Accepted Manuscript

Prediction of prior austenite grain growth in the heat-affected zone of a martensitic steel during welding

L. Shi, S.A. Alexandratos, N.P. O'Dowd

PII: S0308-0161(18)30162-5
DOI: 10.1016/j.ijpvp.2018.08.005
Reference: IPVP 3746

To appear in: International Journal of Pressure Vessels and Piping

Received Date: 11 May 2018
Revised Date: 7 August 2018
Accepted Date: 18 August 2018

Please cite this article as: Shi L, Alexandratos SA, O'Dowd NP, Prediction of prior austenite grain growth in the heat-affected zone of a martensitic steel during welding, International Journal of Pressure Vessels and Piping (2018), doi: 10.1016/j.ijpvp.2018.08.005.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.
Prediction of prior austenite grain growth in the heat-affected zone of a martensitic steel during welding

L. Shi, S. A. Alexandratos, N. P. O’Dowd*

School of Engineering, Bernal Institute, University of Limerick, Limerick V94 T9PX, Ireland

Abstract
Engineering components operating at high temperature often fail due to the initiation and growth of cracks in the heat-affected zone (HAZ) adjacent to a weld. The size and morphology of the prior austenite grains (PAGs) in the HAZ of a tempered martensite steel weld can have a strong influence on the final martensitic microstructure. However, there are few available models to predict PAG size in the HAZ of martensitic steel welds. In this work two approaches are examined to predict PAG growth in the HAZ of a martensitic steel (P91) weld. Phase field (PF) methods, which explicitly represent the changing morphology of a representative volume of martensite grains, and approximate analytical solutions for grain growth at high temperature are examined. The predicted grain growth kinetics and final grain diameter using a two term analytical solution is shown to agree well with experimental data and with the validated PF simulation. The two term analytical model provides a versatile tool to analyse PAG growth at low computational costs. In addition, a simplified equation for predicting the final PAG diameter in the HAZ of P91 welds is proposed for engineering applications. The methods have been used to estimate the final grain diameter in the HAZ of a single bead-on-plate weld.

Keywords: Martensitic steel, Prior austenite grain growth, Welding thermal cycle, Heat-affected zone, Grain growth modelling

*Corresponding author
Email address: Noel.ODowd@ul.ie (N. P. O’Dowd)

Preprint submitted to International Journal of Pressure Vessels and Piping August 21, 2018
1. Introduction

Engineering steels, such as modified 9Cr-1Mo-V-Nb (P91) steel, widely used in high temperature piping and steam headers in power plant, have optimised microstructures to enhance their operating performance [1, 2, 3]. However, thermo-mechanical process (e.g. welding and associated post weld heat treatment) may significantly change the original microstructure of the base material, leading to microstructural degradation and premature failure of components [4, 5]. It is reported that crack initiation has been observed mainly in the heat-affected zone (HAZ) of P91 welds [6, 7, 8].

The welding thermal cycle induces many changes in the final microstructure of the HAZ in a welded joint [9, 10, 11, 12]. In particular, for martensitic steels, prior austenite grain (PAG) size and morphology determine the martensite start temperature and the final martensite microstructure and have a significant influence on welding-induced residual stresses [13, 14]. The HAZ of a P91 weld is divided into a number of sub-zones depending on the peak temperature, \( T_p \), reached during welding in these regions [15, 16]: coarse-grain (CGHAZ, \( T_i \leq T_p < T_s \)), fine-grain (FGHAZ, \( A_{c3} \leq T_p < T_i \)) and intercritical (ICHAZ, \( A_{c1} \leq T_p < A_{c3} \)), where \( T_s \) is the solidus temperature (= 1773 K for P91), \( A_{c1} \) is the temperature at which transformation from martensite to austenite starts during heating (= 1063 K for P91), \( A_{c3} \) is the temperature at which transformation from martensite to austenite is completed during heating (= 1193 K for P91) and \( T_i \) is an intermediate temperature to be discussed in Section 2.2 (= 1373 K for P91).

There are numerous models for predicting the thermal field during welding [17, 18] and numerous models for predicting the influence of microstructure on thermo-mechanical properties [19, 20]. However, to make full use of such models, it is necessary to develop relevant microstructure evolution models to link process–microstructure–property models as shown in Figure 1. Such a multi-scale multi-physics modelling scheme would make it possible to integrate welding process models, microstructure evolution models and structural deformation models for process parameter optimization and ultimately component lifetime prediction. The application of multi-scale multi-physical simulations to develop process-microstructure-property models to aid in process optimisation and microstructure design has been reported [21, 22]. In [21], a combined phase-field and finite-element model has been used to analyse the process-microstructure-property relations in a Ni-base superalloy. In [22] an overview of multi-scale multi-physics modelling
of process–microstructure–property–performance relationships in additive manufacturing has been given.

Figure 1: Multi-scale modelling framework to facilitate process–microstructure–property predictions for materials design and process optimization [21]. (a) process model [22], (b) microstructure evolution model [24], (c) property prediction model [20].

