Abstract: This paper presents a crystal plasticity model to predict the tensile response and crack initiation in a mixed ferrite-martensite material with a low volume fraction of proeutectoid ferrite, representative of a welding-induced inter-critical heat-affected zone (IC-HAZ). It is shown that small volume fractions of ferrite can have a significant effect on material strength and ductility depending on the ferrite grain orientation. For relatively ‘soft’ ferrite grains, micro-cracks can grow across inter-ferrite ligaments with damage accumulating in the ferrite, leading to a reduction in strength and strain hardening, but with little influence on ductility; in contrast, relatively ‘hard’ ferrite grains act to accelerate micro-crack initiation, leading to reduced ductility, with negligible influence on strain hardening up to the maximum load.

Keywords: Crystal plasticity, IC-HAZ, dual phase, crystallographic orientation, damage.

1. Introduction

P91 is a tempered martensitic steel (containing 9% chromium, 1% molybdenum) which has been widely used in high temperature piping systems for fossil fuel power plant, due to its high creep resistance, low thermal expansion and good weldability. P91 is also a candidate material for next generation ultra-supercritical (USC) thermal plant [1,2]. Welding plays a pivotal role in the manufacture of complex piping system in such power plant [3]. The thermal history experienced at each material point within a welded joint depends on the
distance from the welding heat source, leading to heat affected zones (HAZ) in the weld. These are further classified, according to their characteristic microstructure into coarse-grained (CG-HAZ), fine-grained (FG-HAZ) and inter-critical (IC-HAZ) [4]. Under complex operational loading conditions, failures can often initiate within the IC-HAZ, a phenomenon known as Type-IV cracking [5–10].

Figure 1 (adapted from [6]) shows the relationship between peak temperature, $T_p$, and the key phase transformation temperatures for a P91 weld. For the CG-HAZ, $T_p$ is significantly greater than $A_{c3}$ (the upper austenite transition temperature) so that significant austenite grain growth occurs, whereas in the FG-HAZ region, re-crystallisation dominates leading to grain refinement; in the IC-HAZ region, $A_{c1} < T_p < A_{c3}$, leading to partial transformation to austenite and the development of a mixture of ferrite and tempered martensite following cooling [6,7]. The temperature in this region is not sufficiently high to cause dissolution of carbides, leading to the formation of carbide-free ferrite in the IC-HAZ region [8].

It is important to understand the influence of the IC-HAZ microstructure on mechanical behaviour as failure generally occurs in the IC-HAZ under long term service [9-11]. Limited information is available on the effect of weld microstructure on inelastic deformation in P91 and related materials, due to the complexity of the IC-HAZ microstructure and the difficulty of extracting test samples from the IC-HAZ. However, it is reported that the IC-HAZ material has the lowest hardness compared to the other regions of the weld after PWHT [8-10; 12, 13]. The IC-HAZ is a partially transformed region, resulting in a mixture of metallurgical features [12–14]. In [15] the existence of small amounts of pro-eutectoid ferrite in the IC-HAZ is reported. The low values of micro-hardness in the IC-HAZ have been attributed to the presence of this soft ferrite phase within a martensite matrix. (Transmission electron microscope images indicate that the IC-HAZ exhibits a lower dislocation density than parent material [16, 17], which is another possible explanation for the lower hardness of the IC-
HAZ.) In this work we examine the influence of a low volume fraction of ferrite within a martensite matrix on the microstructural deformation and the initiation of micro-cracks under tensile loading.

Modern modelling techniques provide the opportunity to gain unique insight into, and quantify, specific microstructure effects on constitutive response. For example, a continuum damage mechanics (CDM) model [18] was used to account for multiple precipitate types within a 9Cr steel and the results indicate that the volume fraction of MX carbide is a vital factor for creep behaviour of 9Cr steel at elevated temperature [19]. Crystal plasticity finite element (CPFE) approaches have provided information on inelastic deformation at the micro-scale [20–22]. A dislocation-density grain boundary interaction scheme has been developed and incorporated into a CPFE approach by Shanthraj and Zikry [20], to analyse crack nucleation and evolution based on the unique variant morphologies and inherent orientation relationships in martensitic microstructures. The extended finite element model (XFEM) approach was used in [23] to simulate martensite cracking in a dual phase steel. A combined CPFE and continuum damage model for a single crystal superalloy showed that effects such as crystallographic orientation, self- and latent-hardening and rate sensitivity can significantly influence creep and damage [24]. The authors are not aware of any previous work on modelling of the failure mechanisms using the CPFE approach for IC-HAZ, especially for 9Cr steels. Therefore, this work investigates the application of a crystal plasticity model combined with a strain-controlled damage model at the micro-scale, to investigate the failure response of P91 steel under monotonic tensile loading.

