026.



Geometrically necessary dislocations are extracted from the mean average misorientation angle captured during EBSD



slope = 0.0032 deg./μm

$$\rho_{\text{GND}} = \frac{0.0032 \cdot \left(\frac{\pi}{180}\right) \cdot 10^{-6}}{b}$$

... and, for FCC: $\rho_{\text{GND}} \approx \rho_m$

with