Several methods have been developed to simulate temperature-driven grain growth in the HAZ of a welded joint, such as the Monte-Carlo (MC) method [25, 26, 27], the cellular automata (CA) method [28, 29] and the phase field (PF) method [9, 30]. The MC and CA methods provide very flexible frameworks to study microstructural changes in materials. However, both methods are implemented by considering a time-dependent probability of grain growth due to the thermal history. For these models the real time of the physical system is not considered, due to the probabilistic nature of the techniques [31, 32]. Thus, it is difficult to scale the numerical time step of these methods to the physical time, particularly in non-isothermal grain growth studies where time dependence is important and the time increment may vary throughout the analysis [30, 32, 33]. For example, in the MC method for grain growth the experimental data based (EDB) model can be used to relate the dimensionless model simulation time and real physical time, t. Alternatively, an atomistic model or a grain boundary migration model can be used [20]. Thus, the validity of these models depends on the reliability of the models used to establish the relationship.
of the simulation time with the real physical time. The PF method is more suitable for simulation of non-isothermal grain growth and grain morphology in the HAZ since the thermal history can be directly included in the analysis without establishing a relationship between the simulation time with physical time. The overall intention of the work (Figure 1) is to couple microstructure evolution models with constitutive (stress-strain) behaviour using crystal plasticity finite-element approaches. Such approaches have been successfully implemented using a fully coupled PF and FEA [21, 22]. Thus, the PF method seems more suitable for simulation of grain growth and prediction of the grain morphology in the HAZ for multi-scale modelling. However, we would expect that an appropriately calibrated MC/CA model would provide a similar level of accuracy to the PF model used in our work and there has been some success in combining CA models and crystal plasticity FEA models [31]. Analytical solutions for predicting grain growth in HAZ have been reported [34, 35, 36]. In our previous work, application of the existing analytical solutions show poor prediction of grain growth in the HAZ of a precipitation strengthened martensitic steel, such as P91 [24]. This is because the existing analytical solutions do not consider the dissolution of precipitation at high temperature (above 1373 K), which is the determinant factor for final austenite grain size during welding of P91 steel. A modification of these solutions is therefore necessary to allow its application in precipitate strengthened martensitic steels such as P91.

To date, there are limited studies investigating the influence of thermal cycles on PAG growth in the HAZ of P91 welds [24]. Pandey et al. [37, 38] has studied the influence of post-weld heat treatment (PWHT) on microstructure evolution in various zones of gas tungsten arc welded P91 pipe weldments. Austenite grain growth during austenitization in T91 steel has been studied experimentally using a Gleeble thermo-mechanical simulator, which indicates that austenite grain growth was relatively insensitive to heating rate [39]. In [40] a physically-based macroscale thermomechanical model was developed to predict PAG and lath size in P91 welds, based on a grain growth model used in the annealing process [41]. However, grain morphology and grain growth kinetics cannot be captured explicitly using this type of macroscale model. Recently, Shi et al. [24] have employed the finite element method in conjunction with the PF method to predict grain growth in the HAZ of a single bead-on-plate weld geometry. However, the effects of welding thermal cycle parameters (i.e., heating and cooling rate, peak temperature) on grain growth kinetics have not been quantitatively studied. Furthermore,
as it is computationally expensive and time consuming to use PF method to analyse grain growth kinetics, alternative methods are required to meet the demands of industry and academia to develop a full understanding of grain growth in the HAZ of precipitate strengthened martensitic steels. In the current work, three methodologies have been proposed for predicting prior austenite grain growth in the HAZ of a martensitic steel to aid in process optimisation. The influence of the heating rate, peak temperature and cooling rate on grain growth in the HAZ of a P91 steel is quantified using PF simulation in conjunction with a macroscale analytical solution. A modification of an existing macroscale grain growth model is proposed to account for the precipitate dissolution in P91 steel during welding. In addition, a simplified equation is proposed to predict the dependence of PAG size in the HAZ on thermal history. The PF method, the modified two term analytical solution and the simplified equation are calibrated and validated from independent experimental data.

2. Methods for predicting grain growth

2.1. Welding thermal cycle

Figure 2 shows a typical welding thermal cycle at a material point calculated by finite element analysis for a single bead-on-plate geometry [23, 42]. During welding, the heating rate and cooling rate of the thermal cycle vary with time, making it difficult to quantitative analyse which factors (i.e., heating and cooling rate, peak temperature) determine the final grain size and morphology in welding. To quantify the effects of the welding thermal cycle on PAG growth in the HAZ, the ‘real’ welding thermal cycle predicted numerically or measured experimentally may be simplified using linear approximations, as shown in Figure 2. The heating rate, \( \dot{T}_h \), and cooling rate, \( \dot{T}_c \), are defined as the absolute values of the slope of the ‘simplified’ thermal cycle at the heating stage and cooling stage, respectively. Thus, the linear approximated thermal history, \( T(t) \), in the austenization zone during heating from \( A_{c3} \) to its peak value, \( T_p \), at time \( t_p \) is expressed as,

\[
T(t) = A_{c3} + \dot{T}_h t
\]

where

\[
\dot{T}_h = \frac{T_p - A_{c3}}{t_p},
\]

5
is the heating rate. Similarly, the temperature during the cooling stage from $T_p$ to $A_{c3}$ over time $t_f$ is expressed as,

$$T(t) = \frac{(\dot{T}_h + \dot{T}_c)T_p - \dot{T}_c A_{c3}}{\dot{T}_h} - \dot{T}_c t$$  \hspace{1cm} (3)

where

$$\dot{T}_c = \frac{T_p - A_{c3}}{t_f - t_p}, \hspace{1cm} (4)$$

is the cooling rate.

Figure 2: A schematic of a ‘real’ welding thermal cycle and its linear approximation to represent the welding thermal history. The heating rate, $\dot{T}_h$, peak temperature, $T_p$, and cooling rate, $\dot{T}_c$ (both positive numbers) are defined as indicated in the figure.

It should be noted that the heating and cooling rate are linearised to simplify the analysis of the effects of heating and cooling rate on final grain size and morphology. This linearisation of the thermal history is a reasonable approximation for the typical heating and cooling rates observed during welding, as shown in Section 3.3. It should also be pointed out that thermal histories with varying heating and cooling rate can be implemented in the PF simulation and the two term analytical solution, as in Section 3.3.
2.2. Phase field simulation

The PF method for simulation of grain growth in HAZ during welding has been described in our previous work [24], and there are numerous works on PF simulation of grain growth at constant temperature [43, 44, 45]. Thus, only the important relevant aspects of the method are reviewed here. The PF method is based on the so-called phase field parameter which in the current context represents each individual grain. In the case of grain growth, the driving force in the PF model is the minimisation of the total interfacial energy. The evolution equation for the phase field parameters are then given by [30],

\[
\dot{\phi}_i = \sum_{j \neq i} \mu \sigma \left[ (\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j) + \frac{\pi^2}{2\eta^2} (\phi_i - \phi_j) \right],
\]

where \(\phi_i\) and \(\phi_j\) are the phase field parameter for grain \(i\) and \(j\), respectively; \(\eta\) is the grain boundary thickness, which in this work is taken as 0.6 \(\mu\)m, \(\sigma\) is the grain boundary energy and is taken as 0.24 J/m\(^2\), and \(\mu\) is the grain boundary mobility, which is temperature dependent and can be expressed using the following Arrhenius relationship [24],

\[
\mu = \mu_0 \exp \left( -\frac{Q}{RT} \right),
\]

where \(Q\) is the activation energy, \(R\) is the universal gas constant and \(\mu_0\) is a pre-exponential factor.