Small amounts of ferrite can induce significant stress concentrations and associated strain gradients at the ferrite-martensite grain boundaries, as shown in our previous work [7]. This may lead to premature micro-crack initiation and influence the fatigue life of welded joints. It has been shown experimentally that the presence of soft ferrite grains in a hard martensite
matrix has a detrimental effect on the low cycle fatigue life of 9Cr-1Mo steel, leading to acceleration of fatigue crack initiation [25]. In this work a modified two-dimensional Voronoi tessellation model is implemented, which explicitly accounts for the packet/block microstructure of the martensite. The Kurdjumov-Sachs (K-S) orientation relationship [26] is used to describe the crystallographic orientation of the martensite grains at each material point [27]. A strain controlled damage model is incorporated to assess the influence of the soft ferrite phase on the development of micro-plasticity and damage to provide insight into the mechanical behaviour of welded joints.

2. Finite element modelling framework

2.1 Implementation of finite element model for IC-HAZ

A typical tempered martensite grain has a BCC lattice structure comprised of three different types of slip systems (see Table 1), twelve \{110\}<111> slip systems, twelve \{112\}<111> slip systems and twenty-four \{123\}<111> slip systems. Figure 2 shows examples of a slip system for each of these slip families. The hierarchical microstructure of martensite grains is shown schematically in Fig. 3. The prior austenite grain (PAG) is divided into martensite packets containing blocks with specific misorientations as described in [26], while each block consists of collections of laths with similar orientations separated by low angle grain boundaries [28]. In recent work [29], the K-S relationship was introduced into a Voronoi Tessellation (VT) code, providing a physical description of the orientation relationship between the neighbouring blocks and packets within a PAG.

Figure 4(a) shows a micrograph of the IC-HAZ region from a sample of ex-service P91. The micrograph shows a region, without internal block boundaries, which may be identified as a ferrite region within a matrix of martensite grains [30]. Similar microstructures have been reported in [15, 31]. The present work is focused on assessing the influence of such an isolated ferrite region within a martensite matrix. The corresponding idealised FE
representation derived from the modified VT code is shown in Fig. 4(b), including one randomly distributed ferrite grain (approximately 5% by volume based on experimental observations [15]). The colour contours correspond to one of the Euler angles for each martensite block, obtained from the K-S relation based on a random distribution of PAGs. The grain size of the martensite PAG in the IC-HAZ is typically 10 µm [2], whereas the mean block width within the PAG is approx. 1.5 µm [32]. In this paper, attention is focussed on the tensile response of the IC-HAZ material, with particular focus on the in-plane interactions between grains, packets, blocks within the PAG and between the ferrite and martensite phases. Hence, it is assumed here that the grains are columnar in the out-of-plane direction (with one element in that direction), following the approach adopted previously for modelling of single-phase P91 martensitic steel [21]. Three-dimensional, linear brick elements are used within the framework of the fully three-dimensional user material constitutive model presented below, with periodic boundary conditions in both the in-plane and out-of-plane directions, as described below (Section 3) and illustrated in Fig. 4(c). The present quasi-2D representation is considered appropriate to capture the dominant in-plane interactions of the ferrite-martensite phase mixture in the IC-HAZ, at least as a first step towards more detailed application of a full 3D modelling approach, which would be actually be prohibitively onerous, in terms of computational overheads. Previous work [21] has directly compared 3D columnar, 3D equiaxed and test data, for the same boundary conditions and deformation mode as use here, for a stainless steel; it was shown that the 3D columnar gave almost identical tensile stress-strain response to the 3D equiaxed up to 10% strain, as the most important grain interactions in the in-plane directions are accounted for. The present quasi-2D gives the same response as the columnar 3D. The key differences will, of course, be in terms of fracture and failure modes, e.g. clearly, 3D aspects of the fracture surfaces and
crack morphology will not be captured in the quasi-2D approach. It is intended to develop 3D models of the martensite-ferrite grain interactions in future work.

The crystal plasticity model used to represent the constitutive response is discussed in Section 2.2.

