

FEMS 2025 EUROMAT

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Multiscale Modeling of Creep Deformation in 30CrMoNiV11- 5 Steel: Integrating Mean- Field Theory, Dislocation Dynamics, and Experimental Validation

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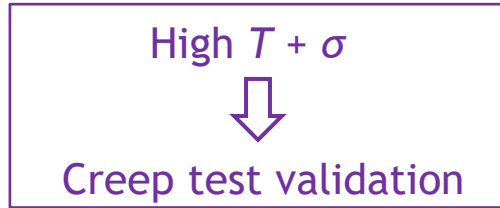


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AID4Greenest: Creep prediction

AID4Greenest target (aid4greenest.eu): IA and other models to avoid waste

Large forged shaft with high-temperature service



To avoid waste of material energy time



Life prediction before forging & thermal post processing



Large forged shaft (target component in AID4Greenest)



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Material - 30CrMoNiV5-11 Steel (heat-resistant steel)

%C	%Si	%Mn	%Cr	%Mo	%Ni	%V	%Cu	%S	%P
0,28	0,10	0,65	1,37	1,08	0,63	0,29	0,10	0,01	0,009

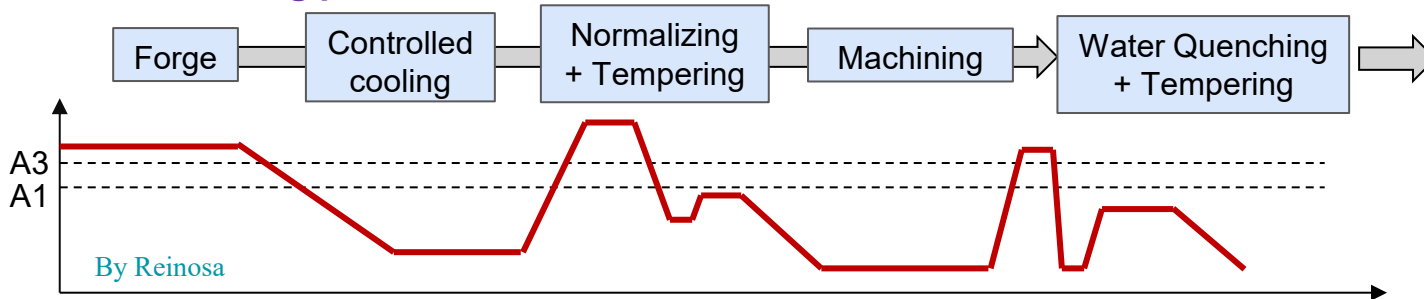
30CrMoNiV5-11 (Turbine manufacturers) → Different designations: DIN1.6946, SEW555

Family materials:

First developed: 1CrMoV → After 1990: 26CrMoNiV3-8 (in UK)

GX12CrMoVNbN9-1, 9Cr-1Mo, 2.25Cr steel, 9Cr steel, 12Cr steel, 28CrMoNiV4-9, 1Cr-steel, ...

Manufacturing process:



Observed phases:
BCC_A2 (Bainite, Ferrite)
Different carbides nature,
shape density

1. Process modelling and Process characterization (heat transfer coefficient)

- FEM simulations provide thermal field
- Mean Field + Cellular automata
- Microstructure 1 validated by characterization



2. Thermodynamic approach (Thermocalc Prisma) + sample characterization

→ Microstructure 2, after heat treatments, before creep



3. Creep behavior

Today

- Standard tests
- Phenomenologic model
- Machine Learning approaches



-Mean Field Creep model



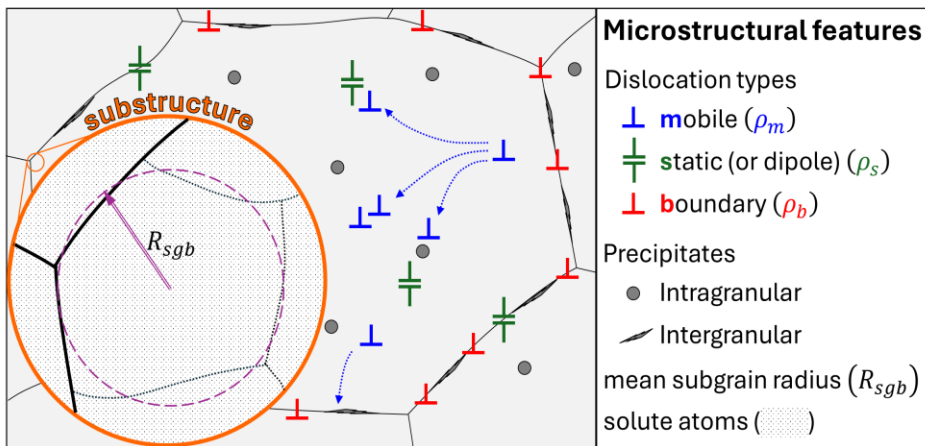
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Mean field creep (MFC) model framework

Why?

ML rupture/time predictions \neq mechanistic understanding
Classical creep fits \neq evolving microstructure

Creep deformation \leftrightarrow Microstructure evolution



MFC predicts the 3 creep stages +
comparison of 2 damage approaches
Identification Validation : experiments

...in math terms...

$$W = \begin{bmatrix} \epsilon \\ \rho_m \\ \rho_s \\ \rho_b \\ R_{sb} \end{bmatrix} = \begin{bmatrix} f(\epsilon, \rho_m, \rho_s, \rho_b, -) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(-, \rho_m, \rho_s, \rho_b, R_{sgb}) \end{bmatrix}$$

Vector of unknowns
(co-dependent functions)

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

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

Creep strain rate (s^{-1})

Mobile dislocation density (m^{-2})

Burgers vector (m)

Velocity (ms^{-1})

Taylor factor (-)

By Carlos Rojas

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Modeling framework

Particle kinetics

- Type of precipitate, location of nucleation, ...
- N_p : Number density of particles (m^{-3})
- r_p : Mean radius of particles (m^{-3})