It is reported that at temperatures above 1373 K, the pre-existing precipitates (e.g., \(M_23C_6\) carbides and MX carbonitrides) in P91, which act to pin the grain boundaries, are completely dissolved into the austenite matrix [46, 47]. This results in an increase in the rate of grain growth above this temperature and the development of fine grain \((T_p < 1371\) K) and coarse grain \((T_p > 1373\) K) regions in the HAZ. In order to account for precipitate dissolution at high temperatures, two regimes are therefore considered when calibrating Eq. 6 [24]. Data from Gleeble simulated welds for P91 [5] have been used to calibrate Eq. 6 and the constants, \(Q\) and \(\mu_0\) for the two temperature regimes, are provided in Table 1. It is noted that the activation energy at low temperature is lower than that in the case of high temperature which is consistent with the result of Toloui and Militzer [30]. This is because the activation energy \(Q\) does not have explicit temperature dependence but is related to the interfacial energy density through the microstructure [30]. The
interfacial energy density is high for fine grained structures (which occur at low temperatures in our analysis) while it is low for coarse grain structures (which occur at high temperatures). With high interfacial energy density the system is unstable, in other words, it is easy to mobilise the grain boundaries. Therefore, the activation energy $Q$ at low temperature will be low. The converse argument applies at high temperatures when the microstructure is coarse grained. However, we should point out that because the grain mobility term is of the form $\exp(-Q/RT)$, overall grain mobility is lower at low temperatures.

Table 1: Calibrated data of grain boundary mobility (Eq. 6) in the PF simulation for P91 [24], $T_t = 1373$ K.

<table>
<thead>
<tr>
<th>Units</th>
<th>$T &lt; T_t$</th>
<th>$T \geq T_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q$ kJ/mol</td>
<td>170</td>
<td>225</td>
</tr>
<tr>
<td>$\mu_0$ m$^2$/J/s</td>
<td>$2.42 \times 10^{-4}$</td>
<td>$2.10 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

2.3. Two term analytical solution

A widely used analytical model for predicting grain growth in metals comes from the classical relationship for isothermal grain growth [34, 35, 36, 48, 49],

$$d^n - d_0^n = k_0 \exp\left(-\frac{Q_s}{RT}\right) t.$$  (7)

Here $d_0$ and $d$ are the initial and final grain diameters, respectively; $k_0$ is a kinetic constant, $t$ is the time at temperature $T$, $n$ is the time exponent and $Q_s$ is the activation energy for grain boundary motion. The similarity between Eq. 7 and Eq. 6 is noted, both have the Arrhenius form, but the terms in the two equations are different. This analytical model can be applied to a thermal cycle by dividing the temperature history into discrete isothermal steps [49, 50]. Grain growth at each isothermal time step is then calculated using the isothermal relationship, and overall growth obtained by summing over the thermal cycle,

$$d^n - d_0^n = k_0 \sum_{i=0}^{t_f} \exp\left(-\frac{Q_s}{RT_i}\right) \Delta t_i,$$  (8)

where $\Delta t_i$ is the time at temperature $T_i$ and $t_f$ is the total time for grain growth. With a continuous thermal cycle (e.g. in a weld), Equation 8 can
be rewritten as follows,

\[ d^n - d^n_0 = k_0 \int_0^{t_f} e^{\exp \left( -\frac{Q_s}{RT} \right)} \, dt. \]  

(9)

Previous work has shown that a single set of thermal kinetic parameters (i.e., \( n \), \( k_0 \) and \( Q_s \)) cannot simultaneously predict the grain size in the FGHAZ and CGHAZ for this precipitation strengthened P91 steel [24]. Thus, as for the PF model, we consider two regimes for Eq. (9) to account for different precipitate pinning regimes, depending on whether the temperature is above or below \( T_t \) (1373 K). As for the PF model, the model parameters have been fitted to the data of [5] for a simulated P91 weld and are summarised in Table 2. A higher value of \( k_0 \) and lower value \( Q_s \) are used to take into account increased grain growth rate above \( T_t \), due to the dissolution of precipitates into the austenite matrix. The other model parameters are independent of temperature.

Table 2: Calibrated thermal kinematic parameters of analytical solution (Eq. 7), \( T_t = 1373 \) K.

<table>
<thead>
<tr>
<th>Units</th>
<th>( T &lt; T_t )</th>
<th>( T \geq T_t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q_s ) kJ/mol</td>
<td>( Q_{s1} = 66.6 )</td>
<td>( Q_{s2} = 53.9 )</td>
</tr>
<tr>
<td>( k_0 ) m(^n)/s</td>
<td>( k_{01} = 2.5 \times 10^{-10} )</td>
<td>( k_{02} = 3.0 \times 10^{-10} )</td>
</tr>
<tr>
<td>( n )</td>
<td>2.2</td>
<td></td>
</tr>
<tr>
<td>( R ) J/mol/K</td>
<td>8.314</td>
<td></td>
</tr>
<tr>
<td>( d_0 ) ( \mu )m</td>
<td>5.0</td>
<td></td>
</tr>
</tbody>
</table>

