

“Scale Bridging Creep : On the Usage of Phase-Field to Model the Carbide Growth in 30CrMoNiV5-11 Alloy During Heat Treatment”

R. Eloudrhiri, G. Bryndza, H. Sepulveda, C. Rojas-Ulloa, F. Chen,
A. Habraken, L. Duchêne

Scale Bridging Creep : an Outline

Context and **motivation**

Phase-Field for **creep** modeling

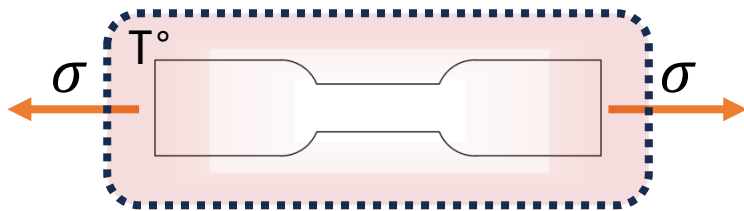
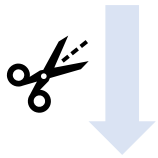
Model-specific **ingredients**

Validation against ThermoCalc

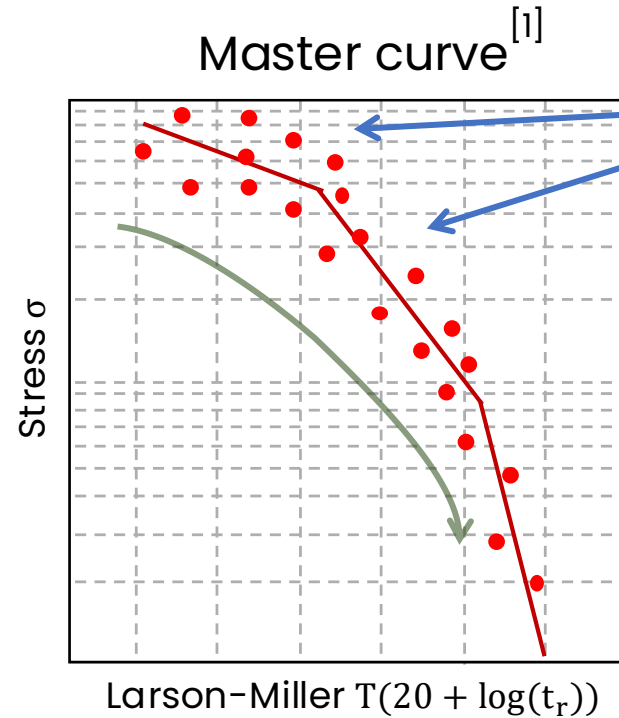
Future **prospects**
and **goals**

Complex microstructural transformations govern creep at the macrostructural level