JAX-coded
solverNumerical SCT
Creep curves

Loadings

Stress + Temperature

Material parameters

- Experimental data
- Adjustable parameters

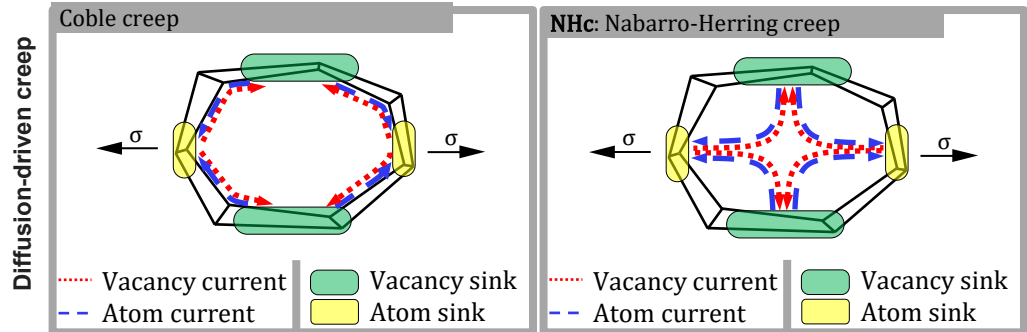
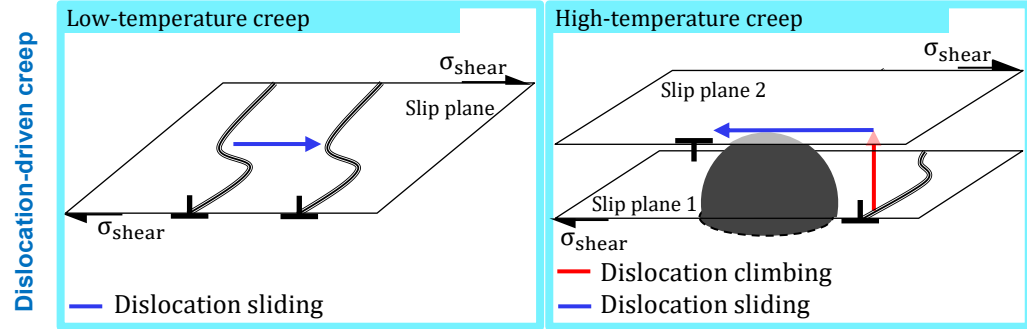
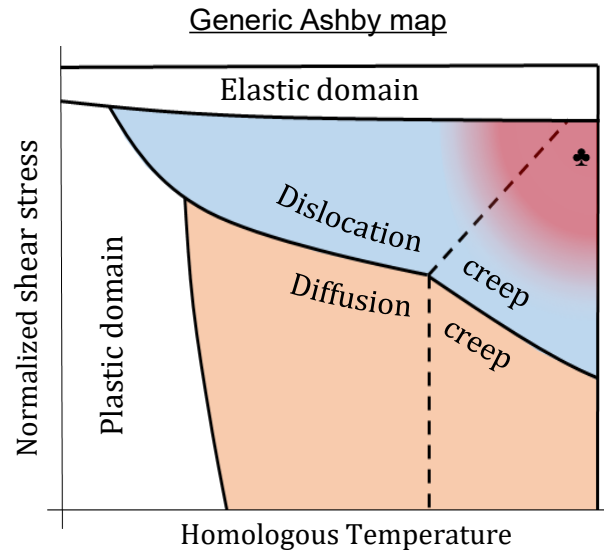
$$\Delta W = \begin{bmatrix} \Delta \epsilon \\ \Delta \rho_m \\ \Delta \rho_s \\ \Delta \rho_b \\ \Delta R_{sgb} \end{bmatrix} = \begin{bmatrix} f(\epsilon, \rho_m, \rho_s, \rho_b, -) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(\epsilon, \rho_m, \rho_s, \rho_b, R_{sgb}) \\ f(-, \rho_m, \rho_s, \rho_b, R_{sgb}) \end{bmatrix}$$

Parameters identification

Experimental
SCT Creep
curves

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Constitutive core





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Model architecture

Stress/Temperature

Dislocation
mechanics
(mean-field)

- > Dynamic recovery
- > Static recovery

Both mechanisms:
(dislocation + diffusion)]

Precipitate
kinetics

By TC PRISMA 2025a

- > Mean radius
- > Number density
- > Grain growth

Particle hardening
within grains

Damage law

- > Cavity
- > Precipitate coarsening

Particle coarsening
at grain boundary
or intra granular

Experiment
loop

- > Standard creep test (SCT)

Zwick Roell Kappa 100DS



- > Stepped iso-stress test (SSM)