2.4. Simplified equation

It may be seen that only the integral term on the right hand side of Eq. 9 is temperature/time dependent. We have integrated the temperature/time dependent term using Maple [51, 52], providing a near-closed form analytical solution, apart from the incorporation of an exponential integral term. The detailed derivation of the simplified equation can be found in Appendix A. The equation for grain size, \( d \) in the FGHAZ (\( T_p < T_t \)) is summarised as,

\[ d = \left[ d_0^n + k_{01} \left( f(T_p) - f(A_{c3}) \right) \right]^{\frac{1}{n}} \]  

(10)

and the equation for grain size in the CGHAZ (\( T_p \geq T_t \)) is,

\[ d = \left[ d_0^n + k_{01} \left( f(T_t) - f(A_{c3}) \right) + k_{02} \left( g(T_p) - g(T_t) \right) \right]^{\frac{1}{n}}. \]  

(11)
The functions $f$ and $g$ in Equations 10 and 11 depend on the relevant temperature and welding thermal cycle parameters, and are given as follows,

$$f(T) = \left(\frac{T}{T_h} + \frac{T}{T_c}\right) \exp \left(-\frac{Q_{s1}}{RT} - \left(\frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c}\right) Ei \left(\frac{Q_{s1}}{RT}\right)\right), \quad (12)$$

$$g(T) = \left(\frac{T}{T_h} + \frac{T}{T_c}\right) \exp \left(-\frac{Q_{s2}}{RT} - \left(\frac{Q_{s2}}{RT_h} + \frac{Q_{s2}}{RT_c}\right) Ei \left(\frac{Q_{s2}}{RT}\right)\right), \quad (13)$$

where $Ei$ is the exponential integral [53], which can be approximated over the relevant range using the following equation [54],

$$Ei(x) = (A^{-7.7} + B^{-0.13})$$

$$A = \ln \left(\left(0.65 + \frac{0.56146}{x}\right) (1 + x)\right) \quad (14)$$

$$B = x^4 \exp (7.7x)(2 + x)^{3.7}.$$ 

In the above equations, $T_h$ and $T_c$ are the heating rate and cooling rate, defined in Section [2.1] respectively. The other parameters are the same as those in Section [2.3] and their values are summarised in Table 2. Note that functions $f(T)$ and $g(T)$ have dimensions of time and consistent temperature and time units must be used in Eqs. 10, 14.

### 3. Results and discussion

#### 3.1. Phase field modelling results

The solution to Eq. 5 is obtained using an open-source PFM code, OpenPhase [44]. The initial grains are randomly introduced by Voronoi tessellation with the initial mean grain diameter at $A_{c3}$ set to be $5 \, \mu m$ [5, 24]. Figure 3 shows a comparison of the predicted mean grain diameter using the PF method with the measured mean grain diameter for a number of different welding thermal cycles from a Gleeble simulated weld in [5]. The predicted mean grain diameters agree well with the experimental measured data. The maximum difference between the PF simulation and measured data is about 20%, which is reasonable since the experimental scatter from different locations of Gleeble simulated welds is estimated to be about 20% [55].

Figure 4 illustrates the predicted grain evolution during a representative welding thermal cycle with a peak temperature of 1250 °C. Figure 4(a) shows the simplified welding thermal cycle with five time periods identified from a
Figure 3: Comparison of the predicted grain diameter in a P91 simulated weld by phase field (PF) simulation and experimental data from [5] indicated by the symbols. The error bars are to indicate a 20% scatter as estimated by [55].

to e. The corresponding grain morphologies predicted from PF modelling at these five times are shown in Figure 4(b) to 4(f), respectively. Figure 5(a) illustrates the statistical grain diameter distributions with lognormal fitting at those five times and Fig. 5(b) shows the evolution of the mean grain diameter and grain number as a function of time. The initial mean grain diameter in Fig. 4(b) is 5 µm at A_c3 with 3,000 PAGs in a region of 250 µm × 250 µm. The distribution of initial grain are well described by a lognormal distribution with almost 60% of the grains at a diameter of 5 µm as shown in Figure 5(a). The maximum grain diameter is 12 µm. As temperature increases from A_c3 to 1150 °C, the mean grain diameter increases from 5.0 µm to 6.1 µm with the corresponding grain number decreasing from 3,000 to 1,964. Figure 4(d) shows the grain morphology at the peak temperature, the mean grain diameter is 8.3 µm with 1,010 grains in the calculation domain. Thereafter, grain growth continues during cooling from peak temperature to 1150 °C with an increase of the mean grain diameter to 17.5 µm (Figure 4(e) with 219 grains). Figure 4(f) shows a slower grain growth rate below 1150 °C as the grain diameter increases to 20.1 µm while the corresponding grain number decreases to 173. The largest grain at the end of the welding thermal cycle is about 45.5 µm as shown in Figure 4(f) and Figure 5(a).
Figure 4: Prior austenite grain (PAG) evolution during a simplified welding cycle.
Figure 5: (a) Statistical grain diameter distributions with lognormal fit at different times, (b) evolution of mean grain diameter and grain number during welding thermal history from PF simulation. The dash line corresponds to the time at which peak temperature is reached.

Figure 6 shows the final grain diameter distributions with lognormal fit for various welding thermal histories. The distributions for \( \dot{T}_h = 100 \, ^{\circ}C/s \) and \( 400 \, ^{\circ}C/s \) predicted by the PF simulation are shown in Figure 6(a). The peak of the relative frequency decreases from 0.19 to 0.16. The PAG diameter is mainly distributed (relative frequency > 10%) from 12 \( \mu \)m to 28 \( \mu \)m for \( \dot{T}_h = 100 \, ^{\circ}C/s \), while it reduces to a range of 12 \( \mu \)m to 25 \( \mu \)m for \( \dot{T}_h = 400 \, ^{\circ}C/s \). The effect of \( T_p \) on the grain diameter distribution is shown in Figure 6(b). The PAG diameter is mainly distributed from 4 \( \mu \)m to 11 \( \mu \)m at a peak temperature of 1050 \( ^{\circ}C \), while it is distributed from 12 \( \mu \)m to 28 \( \mu \)m at a peak temperature of 1250 \( ^{\circ}C \). Figure 6(c) shows the PAG diameter is mainly distributed from 12 \( \mu \)m to 28 \( \mu \)m at a cooling rate of 15 \( ^{\circ}C/s \), which is decreased to a range of 8 \( \mu \)m to 19 \( \mu \)m at a cooling rate of 50 \( ^{\circ}C/s \). For the cases examined, \( T_p \) is the dominant factor in determining the mean PAG diameter, while the influence of cooling rate, \( \dot{T}_c \), is more significant than heating rate, \( \dot{T}_h \).

