

P111: Mean-field modeling of the creep deformation response of alloy 1.4959 addressing precipitate kinetics

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Summary

High temperature creep deformation of austenitic steel alloys is accompanied by a complex process of microstructure evolution induced by internal and environmental factors. Processes such as aging and corrosion (i.e., ripening and precipitation of primary and secondary precipitates) result in non-conventional creep hardening and softening trends that are found beyond the limitations of conventional creep models. In this work, a mean-field creep model adapted to recover the non-classical creep response of austenitic steel 1.4959 alloy is formulated, implemented and validated. The microstructure evolution is considered in terms of precipitate kinetics, and is evaluated by means of ex-situ CALPHAD simulations conducted in ThermoCalc TC-PRISMA. This approach allows to recover the creep hardening and softening effects attributed to phenomena such as solid-solution hardening, precipitate strengthening and precipitate damage accumulation. The numerical implementation of the model follows a fully-implicit 1-level Newton-Raphson resolution algorithm. Physical parameters are obtained from either literature or in-house experiments, whereas fitting parameters are optimized to fit the creep response observed during our creep experimental campaign. Creep curves obtained using the validated set of parameters show reasonable accuracy with experiments. Further extrapolation of results is physically consistent, and reliability is limited to loading regimes sharing the same creep mechanisms. An additional phenomenological cavitation damage formulation is implemented to achieve accurate fracture prediction.

Key Words

Dislocation forest density, Dislocation creep, Solid-solution hardening, Non-classical creep behavior, Incoloy 800H, Thermo-Calc PRISMA

Introduction

Creep life assessment of metallic components required to withstand mechanical loads in high temperature environments is a key design step. Conventional stress-temperature-time to rupture charts such as Larson-Miller parameter (LMP) or Mason-Haferd parameter (MHP) remain a popular choice due to their simplicity and applicability for many alloys. However, these extrapolation methods assume that the creep properties of the material in evaluation remain constant throughout their entire evaluation time. In reality, the macro-mechanical creep resistance of alloys is the result of latent and transient properties of the material [1]. Examples of the latter are, for instance, microstructural effects induced by aging or corrosion in alloy 1.4959 [2]. Otherwise known as Incoloy 800H or Steel X8NiCrAlTi 32-31 [3], it is a popular Fe-Ni-Cr alloy that has seen widespread use in high-temperature applications such as pigtail lines [4, 5] and high-temperature reactors in nuclear power plants [6]. Studies on its creep behavior at temperatures below 760°C and medium stresses ($\lesssim 40$ MPa) reveal a classical creep behavior with clear 1st, 2nd and 3rd stages [7, 8]. However, investigations seeking to certify the alloy suitability for higher temperature applications (e.g., manufacturing of very-high temperature

reactors, reaching temperatures up to 980°C, and within relatively low stresses [9, 10]) reported an inconsistent creep behavior characterized by a two-step creep strain rate minima [11, 12, 13]. The first minimum creep rate (mcr#1) is consequence of a solid-solution creep hardening phenomenon attributed to Cr atoms released after the dissolution of intragranular sub-micron sized Cr₂₃C₆ carbides. These precipitates nucleate during the water quenching (WQ) process, and are dissolved upon high-temperature exposure in favor of the nucleation and coarsening of intergranular precipitates of the same kind. The second minimum creep rate (mcr#2) is the actual steady-state creep rate of the alloy, attributed to the equilibrium state reached between the production and annihilation of crystal defects driving creep deformation. This work deals with the development of a dislocation forest density based creep model to achieve accurate creep deformation and service life predictions for alloy 1.4959 within the stress-temperature regimes where non-classical creep behavior is observed. It computes the uniaxial creep strain (ϵ) based on the variation of the mobile, dipole, and boundary dislocation densities (ρ_m , ρ_d and ρ_b , respectively) affected by key microstructural features of the alloy such as mean dislocation wall (DW) size, precipitate kinetics (PK), and creep damage (D_c).

Mean-field creep (MFC) model

The macroscopic creep deformation is calculated as function of the mean density and effective velocity of mobile dislocations. The physical relationship between these quantities is attained by the Orowan equation [14], integrated into the model in Eq. (1a), where $\dot{\epsilon}$ is the plastic (creep) strain rate, ρ_m is the mobile dislocations density, b is the Burger's vector, v_{eff} is the mean effective velocity of mobile dislocations (see [15, 16]), m_T is the Taylor factor.