Gleeble Fraunhofer IWM

Creep-time curve, creep strain rate, damage evolution, rupture



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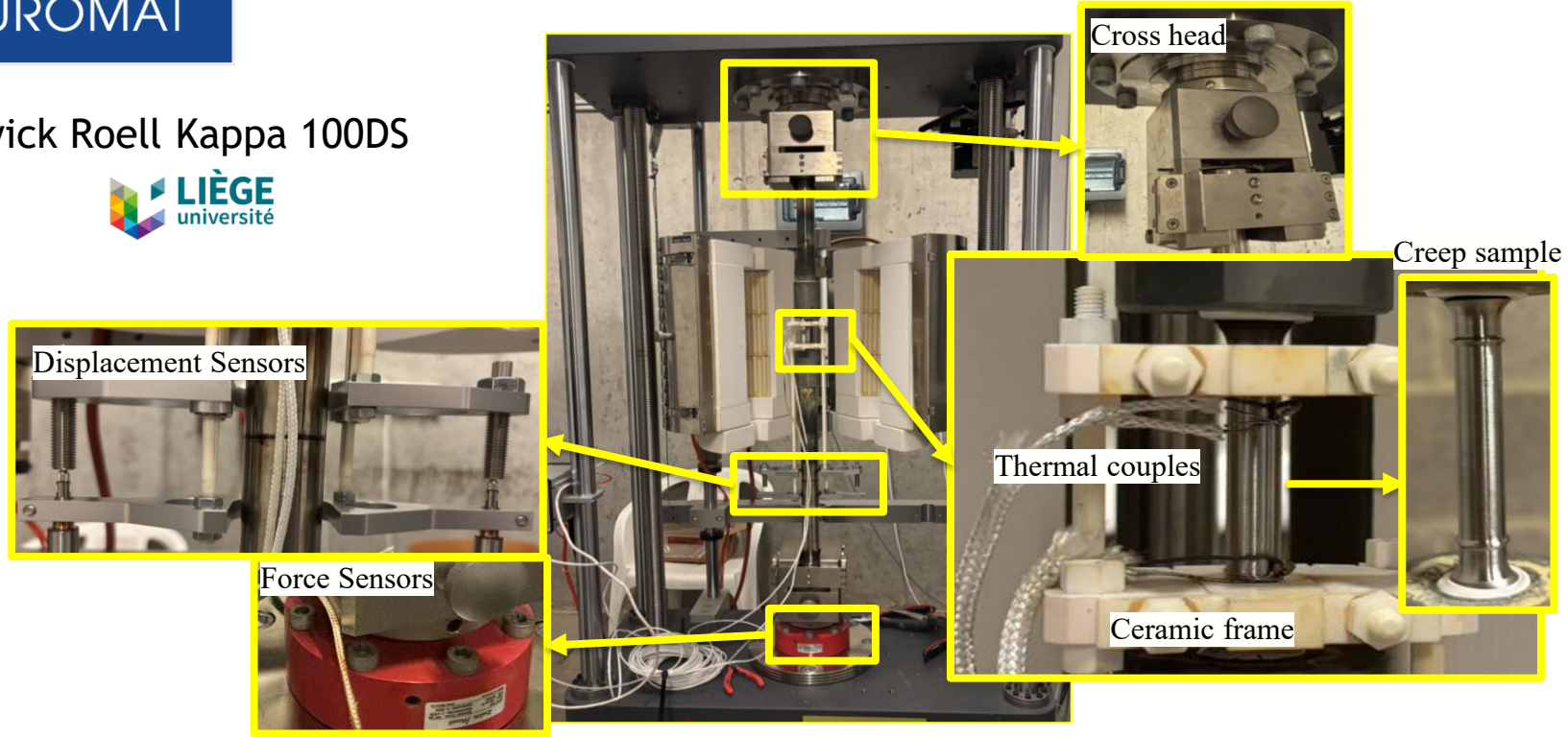
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Experimental campaign - Standard creep test (SCT)

Zwick Roell Kappa 100DS



Following International Organization for Standardization: ISO 204





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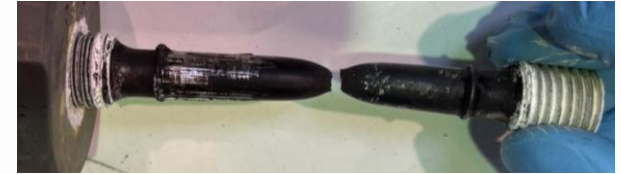
Experimental campaign - SCT

Before test



After test

Sample fractured at the middle



Stress

(283 ~ 450 MPa)

Temperature

(530 ~ 560 °C)

Rupture time

(1 hour ~ 1400 hours)



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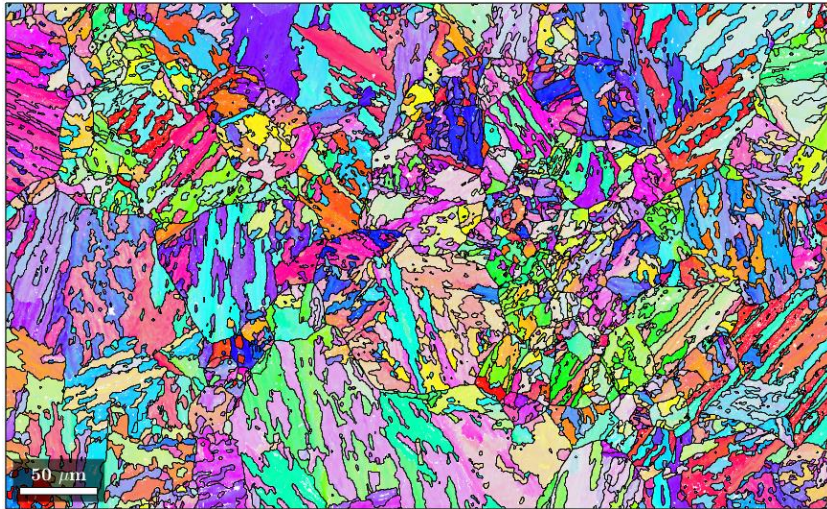


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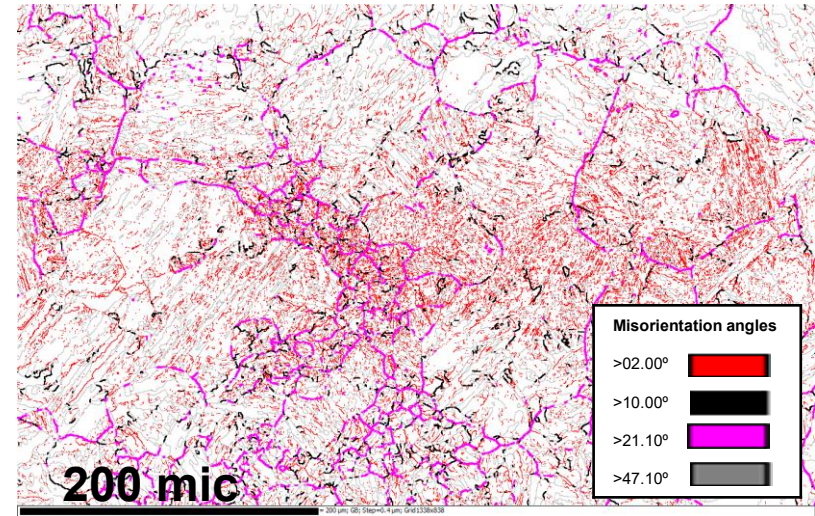
Initial Microstructure measured by

Prior - **austenite grain size** (PAGS) → grain diameter $d=2R_{\text{gbd}}$
Average PAGS: 19.5 μm

Inverse Pole Figure (IPF) map



Grain boundary (high + low angles)