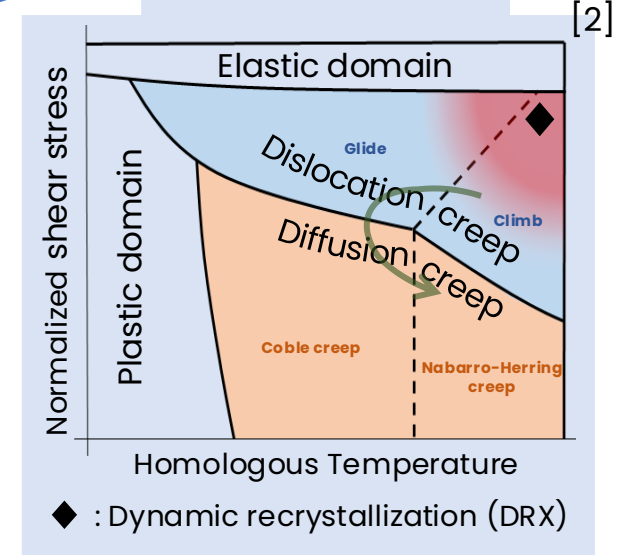
Turbine shaft for power generation



Creep testing



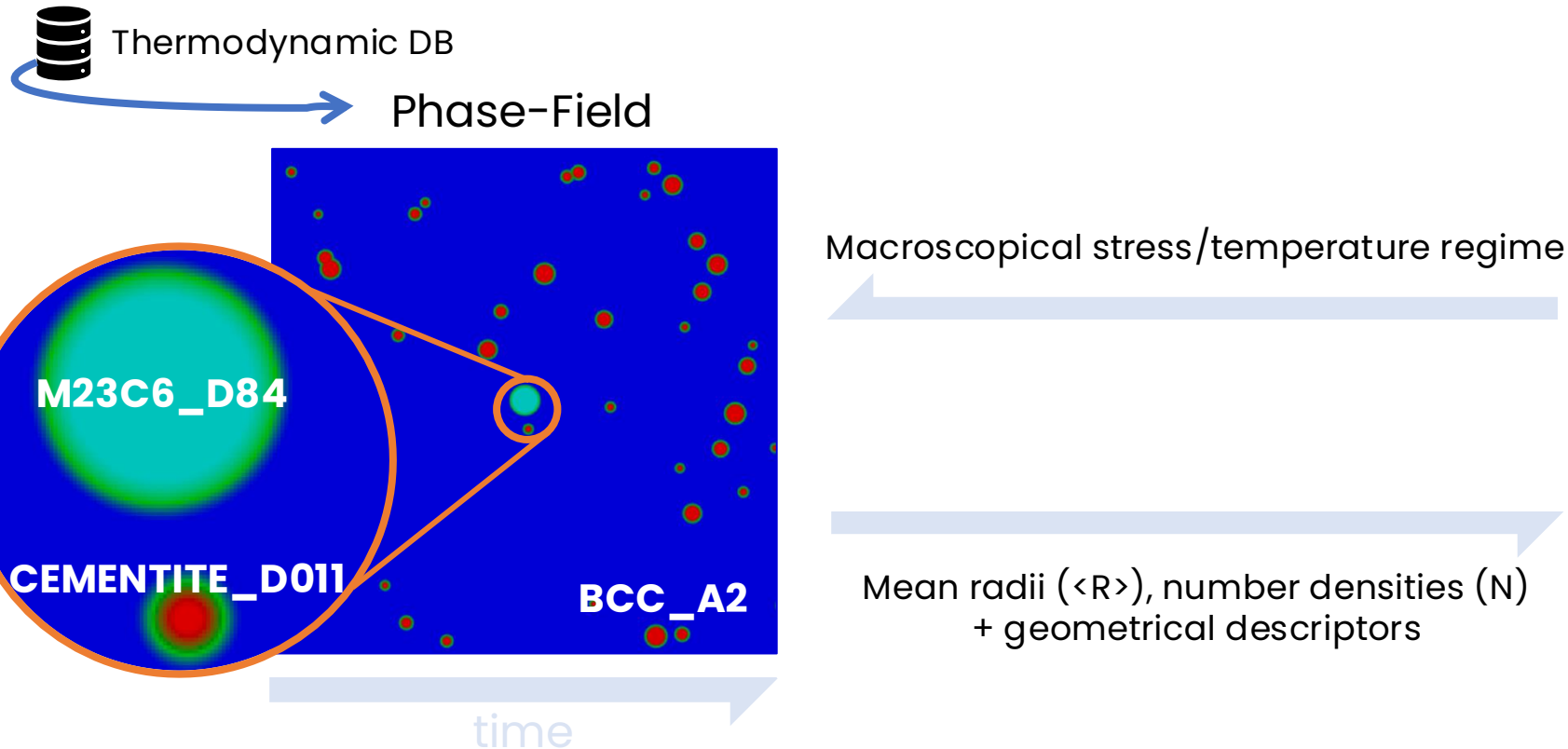
≠ microstructural mechanism



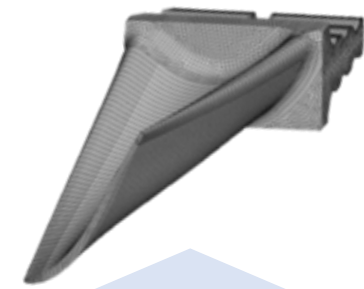
[1] M. Ashby *Acta Metallurgica* (1979)