3.2. Use of analytical solutions

Figure 7 shows a comparison of the predicted grain evolution in the FG and CGHAZ using PF simulation, the new two term analytical solution and the existing classical analytical solution [24, 49]. The time scale is made non-dimensional by dividing by total time. The existing classical analytical solution (dotted line in Figure 7 and labelled classical analytical solution),
Figure 6: Effects of (a) heating rate, (b) peak temperature and (c) cooling rate on final grain size distributions. The initial grain size distribution is shown in Fig. 5(a).

which is generally used to predict grain growth in material processing such as laser surface melting [49] and heating processes [56], provides a reasonable agreement with the PF simulation. The parameters chosen were those which gave the best overall agreement in the FG and CGHAZ. The two term analytical solution, which calibrates the material parameters to account for different precipitate pinning in the FG and CGHAZ, provides closer agreement with the PF solution, as shown by the dash lines in Figure 7.

Figure 8 shows a comparison of the two term analytical solution with the experimental measured data for P91 from [5] (a similar comparison has been made for the PF method in Fig. 3). This figure summarises results from
six experiments with different thermal conditions, representative of welding conditions. We also use the validated PF simulation results to further validate the two term analytical solution by comparing the grain growth kinetics predicted by PF with two term analytical solution as shown in Figs. 9-10. The predicted grain diameter by the two term analytical solution is generally in agreement with experimental measured data and is of similar quality to that obtained using the PF model.

Figure 7: Comparison of predicted grain evolution in the FGHAZ and CGHAZ using PF simulation, with two term analytical solution and classical analytical solution from [24, 49].

Figure 8: Comparison of the predicted grain diameter by two term analytical solution and experimental data in a P91 simulated weld by a Gleeble simulator from [5].
An important aspect of non-isothermal grain growth studies is to capture the grain growth kinetics during rapid welding thermal cycles that are typical of those experienced in the HAZ [55]. Thus the predictive capabilities of the proposed two term analytical model are examined using our previous proposed validated PF model [24] of grain growth for selected simplified welding thermal cycles. Figure 9 compares the austenite grain growth kinetics calculated using the PF simulation with the proposed two term analytical solution at various welding thermal cycles. Grain growth kinetics for \( T_p = 950 \, ^\circ\text{C} \) (in the FGHAZ), \( T_p = 1100 \, ^\circ\text{C} \) and \( T_p = 1300 \, ^\circ\text{C} \) (in the CGHAZ) at different nondimensional times are shown. As expected, the grain diameter in the CGHAZ (1300 °C) is significant larger than that in the FGHAZ (950 °C) at different welding thermal histories. The analyses show that a limiting grain size is reached at approximately 0.6 of the non-dimensional time (60% of the total time in the austenisation zone) for \( T_p = 1300 \, ^\circ\text{C} \), while a limiting grain size is reached at approximately 0.8 of the non-dimensional time for \( T_p = 1100 \, ^\circ\text{C} \) and 950 °C. The result from the proposed two term analytical solution are in good agreement with the PF simulation data for all welding thermal cycles.

Figure 10 compares the predicted final grain diameter from the two term analytical solution with that from the PF simulation at different values of \( \dot{T}_h \) and \( \dot{T}_c \). It is again seen that the influence of \( \dot{T}_c \) on final grain diameter is more significant than that of \( \dot{T}_h \). Figure 10 also shows a significant increase in the mean grain diameter for \( T_p \) above 1100 °C due to precipitate dissolution [6]. The proposed two term analytical model agrees well with both the experimental results (Figure 8) and the PF simulation results (Figure 9 and 10). Although the model cannot directly predict the grain morphology or grain distribution, it can predict the final grain diameter in the HAZ at negligible computational cost. The proposed simplified equation (Eq. 10 and 11) provides an even simpler engineering solution to predict final grain size based on a simplified (linearised) thermal history. The only inputs are the welding thermal cycle parameters \( (T_p, \dot{T}_h \text{ and } \dot{T}_c) \) which can be determined from the welding thermal cycle, as described in Section 2.1 and 6 material constants, as in Table 2. A comparison between the two term analytical model and the experimental data has been provided in Fig. 8. Figure 11 shows the comparison of the final grain diameter calculated by the two term analytical model and the simplified model for a wide range of thermal histories. The figure shows that the prediction of the final PAG diameter by the simplified equation agrees well with the two term analytical model.
Figure 9: Predicted austenite grain growth kinetics by two term analytical solution and PF simulation (left), and the corresponding predicted grain diameter difference (right) (a) and (b) $\dot{T}_h = 100$ °C/s and $\dot{T}_c = 15$ °C/s; (c) and (d) $\dot{T}_h = 100$ °C/s and $\dot{T}_c = 30$ °C/s; (e) and (f) $\dot{T}_h = 400$ °C/s and $\dot{T}_c = 15$ °C/s.
Figure 10: Predicted final mean grain diameter from the two term analytical solution and from PF simulation at different (a) heating rate and (c) cooling rate. Corresponding comparison of the analytical and simulation results at different (b) heating rate and (d) cooling rate.