Vertical cross section - Matlab - mtex 5.9.0

Measurements by Paula Chonillo

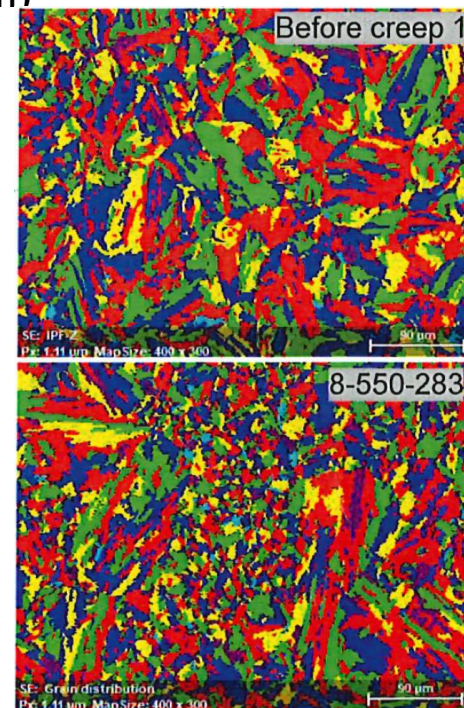


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Microstructure measured by EBSD

EBSD before and after creep: **Bainite grain size** (23~33 μm)

Sample	BG [μm] excl	BG [μm] incl
Before creep 1	32	31.5
Before creep 2	33.5	47.3
550 °C, 450 MPa	33.4	34
550 °C, 350 MPa	26.3	26.7
550 °C, 283 MPa	23.6	25.3



(Measurements by Jérôme Tchoufang Tchuindjang)

Decrease of the grain size when the stress decreases.





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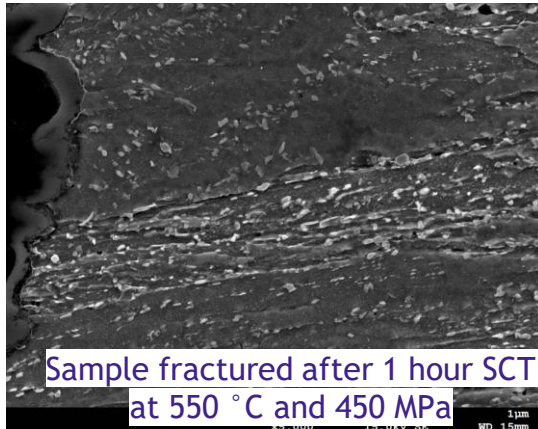
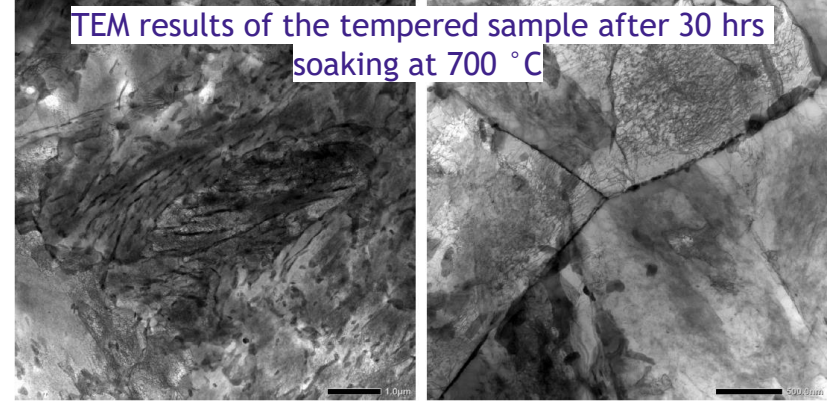
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Microstructure after creep

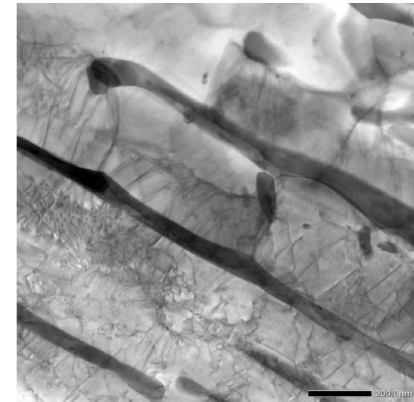
Precipitates observed



- M23C6_D84
- CEMENTITE_D011 (Fe3C, M3C ...)
- M6C_E93
- FCC_A1#2 (V(C,N))



Dislocation density measured using XRD (Cu Kα):
 $\cong 3.4 \times 10^{14}/m^2$



(by University of Oulu)





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Microstructure evolution (550 °C) - Number density

By TC PRISMA 2025a

Main phase: BCC_A2

Precipitate:

- M23C6_D84
- M6C_E93
- FCC_A1#2 (V(C,N))

CEMENTITE begins to eliminate at 1 h

Bulk, dislocation:

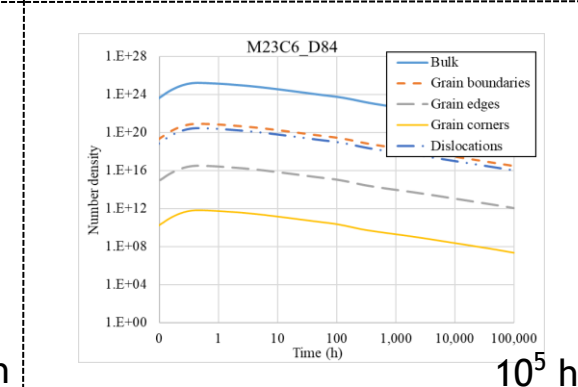
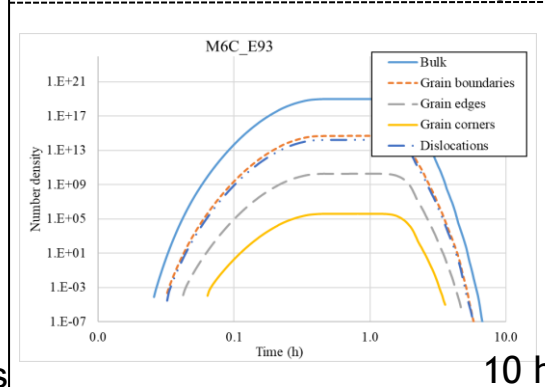
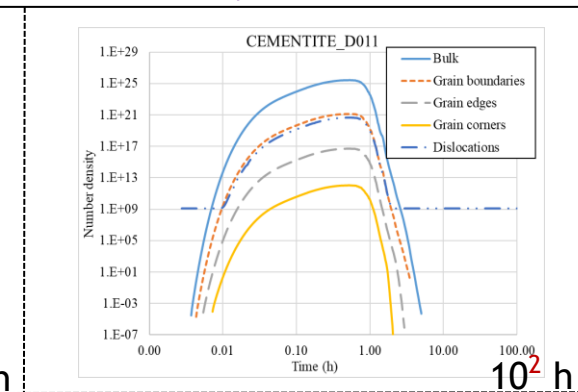
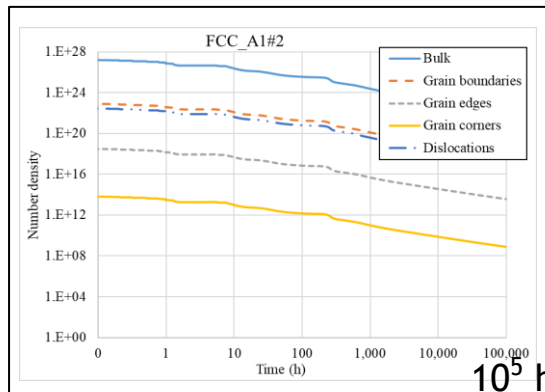
➤ precipitate hardening

