A Coupled Computational Welding Mechanics and Physics-Based Damage Modeling for Prediction of Remaining Useful Life in Welded P91 Alloy

Mahyar Asadi¹*, Jun Zhao⁵, Avi Banerjee³, Leijun Li⁴

Abstract:

Loss of creep resistance in post-weld P91 alloy occurs mainly due to the change in grain size as well as residual stress from the welding process. Post-weld heat treatments can partially improve the creep life, however it remains important to determine the remaining useful life (RUL) particularly in the heat-affected zone under actual service operating conditions. Most creep damage models have focused on the short term creep response at relatively high temperature and stress, where the deformation mechanism is governed by power-law creep (PLC). However, under the actual service temperature and stress (i.e. about half of the melting point) grain-boundary sliding (GBS) is the dominant deformation mechanism that contributes to the creep life. In this paper, a validated deformation mechanisms map (DMM) using low temperature creep strain accommodation processes i.e. GBS, is developed for P91 alloy that predicts the creep rates over a wide range of temperature and stress including those arising under in the actual service conditions. These creep rates are further utilized into a microstructure-based creep damage model for accurate life prediction. A 3D transient computational welding mechanics (CWM) modeling of a pipe in a super-critical water loop, predicts the thermal, microstructure and stress state from welding. It also determines the coarse and fine grain heat affected zone (CGHAZ & FGHAZ). The CWM results are coupled with physics-based creep damage modeling to predict the RUL under the actual service conditions considering the welding residual stress and microstructure states.

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Introduction

Complex engineering alloys that are used for high temperature applications such as P91 and Other CSEF (Creep Strength Enhanced Ferritic) Alloys, are typically precipitation-hardened and their grain boundaries are also strengthened using selective precipitation mechanisms. Their grain sizes are also carefully controlled. The primary objective of using these microstructural design concepts is to optimize their high temperature yield strength as well as creep properties. P91 is widely used in power plants for the last two decades for which time and temperature dependence of creep strain accumulation and formation of a creep crack are the main design criteria used in practice for this class of materials.

The creep deformation is essentially a time dependent and thermally activated plastic strain accumulation processes that are controlled by the competition between the activation energies associated with different mechanisms such as dislocation glide and climb within the grain interiors (Power-Law Creep - PLC) or at the grain boundaries (GBS) or stress assisted vacancy migration leading to grain boundary migration (diffusion creep). All of these processes occur at the atomic scale over time and often lead to time dependent plastic strain accumulation at stresses that are well below the temperature dependent yield strength of the material. Typical constitutive equations that have been developed for different creep deformation mechanisms for simple metals and alloys including some complex alloys are summarized in Table 1.