The rate of change of mobile, dipole and boundary dislocations ($\dot{\rho}_m$, $\dot{\rho}_d$ and $\dot{\rho}_b$, respectively) is calculated after Eq. (1b), Eq. (1c) and Eq. (1d). Each equation term represents a physical phenomena entitled to a dislocation density rate change. These are grouped and labeled accordingly in the equation system of Eq. (1), where "PD" and "DD" stand for particle-dislocation and dislocation-dislocation interaction.

$$\dot{\epsilon} = \frac{b\rho_m v_{\text{eff}}}{m_T(1 - D_c)} \quad (1a)$$

$$\begin{aligned} \dot{\rho}_m = & \underbrace{v_g \rho_m (\rho_m^{1/2} + \rho_d^{1/2})}_{\text{Frank-Read source}} + \underbrace{v_g \left(\frac{\beta \rho_d R_{\text{DW}}}{h_{\text{DW}}^2} - \frac{\rho_m}{2R_{\text{DW}}} \right)}_{\text{Production \& pile-up at DW}} + \underbrace{v_g \left(\frac{\rho_d}{2r_i} - \frac{\rho_m}{\lambda_{\text{eq}}} \right) + v_c \left(\frac{\rho_d}{\lambda_{\text{eq}}} + \frac{\rho_d f_v b}{r_i} \right)}_{\text{PD interaction}} \\ & - \underbrace{v_g \left(\frac{\rho_m}{h_{\text{DN}}} \right)}_{\text{DD interaction}} - \underbrace{v_g \delta_{\text{anh}} \rho_m^2 + \rho_m \rho_d}_{\text{Dynamic \& static recovery}} - v_c 8 \rho_m^{3/2} \end{aligned} \quad (1b)$$

$$\begin{aligned} \dot{\rho}_d = & \underbrace{v_g \frac{\rho_m}{2R_{\text{DW}}} - v_c \frac{\rho_d}{h_{\text{DW}}}}_{\text{Production \& pile-up at DW}} + \underbrace{v_g \left(\frac{\rho_m}{\lambda_{\text{eq}}} - \frac{\rho_d}{2r_i} \right) - v_c \left(\frac{\rho_d}{\lambda_{\text{eq}}} + \frac{\rho_d f_v b}{r_i} \right)}_{\text{PD interaction}} \\ & + \underbrace{v_g \frac{\rho_m}{h_{\text{DN}}}}_{\text{DD interaction}} - \underbrace{v_g \delta_{\text{anh}} \rho_m \rho_d}_{\text{Dynamic recovery}} \end{aligned} \quad (1c)$$

$$\dot{\rho}_b = v_c \left[8(1 - 2\xi) \frac{\rho_d}{h_{\text{DW}}} \right] \quad (1d)$$

An in-depth explanation of each of the parameters and variables contained within Eq. (1) is found beyond the scope of this ECCC26 abstract. Nevertheless, a detailed summary of these modeling aspects can be found in [17].

Thermo-Calc® integration

Physically accurate information on the precipitate kinetics of alloy 1.4959 was attained by means of ex-situ thermokinetic simulations in Thermo-Calc® PRISMA module using with TCFE13 and MOBFE8 databases. Isothermal (stress free, pure aging) thermokinetic simulations were conducted at temperatures ranging from 700°C to 1050°C. The precipitate kinetics quantity (i.e., number density and mean radius) of primary precipitates (Cr₂₃C₆ and Ti(C,N) nucleating at grain boundaries, grain edges, grain corners and dislocations), was then loaded into the model in the form of *.csv files. The right precipitate kinetic quantity is then calculated by means of a temperature and time-dependent linear interpolation as seen in Figure 1a. An example of the interpolation procedure is illustrated in Figure 1b, where the number density of Cr₂₃C₆ at 950°C interpolated between 900°C and 1000°C is compared to Thermo-Calc® results.