Grain edge, corner, boundary:

➤ damage

Log time scale

Big differences in kinetics





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Microstructure evolution (550 °C) - Mean radius

By TC PRISMA 2025a

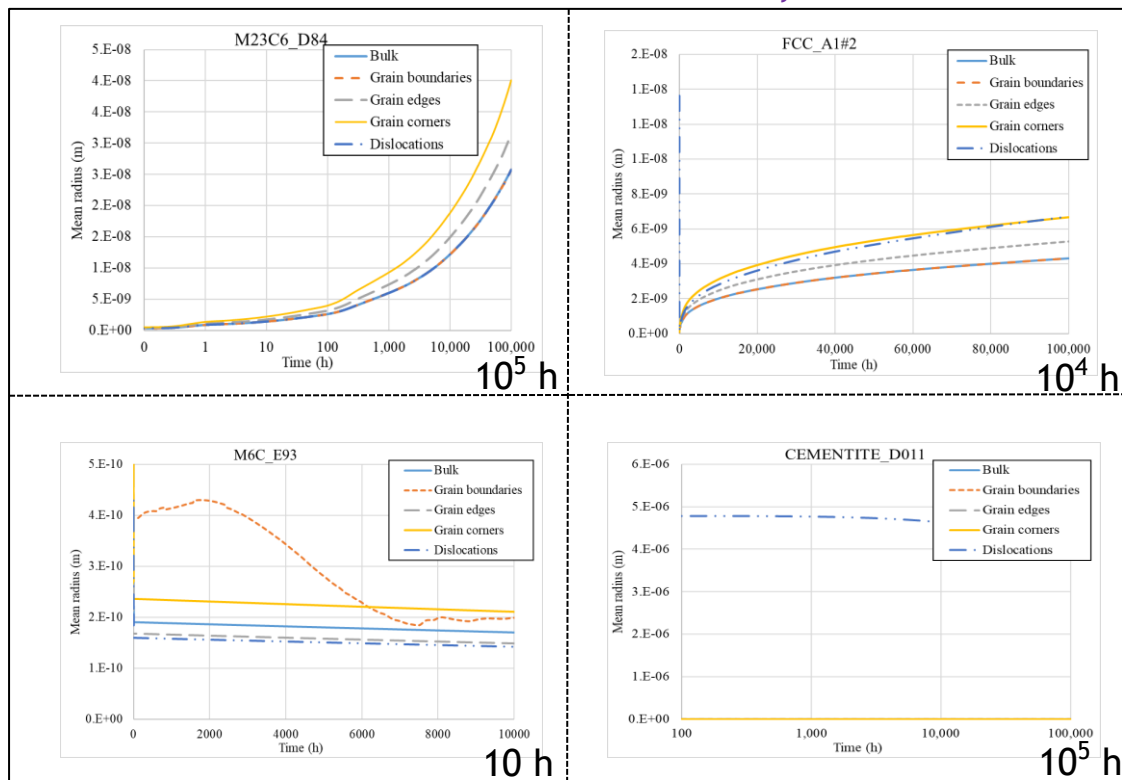
Main phase: BCC_A2

- M23C6_D84
- M6C_E93
- FCC_A1#2 (V(C,N))

CEMENTITE begins to eliminate at 1 h

Bulk, dislocation:
precipitate hardening

Grain edge, corner, boundary:
damage



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Constitutive core modeling framework of literature need revision for our material (Creep 550 °C)

Modified Orowan equation (dislocation creep)

$$\dot{\epsilon}_{disl} = \frac{b \rho_m v_{eff}}{M_T}$$

Internal (Taylor) stress

$$\sigma_i = \alpha M G b \sqrt{\rho_m + c_s \rho_s}$$

Driving stress

$$\sigma_{app} = \sigma_{app,0} (1 + \nu \epsilon)$$

Coble equation (diffusion creep)

$$\dot{\epsilon}_{diff} = K_1(T) \sigma_{app}$$

(More details in backup)

Total rate:

$$\dot{\epsilon}_{creep} = (\dot{\epsilon}_{disl} + \dot{\epsilon}_{diff}) \frac{1}{(1 - D_{ppt})(1 - D_{cav})}$$

Gliding velocity relying on V_r

$$v_g = a_1 \exp\left(\frac{-Q_{self}}{k_B T}\right) \exp\left(\frac{-\sigma_i V_r}{k_B T}\right) 2 \sinh\left(\frac{\sigma_{app} V_r}{k_B T}\right)$$