[2] F. Larson, J. Miller *Transactions of the ASME* (1951)

Phase-Field in a multi-scale framework for physics-based creep simulations



Meso/Macroscale stack



Local creep behavior^[3]

$$\dot{\epsilon}_{creep} = \frac{\rho b v_{eff}}{m_T}$$



[3] F. Chen, C. Rojas-Ulloa, et al.
Material Design (2026)

pyVulcan: *In-house* KKS-based Phase-Field framework

$$F[\eta_i, x_k] = \int_V \boxed{f(\eta_i, x_k)} + \frac{\kappa}{2} \sum_i |\nabla \eta_i|^2 + \cancel{\frac{\epsilon}{2} \sum_k |\nabla x_k|^2} + \sum_s f_{source}^s dV$$

$$\frac{\partial \eta_i}{\partial t} = -L_i \left[-\kappa^2 \nabla^2 \eta_i + w \frac{\partial g}{\partial \eta_i} + \frac{2\eta_i}{\sum_p \eta_p^2} h_j \Delta_{i,j} f + \sum_s \frac{\partial f_{source}^s}{\partial \eta_i} \right] \quad \text{Allen-Cahn equation}$$

$$\frac{\partial x_k}{\partial t} = \tilde{D}_{k,k} \nabla^2 x_k - \tilde{D}_{k,k} \left[\frac{\partial h_j}{\partial \eta_i} x_k^j \nabla \eta_i \right] \quad \text{Cahn-Hilliard equation}$$

$$\frac{\partial f^i}{\partial x_k^i} = \frac{\partial f^j}{\partial x_k^j} = \mu_k, \quad \forall k \text{ species} \quad \text{KKS constraint}^{[4]}$$

$$= w f_0(\boldsymbol{\eta}) + \underbrace{\sum_i h_i(\boldsymbol{\eta}) f^i(\mathbf{x}^i)}_{\text{.tdb}}$$

.tdb

pyVulcan: model-specific ingredients

Thermodynamically-consistent interpolation function : ^[5]

$$h_i(\eta) = \frac{\eta_i^2}{\sum_j \eta_j^2}$$

Polynomial fit of **Gibbs free energy** :

$$f^i(\mathbf{x}^i) = \sum_k A_{k,k}^i (x_k^i)^2 + B_k^i x_k^i + C^i$$

with an **appropriate fit** of **paraboloid coefficients**

- ✓ **Numerically efficient**
- ✓ **Thermodynamically-consistent**

Diffuse filtering scheme for **spectral** methods :

$$\mathcal{F} \cdot \rightarrow \Psi(\mathbf{k}) \mathcal{F} \cdot \quad ; \quad \Psi(\mathbf{k}) = \frac{1}{2} \left(1 - \tanh \left(\frac{|\mathbf{k}| - k_{cutoff}}{\xi} \right) \right)$$

Fully implicit numerical scheme :