<table>
<thead>
<tr>
<th>Mechanisms</th>
<th>Rate Equation ([\varepsilon] [s^{-1}])</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dislocation Climb</td>
<td>(\varepsilon = A \Delta \frac{G_b}{kT} \left( \frac{\sigma}{G} \right)^n)</td>
<td>(A \approx 10^6)</td>
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<tr>
<td></td>
<td></td>
<td>(n=4.5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(G = ) Shear Modulus</td>
</tr>
<tr>
<td>Diffusional Creep</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nabarro-Herring (Bulk)</td>
<td>(\varepsilon = BD \frac{G_b}{kT} \left( \frac{\sigma}{G} \right))</td>
<td>(B \approx 30)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Threshold\ Stress \approx 10^{-7}G)</td>
</tr>
<tr>
<td>Coble (Grain Boundary)</td>
<td>(\varepsilon = CD \left( \frac{D_{GB}}{\sigma} \right) \left( \frac{\sigma}{G} \right))</td>
<td>(C \approx 30)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(B \approx 30)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Threshold\ Stress \approx 0.2G)</td>
</tr>
<tr>
<td>Ashby-Verrall (Diffusional Accommodated Flow)</td>
<td>(\varepsilon = FD \frac{1}{kT} \left( \frac{\delta}{d} \right)^2 \left( \frac{\sigma - \sigma_1}{\sigma_d} \right) \left[ 1 + \frac{\delta}{\delta_d} \left( \frac{D_{GB}}{\delta} \right) \right])</td>
<td>(F \approx 100)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Threshold\ Stress \approx 0.05G)</td>
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<tr>
<td></td>
<td></td>
<td>(\delta = GB) thickness</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\sigma_1 = \frac{6\pi E^2}{\delta})</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\Gamma = GB) free energy</td>
</tr>
<tr>
<td>Grain Boundary Sliding</td>
<td></td>
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<tr>
<td>Controlled by GB Diffusion</td>
<td>(\varepsilon = HD \frac{G_b}{kT} \left( \frac{\sigma}{G} \right)^2 \left( \frac{\sigma - \sigma_1}{\sigma_d} \right)^2)</td>
<td>(H \approx 8 \times 10^5)</td>
</tr>
<tr>
<td>Controlled by Lattice Diffusion</td>
<td>(\varepsilon = LD \frac{G_b}{kT} \left( \frac{\sigma}{G} \right)^2 \left( \frac{\sigma - \sigma_1}{\sigma_d} \right)^2)</td>
<td>(L \approx 10^7)</td>
</tr>
<tr>
<td>Hapert-Dorn</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Complex Engineering Alloy (GBS in Presence of Precipitates)</td>
<td>(\varepsilon = A D \frac{G_b}{kT} \left( \frac{\sigma}{G} \right)^q \left( \frac{\lambda}{b} \right)^q \left( \frac{\sigma - \sigma_{\text{min}}}{\sigma_{\text{min}}} \right)^q)</td>
<td>(A \approx 10^6)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(q = 1) (without particles)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(q = 2) (discrete particles)</td>
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<tr>
<td></td>
<td></td>
<td>(q = 3) (continuous network of particles)</td>
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<tr>
<td></td>
<td></td>
<td>(\lambda : ) interlodge spacing</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(r : ) average particle size</td>
</tr>
</tbody>
</table>

Table 1 Variety of Creep Mechanisms and Formula
Frost and Ashby [1] developed a superposition method for combining different rate equations where one mechanism contributes dominantly to the total creep rate at a given stress and temperature while other mechanisms play a less significant role. This led to the development of a Deformation Mechanisms Map (DMM) which is a diagram that plots normalized stress and temperature and that divides the two dimensional stress and temperature space into different regions in which a specific deformation mechanism is dominant. Different creep strain rate contours are further superimposed on this space to provide a sense of strain rates over which a specific mechanism may dominate during the deformation process. Mohammad and Langdon [2] created their own version of a DMM arguing that GBS, as opposed to Coble type diffusion creep, is likely to dominate at lower stresses because the overall energy barrier required for substantial grain boundary migration is quite large. Koul and Castillo [3] conducted extensive creep testing on IN738LC turbine blade material with a grain size of 1.5 mm and microstructural studies on crept specimens and modified the DMM for a Ni-base superalloy by incorporating a GBS regime in a typical Ashby type DMM. The transition between the PLC and GBS is obtained using experimental Power-Law Breakdown (PLB). Koul et. al. distinguished that that the GBS is the dominant mechanism within the practical range of land based and aircraft turbine operation [4]. They further included an interface reaction controlled diffusion creep regime into the map assuming that, if diffusion creep is operative at very low stresses, the grain boundaries cannot act as perfect sources or sinks for vacancies in complex engineering alloys [5]. Wardsworth et. al. [6] have analyzed a vast amount of creep data that was available on different engineering alloys and concluded that GBS, as opposed to diffusion creep, was the dominant deformation mechanism in complex engineering alloys at lower stresses [7]. Recently, Banerjee et. al. [8] attempted to further subdivide the GBS dominant regime in a Ashby type DMM for a Pb-Sn eutectic solder alloy where the GBS region is further divided into two regions based on the dominance of different GBS accommodation processes. It distinguished that GBS is accommodated by w-type cracking below 0.5 T_m (melting temperature in [K]) whereas creep cavitation accommodation process is dominant above this temperature. Kassner and Hayes [9] explained that creep fracture can occur by w or wedge-type cracking at grain boundary triple points. Waddington et. al. [10] summarized two modes of GBS that one mode suggests w-type cracks form most easily at higher stresses, lower temperature and larger grain sizes when grain boundary sliding is not accommodated. Another mode of GBS has been associated with r-type irregularities or cavities that involves migration of vacancies and voids along the boundary. Diffusion helps transporting along the grain boundary and elevated temperature facilitates the r-type process [11]. The wedges may be brittle in origin or simply an accumulation of r-types voids [12]. These edge cracks may propagate only by r-type void formation [13]. Crack can occur in material from pre-existing flaws, fatigue, corrosion related processes and porosity [14] and [15]. This contrasts the case where cracks form as part of creep or by w-type cracking. Cavity nucleation mechanisms fall into four main categories [9]; a) sliding leading to cavitation from ledges and triple points, b) cavity nucleation from vacancy condensation at a high stress region, c) cavity nucleation from a Zener-Stroh mechanism i.e. a dislocation pile-up [16], and d) the formation of a cavity from a particle-obstacle in conjunction with other mechanisms. Our proposed template of DMM is illustrated in Figure 1 and this is the guide used in constructing DMM for P91 in this paper.
Constructing DMM for P91