F. Riedlsperger, (2023)

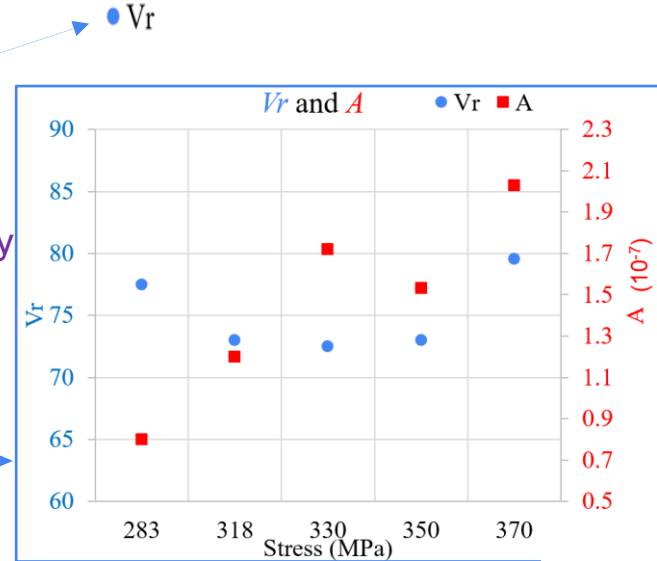
Damage evolution starts at stored-energy threshold SE (stress dependent damage initiation)

$$SE = A \sigma (1 + \epsilon) \epsilon^m \geq SE_{threshold}$$

Lemaitre, J., (2005). Equation (1.105)

$$\dot{\epsilon}_{diff} \propto \sigma_{app}$$

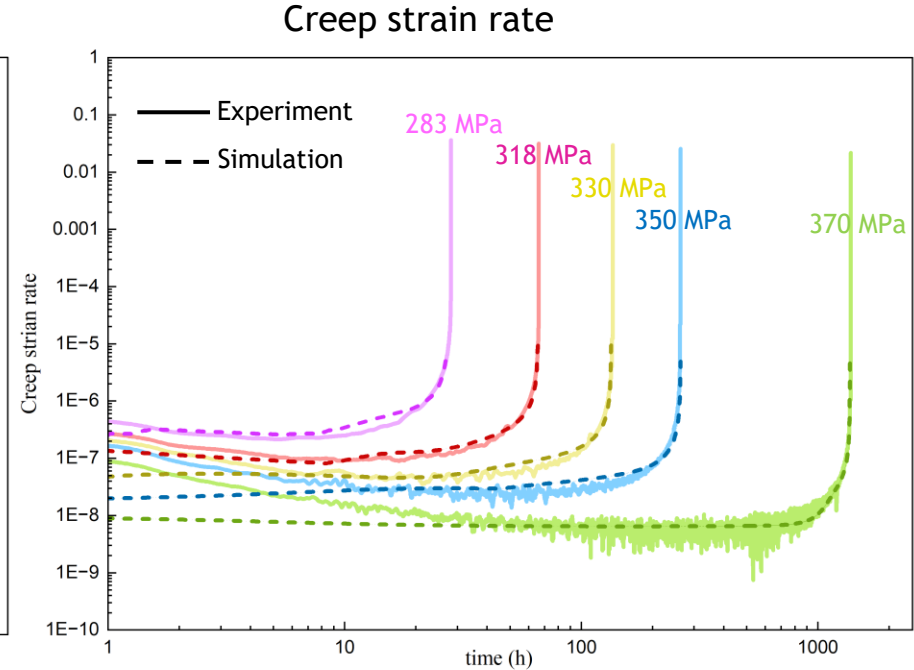
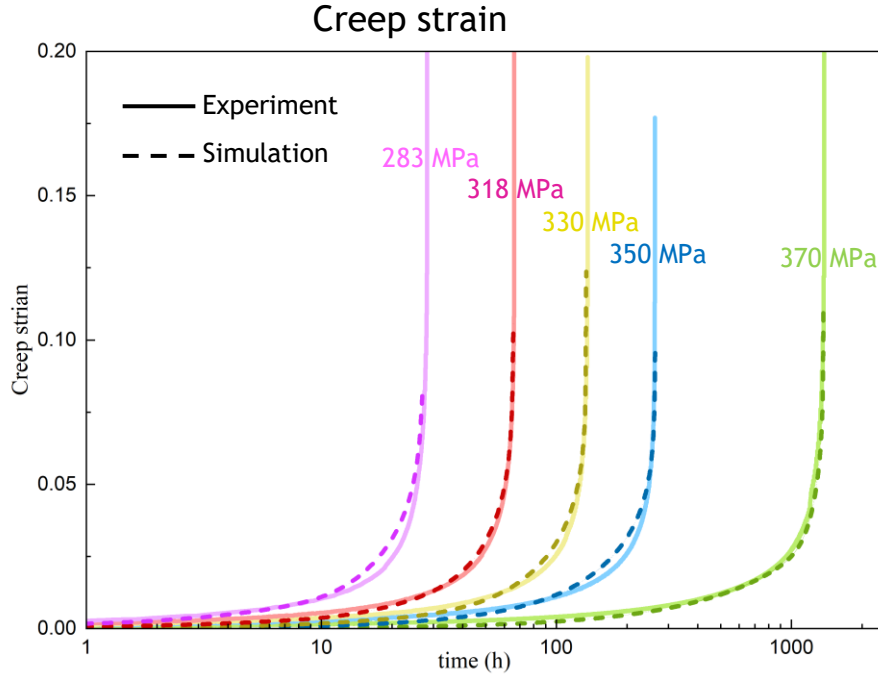
Poor consistent evolution of V_r and $\log(\dot{\epsilon}_{diff})$ to predict experimental creep tests under increasing stress



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Poor Creep strain rate prediction (550 °C) (1st model version of previous slide)

$$\dot{\epsilon}_{diff} \propto \sigma_{app}$$



➤ Primary stage not well predicted

➤ Only Applicable on high stress level



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Constitutive core (Revised modeling framework)

Modified Orowan equation (dislocation creep)

$$\dot{\epsilon}_{disl} = \frac{b\rho_m v_{eff}}{M_T}$$

Internal (Taylor) stress

$$\sigma_i = \alpha M G b \sqrt{\rho_m + c_s \rho_s}$$

Driving stress

$$\sigma_{app} = \sigma_{app,0} (1 + \nu \epsilon)$$

Coble equation (diffusion creep)

$$\log(\dot{\epsilon}_{diff}) = K_1(T) \sigma_{app}$$

(More details in backup)

Total rate:

$$\dot{\epsilon}_{creep} = (\dot{\epsilon}_{disl} + \dot{\epsilon}_{diff}) \frac{1}{[(1-D_{ppt})(1-D_{cav}]}$$