- First order in time
- Picard fixed-point iteration
- Adaptive time step

Light-weight thermodynamically-consistent reduction to ternary systems

Alloying elements: numerically expensive

%Fe	%C	%Cr	%Mo	%Ni	%V	%Mn	%Si
bal.	0,29	1,3	1,02	0,66	0,29	0,74	0,09

form same precipitates

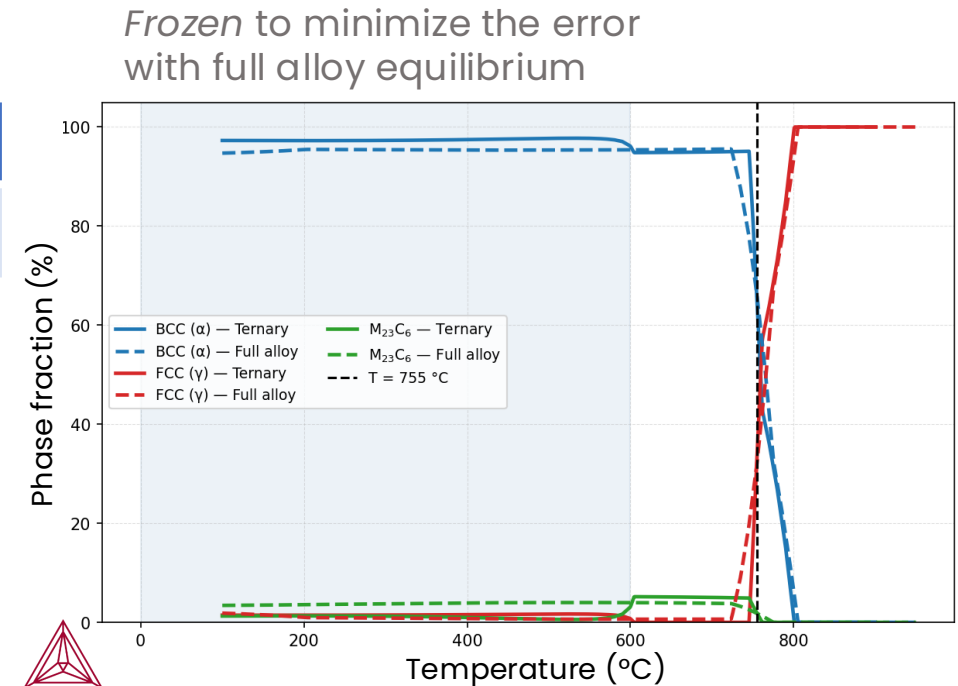
appear in frozen precipitates during aging

Ternary-equivalent alloying elements: ^[6]

%Fe	%C	%Cr
bal.	0,29	1,8444

$$\%Cr_{eq} = \%Cr + 0.533 \%Mo$$

$$\%C_{eq} = \%C$$



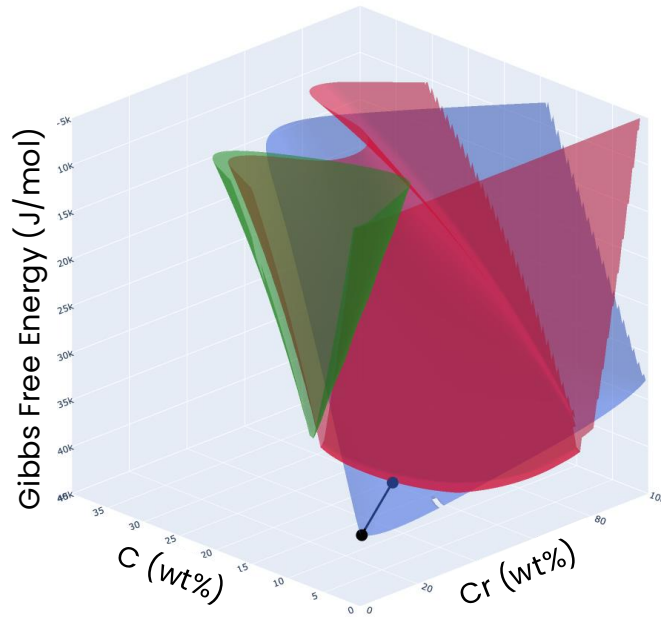
T=550°C is a target temperature



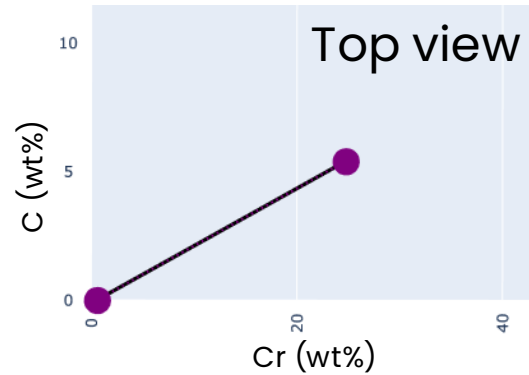
[6] G. Bryndza, R. Eloudrhiri et al. (To appear...) (2026)