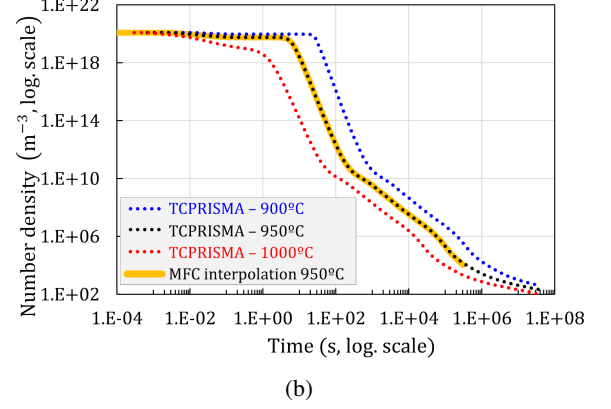
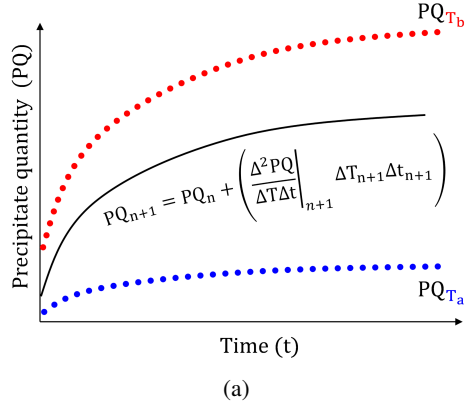
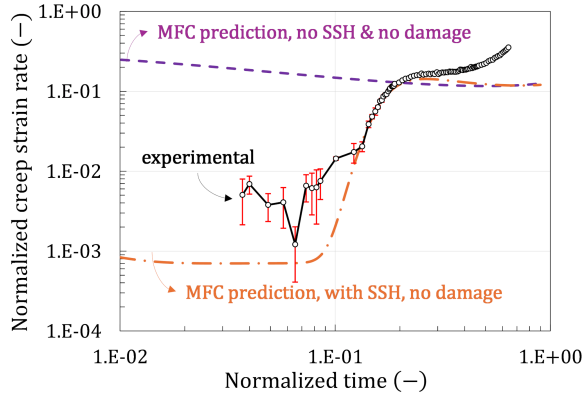


Figure 1: (a) Illustration showcasing the time-temperature interpolation method implemented into our MFC model to calculate precipitate kinetic quantities (mean radius and number density) from ex-situ thermokinetic Thermo-Calc® PRISMA simulations. (b) Verification of interpolation method approach accuracy; the time-dependent number density of Cr_{23}C_6 carbides nucleating at dislocations calculated by MFC interpolation between 900°C and 1000°C is compared to the actual thermokinetic (TCPRISMA) data for the same temperature. The interpolated 950°C curve shows remarkable resemblance to that computed by TCPRISMA.

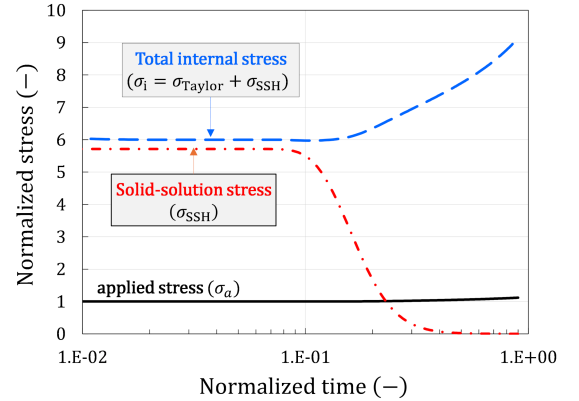
Results

Solid-solution hardening

The prediction of the SSH stress (σ_{SSH}) contribution to the initial (σ_i) is achieved by integrating a kink-pair formation Arrhenius-type formulation that represents the probability of dislocations moving forward as function of the applied stress (σ_a) while in presence of obstacles, generating an opposite contribution ($\sigma_i = \sigma_{\text{Taylor}} + \sigma_{\text{SSH}}$). The integration of the SSH formulation enables the prediction of two creep strain rate minima, located approximately at 2×10^{-3} and 2×10^{-1} respectively in the normalized creep strain rate scale shown in Figure 2a. Figure 2b showcases the σ_{SSH} contribution to the internal stress history ($\sigma_i = \sigma_{\text{SSH}} + \sigma_{\text{Taylor}}$, where σ_{Taylor} is the Taylor stress).



(a) Experimental normalized creep strain rate vs. time curve compared to MFC predictions with and without solid-solution hardening.



(b) Normalized solid-solution (σ_{SSH}), Taylor (σ_{Taylor}) and applied (σ_a) stress history calculated for a MFC simulation of the experimental creep test showcased in (a).