### 2.2 Micro-mechanical crystal plasticity constitutive formulation

The CPFE model describes the microstructural deformation at the block level, accounting for elastic and plastic flow anisotropies for each block, without considering a size effect (length scale dependent plasticity) for simplicity. Length scale effects may be important when block size is lower than \( \sim 1 \ \mu m \) [33], which will be considered in our future work. Martensite laths are not explicitly modelled; the constitutive model at the block level accounts implicitly for the lath contributions, as described in [21].

Following [34], the deformation gradient \( F \) is decomposed into components, \( F^e \) and \( F^p \), as follows:

\[
F = F^e F^p, \tag{1}
\]

where \( F^e \) is the elastic deformation gradient due to the reversible response of the lattice to external loadings and rotation, while \( F^p \) is an irreversible deformation gradient due to slip.

The inelastic slip rate on a slip system \( \alpha \), \( \dot{\gamma}^\alpha \) is represented by a thermally activated flow rule [35] dependent on the resolved shear stress \( \tau^\alpha \), as follows:

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp \left\{ -\frac{F_0}{kT} \left[ 1 - \left( \frac{\tau^\alpha - S^\alpha}{\tau_0} \right)^p \right]^q \right\}, \tag{2}
\]

In Eq. (2), \( T \) and \( k \) are absolute temperature and Boltzmann constant, respectively. The material constants are: \( F_0 \), the total free activation energy needed to overcome the lattice resistance; \( \tau_0 \), the lattice friction stress at absolute temperature; \( p \), \( q \) and \( \dot{\gamma}_0 \), are the exponents
and pre-exponent constant, respectively. The resolved shear stress $\tau^\alpha$ on a given slip system, is defined as follows:

$$\tau^\alpha = (F^e)^T F^e \mathbf{T}^{*} : (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha),$$

(3)

where $\mathbf{m}^\alpha$ and $\mathbf{n}^\alpha$ are unit vectors to define slip direction and slip plane normal in the reference configuration; $N$ denotes the total number of slip systems. In Eq. (3) $\mathbf{T}^{*}$ indicates the stress elastically work-conjugate to the elastic Green strain

$$\mathbf{T}^{*} = (F^e)^{-1} J \sigma^e (F^e)^{-T},$$

(4)

where $J=\text{det}(F)$, $\sigma$ and $J\sigma$ are the Cauchy and Kirchhoff stress, respectively. The slip resistance $S^\alpha$ in Eq. (2) is defined as,

$$\dot{S}^\alpha = \sum_{\beta=1}^{N} h^{\alpha\beta} \left( \frac{S_{\text{sat}} - S^\beta}{S_{\text{sat}} - S_0} \right) \left| \dot{\varepsilon}^{\beta} \right|,$$

(5)

where $h^{\alpha\beta}$ in Eq. (5) is the hardening matrix and $S_{\text{sat}}$ is the saturated slip resistance with initial value $S_0$. The hardening matrix, $h^{\alpha\beta}$, can be written as

$$h^{\alpha\beta} = h_s \left[ \omega_1 + (1 - \omega_2) \delta^{\alpha\beta} \right],$$

(6)

where $h_s$ is a material constant for all slip systems (active and inactive) and $\delta^{\alpha\beta}$ is the Kronecker delta. The slip resistance $h^{\alpha\beta}$ depends not only on the active slip systems $\alpha$ (self-hardening) but also on the non-active slip system $\beta$ (latent hardening), through the constants $\omega_1$ and $\omega_2$ [27]. If $\omega_1 = 1$, $\omega_2 = 1$ all slip systems harden equally, irrespective of whether active or not, leading to isotropic crystallographic hardening (Taylor hardening, [36]). Based on recent studies [37, 38] this model ($\omega_1 = 1$, $\omega_2 = 1$) has been used here.

2.3 Damage model

The accumulated equivalent plastic strain ($\varepsilon_{eq}^{pl}$) has been proposed by a number of authors as an important indicator parameter for crack initiation [39, 40]. In this paper, we adopt a strain-
controlled damage progression model in conjunction with micro-plasticity in order to describe the localized deformation. This damage model has previously been applied for austenitic stainless to account for damage development [41]. The accumulated equivalent plastic strain $\varepsilon_{eq}^{pl}$ is defined as:

$$
\varepsilon_{eq}^{pl} = \int_0^t \left( \frac{2}{3} D^p : D^p \right)^{\frac{1}{2}} dt,
$$