Other macroscale grain growth models are available, e.g. [40], [41], which, suitably adapted, can provide a similar agreement with experimental data and PF simulations to that provided by Eq. [9]. The focus in this work is the development of a simplified flexible framework for prediction of grain growth under relatively simple thermal histories for quantitative analyzing the welding thermal histories on grain growth kinetic and the use of Eq. [9] provides an excellent basis for this approach. For a precipitate strengthened martensitic steel such as P91, the initial austenite grain after being fully transformed from martensite at $A_{c3}$ determines the final grain size, while the
primary austenite grain of the parent material, which is also referred as the prior austenite grain, has little effect on the final grain size after welding. In this paper, the initial grain size $d_0$ used in Eqs. 9–11 is the austenite grain size at $A_{c3}$. It has been found that the size of the newly formed austenite grain is not sensitive to heating rate [30]. Thus, the grain size with a peak temperate at $A_{c3}$ measured in [5] is used as the initial grain size in this work.

Figure 11: A comparison of the final grain diameter calculated by simplified equation and two term analytical model for various thermal histories.

3.3. Prediction of grain sizes in the HAZ of a bead-and-plate weld

As a final comparison, Fig. 12 shows the predicted grain diameter in the HAZ of a single bead-on-plate weld during GTA welding of P91 steel predicted by the PF simulation, the two term analytical solution and the simplified equation. The ‘real’ welding thermal cycles predicted by a finite element analysis were used in the PF simulation and the two term analytical solution, while the linearised welding thermal cycle was used in the simplified equation to predict the final grain diameter. The three methods predict similar results. As expected, the final grain diameter decreases with an increase in distance from the fusion boundary since the material near the fusion boundary experiences the highest peak temperature. The final grain diameter in the CGHAZ near the fusion boundary is about three times larger than that in the FGHAZ as shown in Figure [12]. The final grain diameter in the HAZ through the plate thickness (i.e., along $yy'$) shows similar trends
to that along the plate surface (i.e., along \(xx'\)). However, the width of the HAZ along the plate surface is 0.9 mm (Figure 12(a)), which is narrower than that through the plate thickness (1.2 mm, Figure 12(b)). This is because the plate surface (along \(xx'\)) experiences both convection and radiation, leading to a more rapid heat transfer and a reduced surface temperature compared to that through the plate thickness (along \(yy\)). The predicted grain diameter from the simplified equation is smaller than that predicted from the two term analytical solution, particularly in the CGHAZ. This is mainly due to the fact that the temperature for the simplified welding thermal history is lower than the ‘real’ welding thermal cycles, as shown in Figure 2.

Figure 12: Prediction of the grain diameter in the HAZ of a single bead-on plate P91 weld by PF simulation, two term analytical solution and simplified equation. (a) along plate surface (\(xx'\)), (b) along plate thickness (\(yy'\)). The welding direction is normal to the plane shown (in the \(z\) direction).

4. Conclusions

In this paper, the phase field method (PFM), a two term analytical solution and a simplified closed-form equation have been used to predict PAG growth in the heat-affected zone (HAZ) of a P91 steel weld. The models have been calibrated using Gleeble thermo-mechanical simulation data from the literature. The calibrated PFM has been used to analyse the grain growth kinetics during a welding thermal cycle. To avoid the time-consuming PF simulation (a typical 2D PF problem takes 21 hours on a 24 core machine)
A two term analytical solution is proposed. The grain growth kinetics predicted by the validated PF simulation and the two term analytical solution show consistent results. For the cases examined, it has been found that the peak temperature \( (T_p) \) is the most important parameter in determining the final grain size. It has also been found that the effect of cooling rate \( (\dot{T}_c) \) on final grain size is more significant than heating rate \( (\dot{T}_h) \).

The proposed methodologies provide useful tools to predict PAG growth in the HAZ of P91 for different welding thermal histories. The methods can be easily extended to analyse grain growth in other materials which experience a similar thermal history such as post weld heat treatment. Further work on linking the microstructure evolution model with models for predicting thermomechanical behaviour is required in order to obtain quantitative information for optimising welding process parameters as well as predicting and controlling the mechanical properties of welded joints.

**Acknowledgments**

This work was funded by Science Foundation Ireland (SFI) under Grant No. 14/IA/2604. The modelling work was supported by the Irish Centre for High-End Computing (uleng050b). The authors are grateful to Dr Oleg Shchyglo of the Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany for useful discussions on implementing the OpenPhase code. Helpful discussions with Mr Edward Meade and Dr Fengwei Sun of the Bernal Institute at University of Limerick, Ireland; Dr Richard Barrett, Prof Sean Leen, Mr Ming Li, and Prof Padraic O’Donoghue of National University of Ireland, Galway; and Dr David Allen, Mr Bartosz Polomski and Mr Rod Vanstone of the IMPEL project team are gratefully acknowledged.

**Appendix A. Derivation of the simplified equation for predicting grain diameter**

The thermal history from an experimental measurement or numerical simulation is simplified by linear approximations during heating and cooling as described in section 2.1. Figure A.13 shows a schematic of the linear approximated thermal history in the FGHAZ and CGHAZ. The grain growth equation is,

\[
d^n = d_0^n + \int_0^t \exp \left( -\frac{Q_s}{RT} \right) dt
\]

(A.1)
where $d_0$ and $d$ are the initial and final grain diameter, respectively, $k_0$ is the kinetic constant, $t$ is the time at temperature $T$, $n$ is the time exponent and $Q_s$ is the activation energy. Calibration of the constants $k_0$ and $Q_s$ are divided into two regimes to account for different precipitate pinning during welding thermal history. Separate equations are derived to describe grain growth in these two regions which correspond to the FGHAZ and CGHAZ regions.

**A1. FGHAZ (peak temperature is lower than $T_t$)**

We consider the heating and cooling stage separately and evaluate the total grain growth over the whole welding thermal cycle.