Constrained least-square fit to recover thermodynamic phase equilibria

Thermo-Calc Gibbs Energy

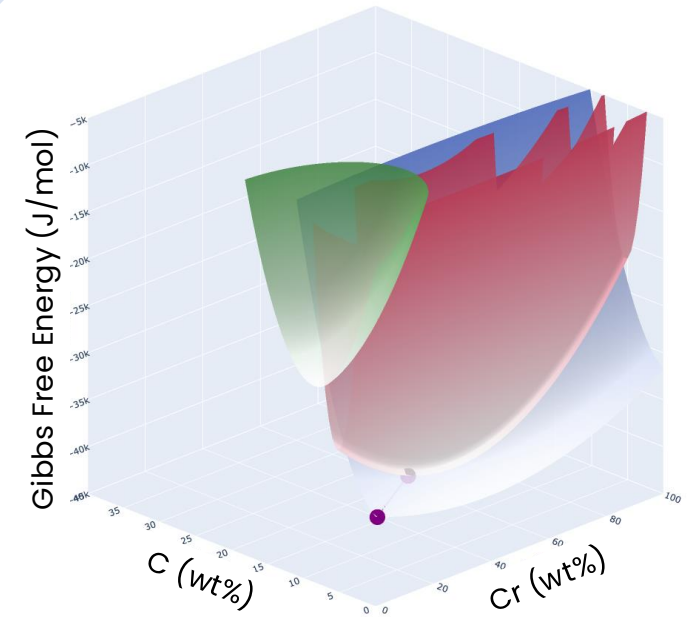


Constrained on the tie-line



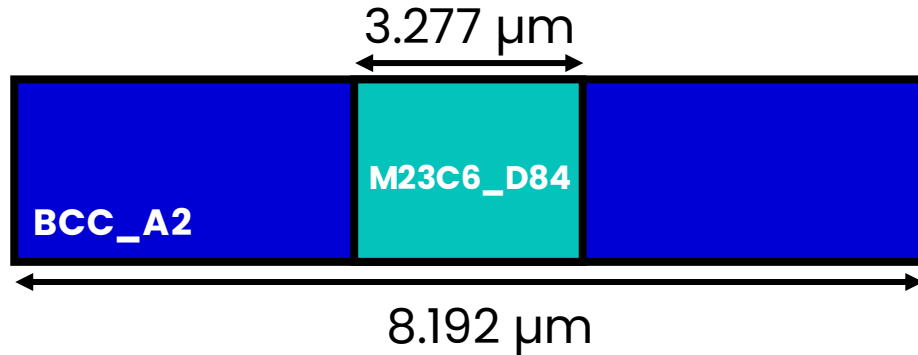
→ Both tie-line **overlap**

Parabolic Gibbs Energy

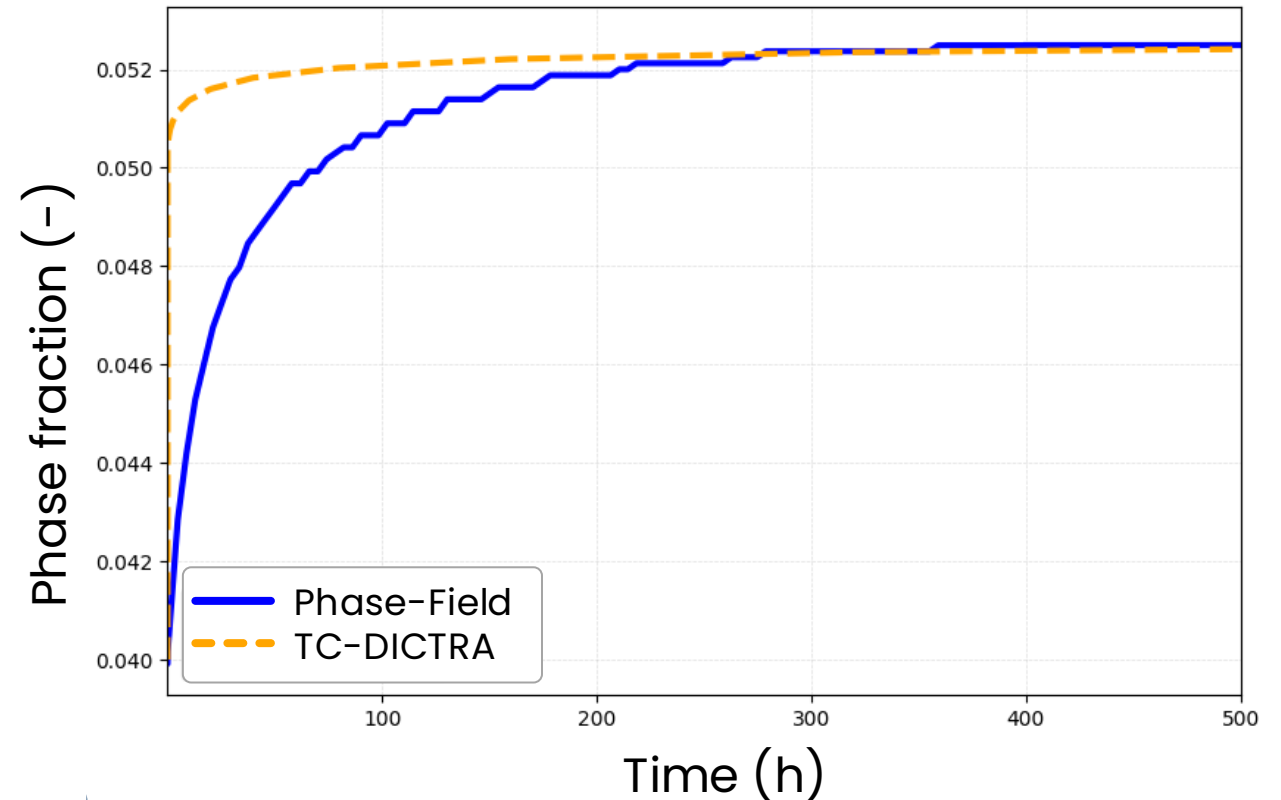