(7)

where $t$ is the current simulation time and $D^p$ is plastic strain rate, expressed as:

$$
D^p = \frac{1}{2} \sum_{\alpha=1}^N \mathbf{F}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \left( \mathbf{F}^\alpha \right)^{-1} + \left( \mathbf{F}^\alpha \right)^T \mathbf{n}^\alpha \otimes \mathbf{m}^\alpha \left( \mathbf{F}^\alpha \right)^T
$$

(8)

A microstructural damage variable, $\omega$, varying from 0 (no damage) to 1 (fully damage), is adopted to describe the degradation of the elastic stiffness. The modified local elastic stiffness matrix is written as follows:

$$
\mathbf{C} = \mathbf{C}_0 (1 - \omega),
$$

(9)

where $\mathbf{C}_0$ is the material elastic stiffness without damage. A continuously varying $\omega$ is assumed using a modified Cauchy-Lorentz cumulative distribution function [42] as follows:

$$
\omega = 1 + \left[ \frac{1}{2} + \frac{1}{\pi} \arctan \left( \frac{d}{\varepsilon_c} \right) \right]^{-1} \left[ \frac{1}{\pi} \arctan \left( \frac{\varepsilon_{eq}^{pl} - \varepsilon_c}{d} \right) - \frac{1}{2} \right].
$$

(10)

The Cauchy-Lorentz function in Eq. (10) provides a phenomenological description of a damage transition with $\omega = 0$ at $\varepsilon_{eq}^{pl} \leq 0$ and $\omega \rightarrow 1$ as $\varepsilon_{eq}^{pl} \rightarrow \varepsilon_c$ and $\varepsilon_c$ is the critical strain.

The width of the damage transition region is defined by $d$.

The material model defined in Section 2.2 and 2.3 is implemented in a material user subroutine (UMAT) in the non-linear commercial finite-element code Abaqus (2016) [43].

3. Model calibration and material parameters identification
A methodology to obtain the visco-plastic constitutive response in heterogeneous (welded P91) material using digital image correlation (DIC) is described in [44]. The material parameters for the constitutive model described in Section 2 were determined by fitting to the experimental data in [44] for the IC-HAZ at room temperature. The representative volume element (RVE), constructed as described in Section 2.1, has been checked to establish a sufficient number of blocks to give a consistent macroscopic response using the polycrystalline FE model [7, 29, 45]. Two RVEs were first generated: an all-martensite RVE and an all-ferrite RVE as shown in Fig. 5. The all-martensite RVE consists of 20 PAG grains, containing 444 blocks; the smallest element size is about 0.24 µm, giving about 4 or 5 elements across the width of each block (see Fig. 5a, inset). The model contains about 30,000 elements. The all-ferrite RVE (see Fig. 5b, inset) consists of 200 PAG grains with 35,000 elements, following our previous work [7]. In both cases periodic boundary conditions (see Fig. 4c) are used to represent the overall material microstructure, as in [7, 21].

Micro-hardness indentation tests for the ferrite and martensite phases in the IC-HAZ demonstrated a hardness value for martensite of approximately 1.25 times that of the ferrite phase [31]. In the CPFE model, the lattice friction stress (Eq. 2) largely controls the material strength. Therefore, in this work the constitutive response of the ferrite phase is represented by scaling \( \tau_0 \) according to this micro-hardness ratio between the two phases; the martensite and ferrite lattice friction stresses are given by \( \tau_{0m} \) and \( \tau_{0f} \), respectively. The resulting predictions of the macro stress-strain responses of both martensite and ferrite phases are shown in Fig. 6, taken from the RVEs of Fig. 5. Table 2 presents the identified elastic constants and flow parameters used in the analysis. Table 3 gives the parameters associated with the strain hardening for both phases. Numerous researchers, e.g. [46], have argued that for BCC crystals, the slip along \{110\} slip planes is the dominant deformation mode at room
temperature. Therefore, only the dominant twelve \{110\} slip systems of BCC are considered in the remainder of this paper. Table 4 gives the list of \{110\} slip systems used in the UMAT.

4. Results

4.1 Crystal orientation effect on global response

The global and local deformation mechanical responses induced by different ferrite orientations are first investigated.

Figure 7(a) illustrates the approach with an isolated ferrite grain embedded within the martensite matrix. The darkest lines correspond to the PAGs (or ferrite phase), the heavy lines correspond to packet boundaries and the lightest lines are the block boundaries. The regions A, B, C D in Fig. 7(a) and the path have been identified for further analysis in Section 4.2 and 4.3. Three orientations are chosen for the single crystal ferrite grain, as shown in Fig. 7(b); the loading direction is [010] in all cases.