Figure 2: Solid-solution hardening (SSH) contribution in the context of (a) the creep strain rate vs. time response and (b) the stress history of a creep test. Both curves have been purposely normalized for confidentiality reasons. Damage is neglected in all simulations for illustrative purposes.

Creep prediction

MFC simulation results for a single temperature and multiple stress levels are compiled in Figure 3. Results displayed in a single plot allow to identify the transitional trend of both minimum creep rates #1 and #2 across the different stress levels. In addition, numerical creep curves σ_6 and σ_8 are found in good agreement with their experimental equivalents. Creep damage in MFC (D_c in Eq. (1a)) considers contributions of two damage mechanisms: cavitation and precipitate coarsening [16]. Creep rupture, signaled with orange crosses in Figure 3, signifies a user-defined creep damage threshold is reached. Rupture predictions of the identified model are found within -5% and +15% of the experimental time-to-rupture within the stress-temperature configuration where non-classical creep responses are observed.

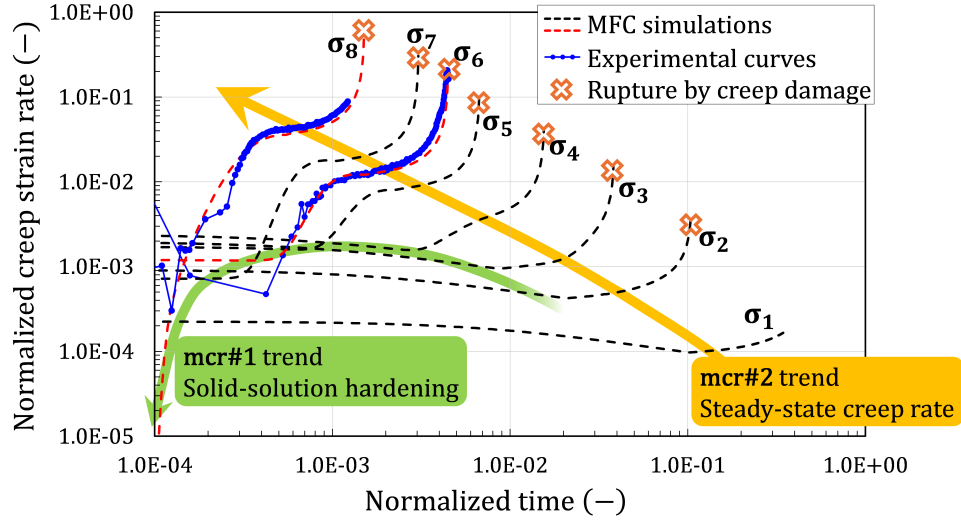


Figure 3: Experimental and numerical normalized creep strain rate vs. time curves showcasing the minimum creep rate trends of alloy 1.4959 for a single temperature and multiple stresses ($\sigma_1 < \sigma_2 < \dots < \sigma_8$). The orange crosses indicate that the simulation stopped after a critical creep damage value (rupture) was reached. Please note that test corresponding to the stress level σ_8 was not conducted until rupture.

Conclusions and prospects

In this work, prediction of the non-classical creep behavior of alloy 1.4959 is achieved via a dislocation-density based creep model. The validated model allows for a physically accurate description of the uniaxial creep strain, damage evolution, and dislocation forest density of the material.

The integration of ex-situ Thermo-Calc® PRISMA thermokinetic simulations information to recover the precipitate kinetics of alloy 1.4959 during creep provides an added layer of physicality while maintaining low computational costs during MFC creep simulations. The feasibility of this approach for other material compositions or the consideration of secondary precipitates is projected.

Exploitation of the model capabilities as a physically accurate inter- and extrapolation tool to complement creep behavior information while shortening experimental campaigns is envisioned.

Acknowledgments

All ULiège authors acknowledge the financial support of the European project AID4Greenest HORIZON-CL4-2022-RESILIENCE-01-19. In addition, Carlos Rojas-Ulloa acknowledges the FNRS FRIA grants B1 4000-8987 and B2 4002-1907 and as Research Director F.R.S. - FNRS, Anne Marie Habraken acknowledges the F.R.S. - FNRS (Fonds de la Recherche Scientifique, Belgium, Walloon Region). Víctor Tuninetti and all ULiège authors acknowledge the international research cooperation agreement WBI/AGCID 2023-2025 RI-02 (DIE23-001).

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