**A1.1. Heating stage**

The linear approximated thermal history during heating from $A_{c3}$ to its peak value ($T_p$) over time $t_1$ can be expressed as Eq. 1. Substituting into the integral term in Eq. (A.1), that the kinetic growth term of Eq. (A.1) can be expressed as,

\[
A_{h1} = \int_{0}^{t_1} k_0 \exp \left( -\frac{Q_{s1}}{RT} \right) dt \\
= k_0 \int_{0}^{t_1} e^{\exp \left( -\frac{Q_{s1}}{R \left( A_{c3} + \bar{T}_h t \right)} \right)} dt
\]  

(A.2)
Solving Eq. A.2 using Maple software [51, 52],

\[
A_{h1} = k_{01} \left\{ \left( t + \frac{A_{c3}}{T_h} \right) \exp \left[ -\frac{Q_{s1}}{R \left( A_{c3} + T_h \right)} \right] - \frac{Q_{s1}}{R T_h} E_i \left[ \frac{Q_{s1}}{R \left( A_{c3} + T_h \right)} \right] \right\} \bigg|_{t=0}^{t=t_1}
\]

(A.3)

where \( E_i \) is the exponential integral [53], which can be approximate evaluated using Eq. 14 [54]. Substituting Eq. 1 into Eq. A.3 leads to,

\[
A_{h1} = k_{01} \left[ \left( \frac{T_p}{T_h} \right) \exp \left( -\frac{Q_{s1}}{RT_p} \right) - \frac{Q_{s1}}{RT_h} E_i \left( \frac{Q_{s1}}{RT_p} \right) \right] \bigg|_{T=T_p}^{T=A_{c3}}.
\]

(A.4)

The final expression of the kinetic growth term during heating can be obtained as follows,

\[
A_{h1} = \int_{t_1}^{t_2} k_{01} \exp \left( -\frac{Q_{s1}}{RT} \right) \, dt
\]

\[
= k_{01} \int_{t_1}^{t_2} \exp \left[ -\frac{Q_{s1}}{R \left( T_b - \dot{T}_c t \right)} \right] \, dt.
\]

(A.7)

A1.2. Cooling stage

Similarly, the thermal history during cooling is expressed in Eq. 3. Let

\[
T_b = \frac{\left( \dot{T}_h + \dot{T}_c \right) T_p - \dot{T}_c A_{c3}}{T_h}.
\]

Then Eq. 3 can be rewritten as,

\[
T(t) = -\dot{T}_c t + T_b
\]

(A.6)

and the kinetic growth term of Eq. A.1 for the cooling stage can be expressed as,

\[
B_{c1} = \int_{t_1}^{t_2} k_{01} \exp \left( -\frac{Q_{s1}}{RT} \right) \, dt
\]

\[
= k_{01} \int_{t_1}^{t_2} \exp \left[ -\frac{Q_{s1}}{R \left( T_b - \dot{T}_c t \right)} \right] \, dt.
\]
where \( t_1 \) and \( t_2 \) are defined in Fig. A.13.

Solving Eq. A.7 using Maple software, the final expression of the kinetic growth term during cooling can be obtained as follows,

\[
B_{cl} = k_{01} \left[ \left( \frac{A_{c3}}{T_c} \right) e^{\left( -\frac{Q_{s1}}{RA_{c3}} \right)} + \frac{Q_{s1}}{RT_c} Ei \left( \frac{Q_{s1}}{RA_{c3}} \right) \right] + k_{01} \left[ \left( \frac{T_p}{T_c} \right) e^{\left( -\frac{Q_{s1}}{RT_p} \right)} - \frac{Q_{s1}}{RT_c} Ei \left( \frac{Q_{s1}}{RT_p} \right) \right]
\]  

(A.8)

From Eq. A.1, Eq. A.5 and Eq. A.8, the grain growth kinetic equation can be expressed as follows,

\[
d^n = d^n_0 + A_{h1} + B_{cl}
\]

\[
= d^n_0 + k_{01} \left[ \left( \frac{T_p}{T_h} + \frac{T_p}{T_c} \right) e^{\left( -\frac{Q_{s1}}{RT_p} \right)} - \left( \frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c} \right) Ei \left( \frac{Q_{s1}}{RT_p} \right) \right] - k_{01} \left[ \left( \frac{A_{c3}}{T_h} + \frac{A_{c3}}{T_c} \right) e^{\left( -\frac{Q_{s1}}{RT_C} \right)} - \left( \frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c} \right) Ei \left( \frac{Q_{s1}}{RT_C} \right) \right]
\]  

(A.9)

Define a function which is expressed as,

\[
f(T) = \left( \frac{T}{T_h} + \frac{T}{T_c} \right) e^{\left( -\frac{Q_{s1}}{RT} \right)} - \left( \frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c} \right) Ei \left( \frac{Q_{s1}}{RT} \right)
\]  

(A.10)

Then, Eq. A.9 can be expressed as,

\[
d = [d^n_0 + k_{01} (f(T_h) - f(A_{c3}))]^\frac{1}{n}
\]  

(A.11)

The above Eq. A.11 is the final equation for predicting the grain diameter in the FGHAZ. It is dependent on welding thermal history parameters (i.e., heating rate, cooling rate and peak temperature).

A2. In CGHAZ (peak temperature is higher than \( T_t \))

A2.1. Heating stage

The peak temperature in the CGHAZ is greater than \( T_t \), thus the integral of the kinetic term in heating stage is divided into two regions: \( A_{c3} \leq T < T_t \).
and $T_i \leq T < T_p$. The kinetic term during heating from $A_{c3}$ to $T_t$ over time $t_1$ can be expressed as follows,

$$A_{h1} = k_{01} \int_0^{t_1} e^{x} \left[- \frac{Q_{s1}}{R \left(A_{c3} + \dot{T}_h t \right)} \right] dt. \quad (A.12)$$

That is,

$$A_{h1} = k_{01} \left[ \left( \frac{T}{T_h} \right) e^{x} \left(- \frac{Q_{s1}}{RT} \right) - \frac{Q_{s1}}{RT_h} Ei \left( \frac{Q_{s1}}{RT} \right) \right]_{T=A_{c3}}^{T=T_t}. \quad (A.13)$$