The construction of a practical DMM using numerical techniques requires the availability of long as well as short term creep test data in order to obtain the correct numerical output with respect to the experimental data over a wide range of temperatures and stress conditions. It is not sufficient to perform expedited creep tests at higher temperatures alone where creep rates are dominated with PLC. As a minimum, experimental creep data should be available in both PLC and GBS regimes to capture the transition between PLC and GBS which is Power Law Breakdown (PLB). The practical range of temperatures and stresses in the case of P91 is limited to a small region in GBS and the PLB regime. W-type cracking at the grain boundaries and grain boundary cavitation (r-type) are the main GBS strain accommodation processes in P91. A collection of reliable high temperature mechanical properties on P91 including creep rate is generated by CanmetMATERIALS [17]; and minimum creep strain rate vs. applied stress for different temperature level are shown in Figure 2 taken from [17].
A superimposition model of creep strain rate that combines single-region strains namely, grain boundary sliding (GBS), dislocation glide, and power-law creep (PLC) are used in a computational algorithm scheme to construct DMM. There are constant coefficients that are calibrated to obtain the best agreement with the experimental data shown in Figure 2. The result is a validated P91 DMM presented in Figure 3.

Determining Remaining Useful Life (RUL)

Determining the remaining useful life (RUL) of an engineering component, in damage tolerance analysis, is frequently performed by accumulation of time to crack nucleation and time to crack growth until dysfunctional length. Reliability of RUL, however, has recently shown that depends on short crack propagation [18] i.e. a transition stage between crack nucleation and governing crack growth, which is also the most significant stage in safe life prognostics (Eq. 1). Analyzing either fatigue [19], creep [20], or mixed mode needs different algorithms to calculates each term of the equation based on governing physics of its own.

\[
RUL = \text{Crack Nucleation} + \text{Short Crack Propagation} + \text{Long Crack Growth} \tag{1}
\]

This paper concerns creep life prediction of a P91 pipe (OD 20 [cm]) including calculation of all terms in Eq 1 under operational temperature 700 [K] inside a super critical water loop pipe as well as non-uniform stress distribution including combined residual stress from welding and 1 [MPa] operational stress in super critical water loop condition for this pipe with thickness 2.54 [mm] welded in two passes; root and cap weld pass. The typical failure location of creep for this pipe is well-known to be in inter-critical heat affected zone (ICHAZ) in fine grain region close to the welding line that helps us to compare
the predicted failure location with reported equivalent. This study is not simplified as the uniform uniaxial specimen test but uncomplicated enough to develop a reliable methodology for determining RUL in welded structures while dealing with residual stress from welding.

### Computational Weld Modeling

Using VrWeld, a full 3D transient computational welding mechanics (CWM) modeling of the pipe in a super-critical water loop, predicts the thermal, microstructure and stress state from welding to couple with physics-based creep damage modeling to predict the RUL terms under the actual service conditions considering the welding residual stress and evolution of microstructure states. Mesh and weld cross-section are shown in Figure 4 including root and cap pass. The CWM modeling summary is below;