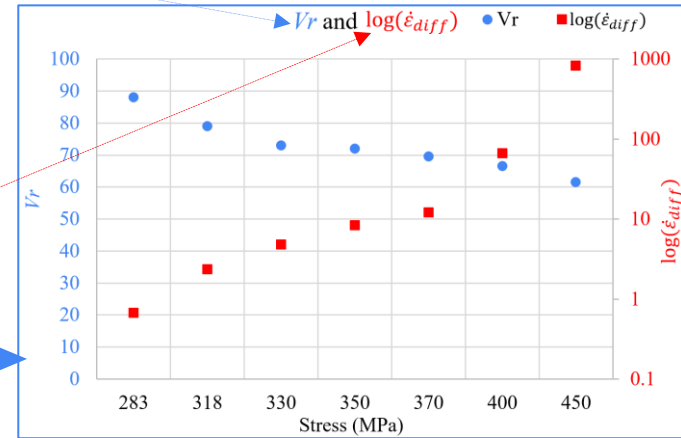
Gliding velocity

$$v_g = a_1 \exp\left(\frac{-Q_{self}}{k_B T}\right) \exp\left(\frac{-\sigma_i V_r}{k_B T}\right) 2 \sinh\left(\frac{\sigma_{app} V_r}{k_B T}\right)$$

F. Riedlsperger, (2023)

$$\log(\dot{\epsilon}_{diff}) \propto \sigma_{app}$$

Both V_r and $\log(\dot{\epsilon}_{diff})$ can be fitted by the functions



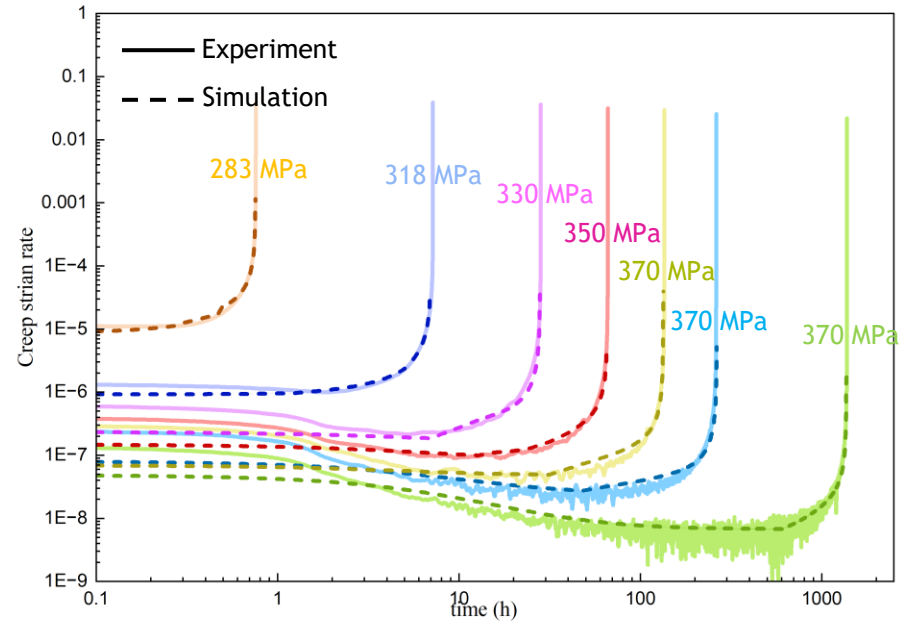
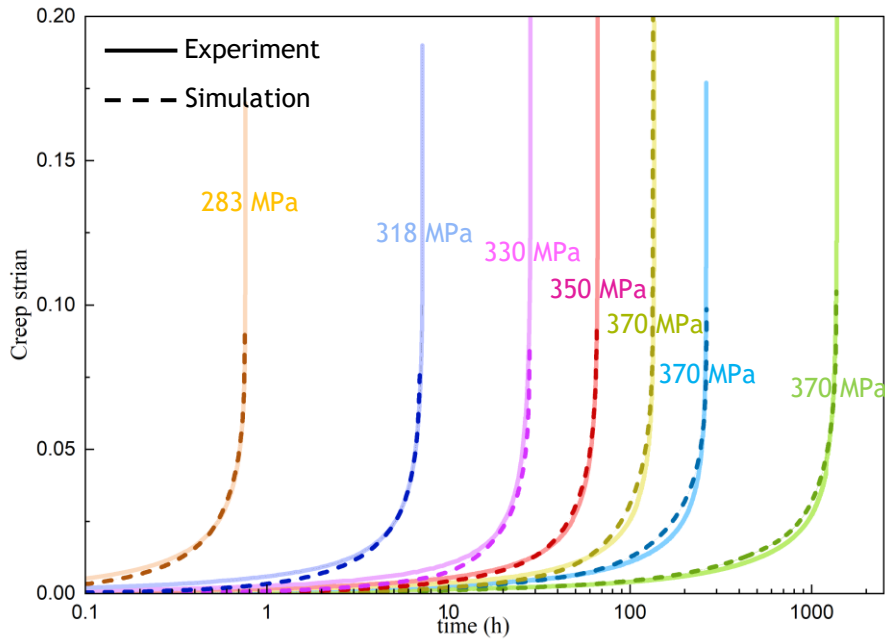
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Creep strain rate at 550 °C (Uliege model)

$$\log(\dot{\epsilon}_{diff}) \propto \sigma_{app}$$

Creep strain

Creep strain rate



➤ Good agreement on all stress levels (different contribution of diffusion and dislocation mechanisms)