Similarly, the kinetic term during heating from $T_t$ to $T_p$ over time $t_1$ to $t_2$ can be expressed as follows,

$$A_{h2} = k_{02} \left[ \left( \frac{T}{T_h} \right) e^{x} \left(- \frac{Q_{s2}}{RT} \right) - \frac{Q_{s2}}{RT_h} Ei \left( \frac{Q_{s2}}{RT} \right) \right]_{T=T_t}^{T=T_p}. \quad (A.14)$$

That is,

$$A_{h2} = k_{02} \left[ \left( \frac{T_t}{T_h} \right) e^{x} \left(- \frac{Q_{s2}}{RT_t} \right) - \frac{Q_{s2}}{RT_h} Ei \left( \frac{Q_{s2}}{RT_t} \right) \right]_{T=A_{c3}}^{T=T_p}. \quad (A.15)$$

A2.2. Cooling stage

Similarly, the kinetic term during cooling from $T_p$ to $T_t$ over time $t_2$ to $t_3$ can be expressed as,

$$B_{c2} = k_{02} \left[ \left( - \frac{T}{T_c} \right) e^{x} \left(- \frac{Q_{s2}}{RT} \right) + \frac{Q_{s2}}{RT_c} Ei \left( \frac{Q_{s2}}{RT} \right) \right]_{T=T_p}^{T=T_t} \quad (A.17)$$
Which is,

\[ B_{c2} = k_02 \left[ \left( \frac{T_i}{T_c} \right) \exp \left(-\frac{Q_{s2}}{RT_i} \right) + \frac{Q_{s2}}{RT_c} E_i \left( \frac{Q_{s2}}{RT_i} \right) \right] + k_02 \left[ \left( \frac{T_p}{T_c} \right) \exp \left(-\frac{Q_{s2}}{RT_p} \right) - \frac{Q_{s2}}{RT_p} E_i \left( \frac{Q_{s2}}{RT_p} \right) \right]. \]  

(A.18)

The kinetic term during cooling from \( T_i \) to \( A_c3 \) over time \( t_3 \) to \( t_4 \) can be similarly expressed as,

\[ B_{c1} = k_{01} \left[ \left( \frac{T_i}{T_c} \right) \exp \left(-\frac{Q_{s1}}{RT_i} \right) + \frac{Q_{s1}}{RT_c} E_i \left( \frac{Q_{s1}}{RT_i} \right) \right] + k_{01} \left[ \left( \frac{T_p}{T_c} \right) \exp \left(-\frac{Q_{s1}}{RT_p} \right) - \frac{Q_{s1}}{RT_p} E_i \left( \frac{Q_{s1}}{RT_p} \right) \right]. \]  

(A.19)

Thus, the final grain diameter in the CGHAZ can be expressed as,

\[ d^n = d_{02}^n + A_{h1} + A_{h2} + B_{c2} + B_{c1} \]

\[ = d_{02}^n + k_{01} \left[ \left( \frac{T_i}{T_h} + \frac{T_i}{T_c} \right) \exp \left(-\frac{Q_{s1}}{RT_i} \right) - \left( \frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c} \right) E_i \left( \frac{Q_{s1}}{RT_i} \right) \right] - k_{01} \left[ \left( \frac{A_{c3}}{T_h} + \frac{A_{c3}}{T_c} \right) \exp \left(-\frac{Q_{s1}}{RA_{c3}} \right) - \left( \frac{Q_{s1}}{RT_h} + \frac{Q_{s1}}{RT_c} \right) E_i \left( \frac{Q_{s1}}{RA_{c3}} \right) \right] + k_{02} \left[ \left( \frac{T_p}{T_h} + \frac{T_p}{T_c} \right) \exp \left(-\frac{Q_{s2}}{RT_p} \right) - \left( \frac{Q_{s2}}{RT_h} + \frac{Q_{s2}}{RT_c} \right) E_i \left( \frac{Q_{s2}}{RT_p} \right) \right] - k_{02} \left[ \left( \frac{T_i}{T_h} + \frac{T_i}{T_c} \right) \exp \left(-\frac{Q_{s2}}{RT_i} \right) - \left( \frac{Q_{s2}}{RT_h} + \frac{Q_{s2}}{RT_c} \right) E_i \left( \frac{Q_{s2}}{RT_i} \right) \right]. \]  

(A.20)

Define a function which is expressed as,

\[ g(T) = \left( \frac{T}{T_h} + \frac{T}{T_c} \right) \exp \left(-\frac{Q_s}{RT} \right) - \left( \frac{Q_s}{RT_h} + \frac{Q_s}{RT_c} \right) E_i \left( \frac{Q_s}{RT} \right). \]  

(A.21)

Then, Eq. (A.20) can be rewritten by using Eq. (A.10) and (A.21) as follows,

\[ d = \left[ d_{02}^n + k_{01} \left( f(T_i) - f(A_{c3}) \right) + k_{02} \left( g(T_p) - g(T_i) \right) \right]^{\frac{1}{n}} \]  

(A.22)

The above Eq. (A.11) and Eq. (A.22) are the final equations for calculating the final austenite grain diameter in the FGHAZ and CGHAZ at various thermal histories, respectively.
References


[48] Z. Jin, D. Yu, X. Wu, K. Yin, K. Yan, Drag effects of solute and second phase distributions on the grain growth kinetics of pre-extruded Mg-6Zn


[56] Xu, Dong and Ji, Cheng and Zhao, Hongyang and Ju, Dongying and Zhu, Miaoyong, A new study on the growth behavior of austenite grains during heating processes, Scientific Reports 7 (1) (2017) 3968.
Three methodologies for prediction of prior austenite grain growth in HAZ of a martensitic steel have been proposed.

Combined phase field and finite element method has been used for analyzing the relationship of process and microstructural evolution in welding.

A modification of an existing macroscale grain growth model is proposed to account for the precipitate dissolution in P91 steel during welding.

A near closed-form equation for calculating the grain size is proposed and validated.

The effect of welding thermal history on grain growth kinetics has been quantitative studied.