\[
\dot{h} + \nabla \cdot (-\kappa \nabla T) + Q = 0
\]  \hspace{1cm} (2)
Where \( h \) is the specific enthalpy, the super imposed dot denotes the derivative wrt to time, \( k \) is the thermal conductivity, \( T \) is the temperature, and \( Q \) is the power per unit volume or the power density distribution. The initial temperature was 300 K. The power density distribution function \( Q \) [\text{w/m}^3] ‘Double Ellipsoid’ heat source model of Goldak [21] was used and the heat source parameters were \( a_1 = 3 \) [mm], \( a_2 = 15 \) [mm], \( b = 15 \) [mm], and \( c = 15 \) [mm] for root pass and \( a_1 = 4 \) [mm], \( a_2 = 12 \) [mm], \( b = 4 \) [mm], and \( c = 2 \) [mm] for cap pass. A convection boundary condition generated a boundary flux \( q \) [\text{w/m}^2] on all external surfaces. This flux is computed from Eq. 3 with convection coefficient temperature dependent \( h_c \) given Eq. 4 and ambient temperature of \( T_{ambient} = 300 \) K.

\[
q = h_c(T - T_{ambient}) \tag{3}
\]

\[
h_{c(Steel)} = 5 + 0.05(T - 300) + 6 \times 10^{-7}(T - 300)^3 \quad \text{[w/m}^2 \text{K]} \tag{4}
\]

The time step length while welding was chosen so that one time step was required to travel one element along the weld path i.e. 8.7 [mm]. Filler metal was added as the welding arc moved along the weld path, i.e., the FEM domain changed in each time step during welding. After each weld pass was completed, the time step length was increased exponentially by a factor of 1.2 per time step during the cool down. The computation involved 154 welding time steps plus 45 cool down time steps. Figure 5 illustrates a snapshot of the transient temperature field when the cap weld passes half way the second layer weld path to fill the gap.

![Figure 5 transient temperature when the cap weld passes half weld path.](image)

**Stress Simulation**
The stress solver solves the conservation of momentum equation (Eq. 5) using the elasticity tensor $D$ as a 6x6 matrix, the body force $b$ and the Green-Lagrange strain $\varepsilon$.

$$\nabla \cdot \sigma + b = 0$$

$$\sigma = D\varepsilon$$

$$\varepsilon = (\nabla u + (\nabla u)^T + (\nabla u)^T \nabla u)/2$$  \hspace{1cm} (5)$$

This partial differential equation was solved for a visco-thermo-elasto-plastic stress-strain relationship using radial return theory and algorithms [22]. The initial state is assumed to be stress free. The Dirichlet boundary conditions is the so-called “Add-to-Diagonal” or “Spring-to-Ground” along the axial direction. If a Spring-to-Ground or Add-to-Diagonal with stiffness coefficient $K$ is stretched with a displacement $dx$, it increases the work of deformation $(dx K dx)/2$. This stabilizes the structure in the sense that it requires work and hence force to stretch the spring along the axial direction of pipe. The system is solved using a time marching scheme with time step lengths used for thermal analysis. Figure 6 illustrates the displacement (in [mm] and visual magnified 50x) at the end of welding (right) and in the transient state of thermal shown in Figure 5 (left).

**Figure 6** Displacement (magnified 50x) at the end of welding (right) and in transient state of thermal shown in Figure 5 (left)

**Figure 7** illustrates Residual stress (effective stress) at the end of welding (right) and in the transient state of thermal shown in Figure 5 (left). Other stresses such as longitudinal, transverse, normal, or principal stresses cane be similarly obtained.
The 3D map of welding residual stress shown in Figure 7 (right) is scaled based on empirical relation developed at the University of Alberta to reflect the post weld heat treatment (PWHT) required by code; and this stress is combined by operational stress (1 [MPa]) at operational temperature (700 [K]) to generate 3D map of the stress that causes the creep deformation during course of service.

**Determining Crack Nucleation Life**

The computational algorithm that constructs the validated DMM for P91 alloy (Figure 3) is integrated with CWM model to read 3D thermal and stress results in order to predict the creep rates over a wide range of temperature and stress including those arising under in the actual service conditions from the 3D CWM results. Additional to stress state, the DMM algorithm requires the local or nodal state of average grain size, average precipitant particle size, and average precipitant particle inter-spacing that are show effective in creep life of engineering alloys. Figure 8 shows the 3D map of these parameters computed based on peak temperature location on different region of the alloy’s phase diagram and typical experimental observation at the University of Alberta’s P91 experience. The 3D map of crack nucleation life is determined as shown in Figure 9.
Determining Long-Crack Growth Life