Simulated phase fractions closely match with reference equilibrium fractions

1D system at $T=650^{\circ}\text{C}$:

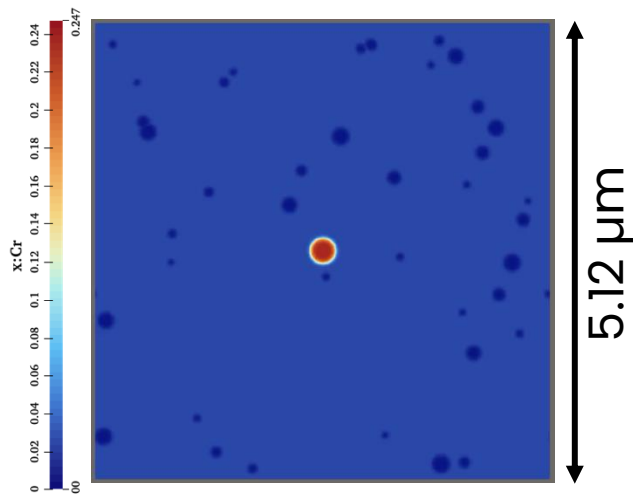


- ✓ Thermodynamic equilibrium
- ✗ Inconclusive kinetics

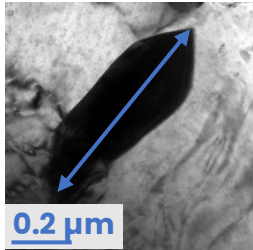
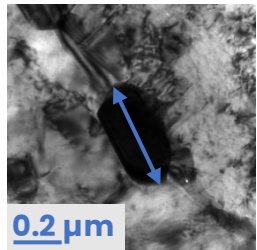