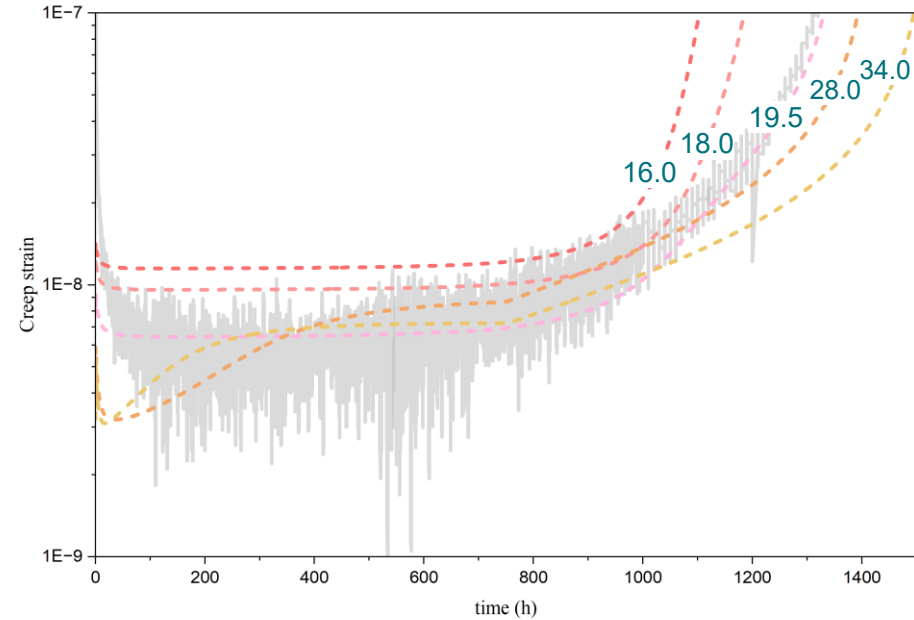
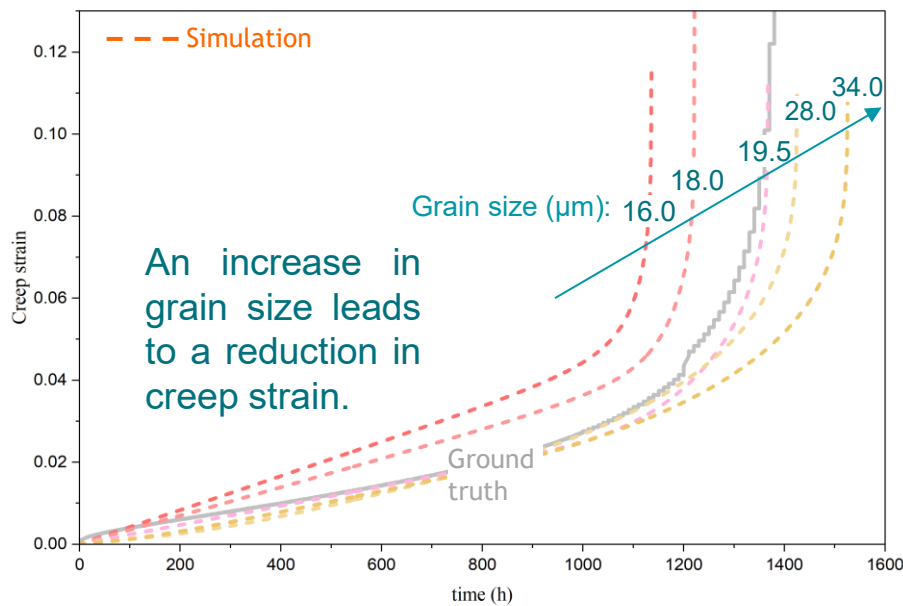


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Parameter sensitivity (1st model)

$$\dot{\epsilon}_{diff} \propto \sigma_{app}$$

Fixed simulation parameters identified at 19.5 μm (PAGS)
> Change grain size only



Takeaways & limitations

- MFC + diffusion creep prediction → accurate secondary creep stage;
damage tertiary stage
- Strengths: clear relation with creep mechanism, parameter-identifiable
- Limits: Numerous data required
Grain evolution neglected,
Still 1D version → need extension to be included in FEM,
particle kinetics data to be validated
- Future work: temperature-dependent $D_{gb}(T)$,
grain growth coupling,
multi-axial constitutive law

Acknowledgments

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Thank you!

Effective velocity:	$\frac{1}{v_{eff}} = \left[\frac{1}{v_g} + 2\pi(\sum r_{p,i}^3 N_{p,i}) \cdot \frac{1}{v_c} \right]^{-1}$
Glide:	$v_g = a_1 \exp\left(\frac{-Q_{self}}{k_B T}\right) \exp\left(\frac{-\sigma_i V_R}{k_B T}\right) 2 \sinh\left(\frac{\sigma_{app} V_R}{k_B T}\right)$
Climb:	$v_c = v_{cl} + v_{cp}$
	<p>Lattice diffusion $v_{cl} = \frac{2\pi\eta_v D_l}{[1-\eta_v \ln(L_\alpha \sqrt{\rho t})]} \exp\left(\frac{-\sigma_i \Omega}{k_B T}\right) 2 \sinh\left(\frac{\sigma_{app} \Omega}{k_B T}\right)$</p> <p>Pipe diffusion $v_{cp} = \left\{ \frac{2\pi b D_p}{L_p^2} \right\} \exp\left(\frac{-\sigma_i \Omega}{k_B T}\right) 2 \sinh\left(\frac{\sigma_{app} \Omega}{k_B T}\right)$</p>

Precipitate strengthening via $\sum r_{p,i}^3 N_{p,i}$ and spacing $L_p = \sqrt{2} a_g \exp\left(\frac{\Delta W}{2k_B T}\right)$

Precipitate coarsening:

$$D_{ppt}(t) = 1 - \frac{L_S^0}{L_S(t)}$$

$$L_S^0 = \sqrt{\frac{\ln(3)}{2\pi \sum_i N_i r_i} + (2r_A)^2} - 2r_A$$

$$L_S = \sqrt{\frac{2 \sum_i N_i r_i^2}{3 \sum_i N_i r_i}}$$

Murchú, C. Ó., (2017), 9Cr steels

L_S^0 : precipitate spacing at damage onset,
 $L_S(t)$: precipitate spacing at current time.

Cavitation:

$$\dot{D}_{cav} = (D_{cav}(t) + a(1 + be^{\frac{T_c}{c}}))\dot{\epsilon}$$

Murchú, C. Ó., (2017), 9Cr steels

Damage evolution starts when stored-energy criterion reaches threshold

$$SE = A\sigma(1 + \epsilon)\epsilon^{\frac{1}{m}} \geq SE_{threshold}$$

Lemaitre, J., (2005). Equation (1.105)

Backup - Parameter identification workflow

- Step 1 (no damage, PK frozen): tune sinks (e.g., annihilation), V_r for stress sensitivity
- Step 2: add diffusion branch to lift entire curve (fit $A_c D_{gb} \delta / d^3$)
- Step 3: re-enable PK evolution;
- Step 4: enable damage for tertiary