Map of crack nucleation life (Figure 9) suggests the critical location for crack to start which is the nucleation shortest life. Fracture mechanics uses stress intensity factor (SIF or K) and fracture toughness (K_{IC}) to determine the time to fracture, and J-integral is an FEM-based technique to calculate K when crack size (a) grows. A crack size 0.5 [mm] i.e. ten times the grain size, is introduced to the critical location of crack nucleation and J is calculated from stress state from the CWM simulation, then converted to K using $K = \frac{EJ}{\sqrt{(1-v^2)}}$ where E, J, and v are modulus of elasticity, J-integral, and Possion ratio respectively. A crack block analysis is shown in Figure 10 that presents the state of stress in crack length 1.5 [mm] introduced to the critical location from nucleation life analysis. The process repeated for crack size 1.5 [mm] and the K plot is shown vs. crack size ,a, in Figure 11.
Potential drop technique is a common method to experimentally measure the creep crack growth rate \((da/dt)\) vs SIF at given temperature. In this paper, \((da/dt)\) vs SIF experimental data is taken from [23] that is measured at 1273 [K] i.e. dash line in Figure 13. Since the operating temperature is 700 [K] therefore the experimental data is adapted from 1273 [K] to 700 [K] i.e. solid line in Figure 13 using Eq 6 where A, K, & m are coefficients of creep rate equation at 1273 [K], \(Q = 30000\) [cal/mol], \(R = 1.987\) [cal/K/mol] the gas constant, and T is new temperature equal to 700 [K] in our case.

\[
\frac{da}{dt} = A (\Delta K)^m \exp\left[-\frac{Q}{R} \left(\frac{1}{T} - \frac{1}{1273}\right)\right]
\]  

(6)
Integration of rate equation over time results in 1136 days for crack to growth to 1.5 [mm] which is about 60% of the thickness. That is too long to be plausible and indicates the importance of using short-crack growth rate in lieu of long crack rate formula when the crack length is less than 10 times the grain size.

**Determining Short-Crack Growth Life**

A term is added (Eq. 7) to the typical Paris-Law creep rate equation to update the rate when it is below 10 times the grain size. In this Eq. the $g$ is grain size, $a$ is crack length, and $\alpha$ is an adjusting parameter which is equal to 1 in most cases. The effect of the new term can be compared in Figure 14 against Figure 13.

\[
\frac{da}{dt} = A [\Delta K \exp(\alpha \frac{g}{a})]^m
\]  
(7)
Time integration of the new equation (Eq. 7) results in 75 days for crack to grow to 1.5 \text{ [mm]} or 60\% of the thickness. Therefore, a realistic life prognostics needs short-crack life prediction and our proposed relationship can be used; however there is a further development to add more microstructure terms in it since the short-crack is microstructurally local phenomena and affected greatly by the local state of material.

**Conclusion**

In this work, a coupled computational welding mechanics (CWM) and physics-based damage modeling for prediction of Remaining Useful Life (RUL) in welded P91 alloy is proposed and a test case implemented. A material physics based DMM has been constructed over wide range of stresses and temperatures and calibrated to P91 alloy by using experimental creep rate data including GBS and PLC, PLBD mechanisms. In the next step, a complete CWM analysis of a typical welded P91 pipe operating under a super-critical loop service condition has been performed to generate the 3D map of stress state including welding residual stress, PWHT recovery, and combined stress. The evolution of microstructure parameters namely, average grain size, average precipitant particle size, and average precipitant particle inter-spacing, during welding has also been computed from 3D transient thermal results from welding. The service operating conditions and the microstructural properties as well as the post-weld stress states were used for physics-based damage modeling to estimate the remaining useful life (RUL) of the typical welded P91 pipe. At first operation dependent fracture critical locations were estimated and then state-of-the-art damage tolerance analysis was applied with Finite Element Analysis to provide time to crack nucleation, time to long-crack growth, and short-crack growth (less than 10 grain size) until a selected dysfunctional length. The result shows synergy of the CWM and physics-based damage modeling to compute the fracture critical locations and RUL, as well as provide analytical support to reduce maintenance cost through optimal weld inspection, repair and replacement.

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**References**