Coarsening kinetics compared against TC-PRISMA simulation

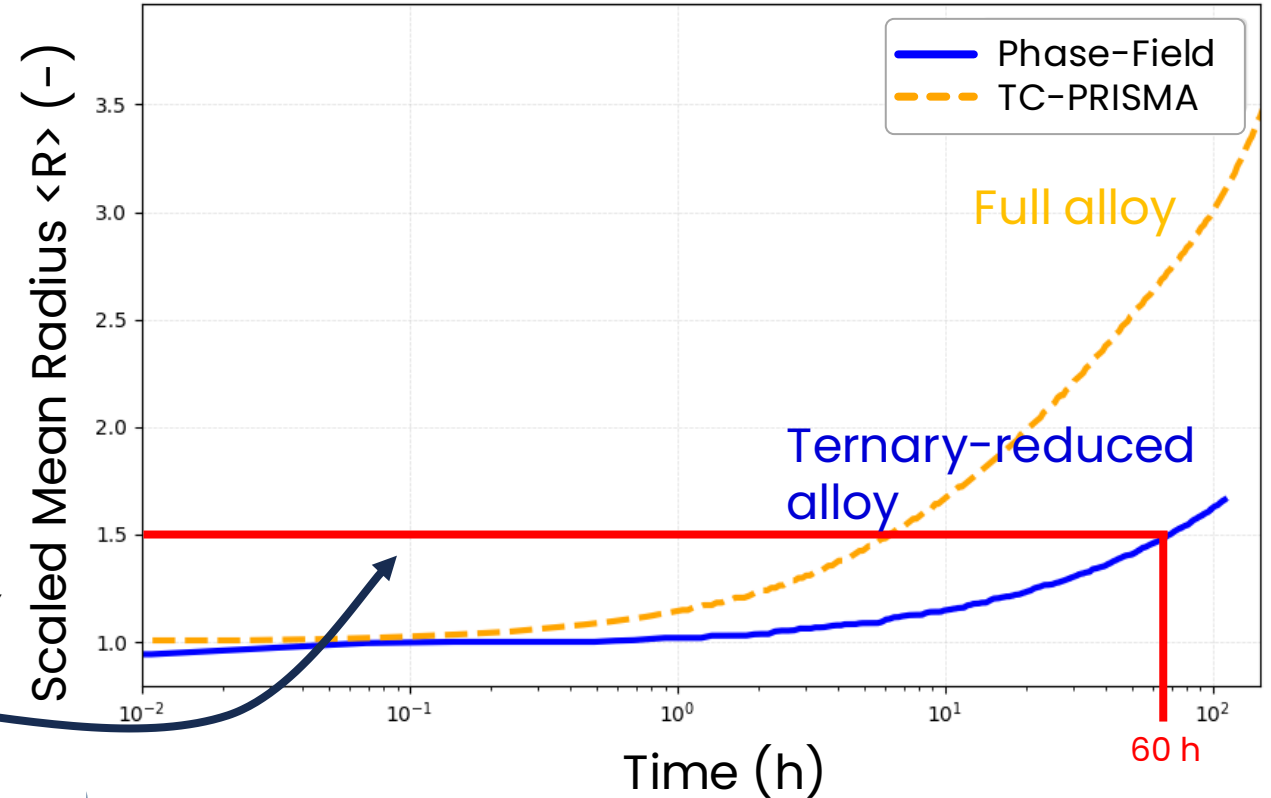
2D Microstructural evolution at $T=550^{\circ}\text{C}$:



v.s. 
TCFE12, MOBF8



Experimental^[7] observation "reveals" **x1.5** size increase after 60h @ 550°C



 [7] AID4Greenest European Horizon Project

Perspectives of this work

Physically-grounded source of microstructural information for creep prediction

**Richer
microstructural
descriptors**

- Morphology
- Relate to micrographs

**Easy access to
multiscale**

- Stronger coupling
(no blackbox)

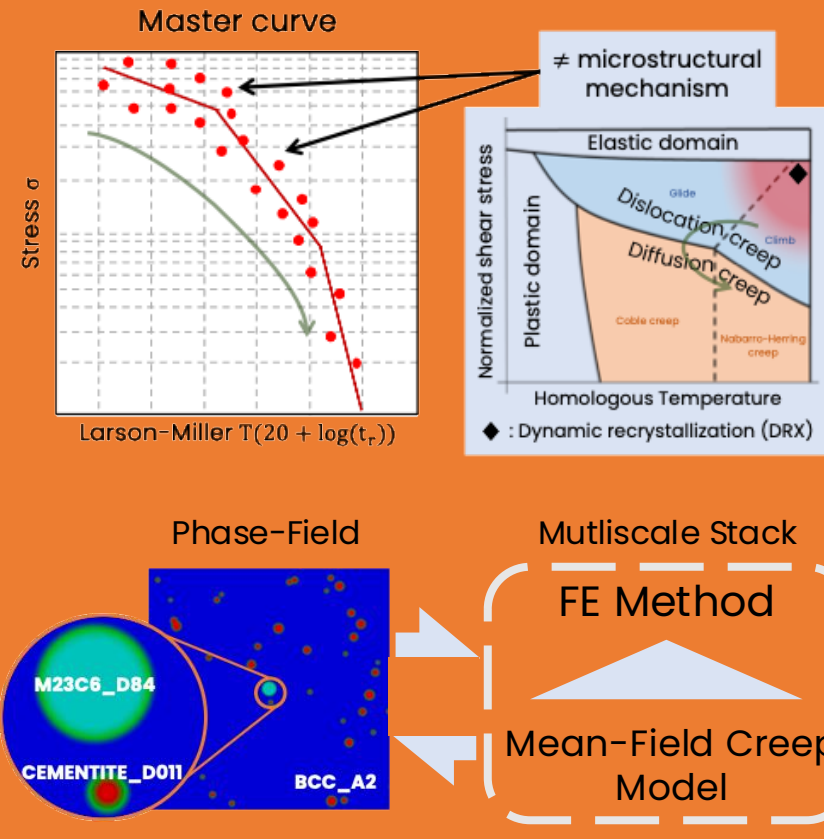
Future physics

- Mechanical coupling
- Nucleation
- Vacancy current

Scale Bridging Creep : a Summary



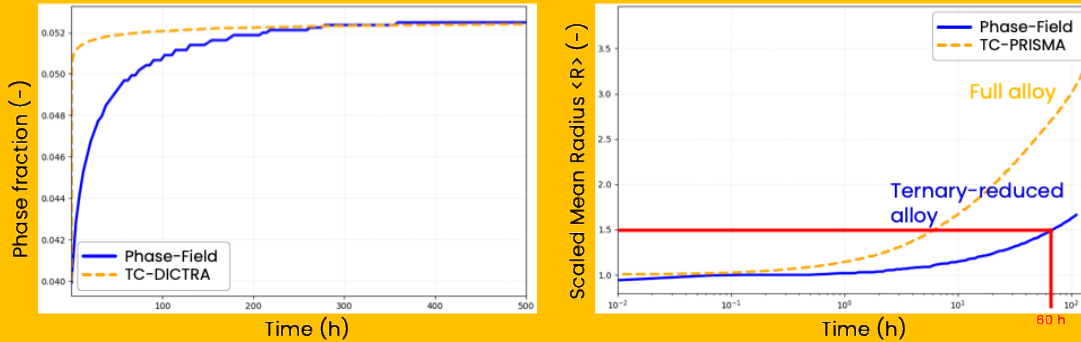
Context, motivation and goals



Reduction to $\text{Fe-C}^{\text{eq}}\text{-Cr}^{\text{eq}}$

$$f^i(\mathbf{x}^i) = \sum_k A_{k,k}^i (x_k^i)^2 + B_k^i x_k^i + C^i \longleftrightarrow$$

Validation and comparison



Perspectives

Physically-grounded source of microstructural information for creep prediction

Connect with me



r.eloudrhiri@uliege.be

www.uee.uliege.be/msm

Scale Bridging Creep

Thank you for your attention!