Figure 8(a) shows a comparison of the global tensile stress-strain responses obtained from the FE analysis for the three different ferrite orientations up to a strain of 5%. Also included is the measured IC-HAZ response from [44]. It is clear that at the macro-scale the influence of the ferrite orientation is weak, with the <100> orientation giving a slightly softer response than the other two orientations and all three cases are similar to the all-martensite response at the macro-scale (Fig. 6). Figure 8(b) provides a comparison of the single crystal stress-strain responses for the three orientations, showing the softest response for the <100> orientation, which is also significantly softer than a typical martensite-only response (compare to Fig. 6). The hardest response is for the <110> orientation, which is a similar response to that of martensite.

4.2 Crystal orientation effect on local micro-mechanical response

Figure 9 shows the $\sigma_{yy}$ distribution at 5% macroscopic strain. The thick solid white lines indicate the prior austenite grain boundaries (PAGB) or ferrite boundary, the thin solid lines
are the packet boundaries and the dash lines are block boundaries. The predictions show a complex pattern of stress due to the orientation mismatch between neighbouring packets and blocks and for Figs. 9(b) to (d) the influence of the ferrite grain with different applied orientations.

Figure 9(b) shows that the introduction of a ‘soft’ \(<100>\) ferrite grain causes reduced stress within the grain, compared to the equivalent PAG in Fig. 9(a); the average \(\sigma_{yy}\) in the ferrite region decreases from \(~610\) MPa for single phase martensite RVE to \(~500\) MPa for the mixed-phase RVE. There is some increase in the local stress in transversely-adjacent martensite grains of the A and B regions (defined in Fig. 7a) and concomitantly, reduced stresses in C and D regions. In contrast, Fig. 9(c) shows that the introduction of a ‘hard’ \(<110>\) ferrite grain increases the local stress in the C and D regions but slightly decreases local stresses in the A and B regions. Figure 9(d) shows that the introduction of the intermediate-hardness \(<111>\) ferrite grain gives an almost identical inter- and intra-granular stress distribution to the ‘no ferrite’ case, Fig. 9(a).

Figure 10 shows the equivalent plastic strain distribution (\(\varepsilon_{eq}^{pl}\)) for the cases examined in Fig. 9. As before, the results are presented at the same macroscopic strain level of 5\%. As discussed in Section 2.3, \(\varepsilon_{eq}^{pl}\) is a key variable controlling prediction of micro-crack initiation for the strain-based damage model. It can be seen from Fig. 10(b), that the introduction of a ‘soft’ \(<100>\) ferrite grain leads to an increase in average \(\varepsilon_{eq}^{pl}\) from 0.054 to 0.069 in this grain (relative to Fig. 10a), and, more importantly, an associated reduction in \(\varepsilon_{eq}^{pl}\) in the transversely-adjacent B region and, especially, in the block and packet of maximum \(\varepsilon_{eq}^{pl}\). In other words, the high plastic strain experienced by this martensite block in region B of Fig. 10a is ‘shared’ with the ferrite phase in this configuration. In contrast, Figs. 10(c) and (d)
show that the ‘hard’ <110> ferrite grain (and to a lesser extent the <111> ferrite grain) further accentuate the $\varepsilon_{eq}^{pl}$ concentration in the most highly strained block location, relative to the original single-phase martensite microstructure. This trend is consistent with CPFE simulations of hard-soft grain interactions for titanium alloy poly-crystals [47].

To further examine this issue and to quantify the trends illustrated in the contour plots of Figs. 9 and 10, Fig. 11 shows the predicted $\sigma_{yy}$ and $\varepsilon_{eq}^{pl}$ distributions (at 5% macroscopic strain) plotted along the path identified in Fig. 7(a) for the all-martensite and mixed-phase analyses. The path traverses the single-phase martensite microstructure from region A to region B. Significantly inhomogeneous distributions of $\sigma_{yy}$ and $\varepsilon_{eq}^{pl}$ are predicted in Figs. 11(a) and (b), due to traversing of multiple block boundaries within the fully martensitic microstructure. Figure 11(c) shows the increased stresses within adjacent martensite grains for the ‘soft’ <100> case, relative to both the <110> and martensite-only cases; the highest localisation of stress occurs at the ferrite-martensite grain boundaries for the case of the ‘soft’ <100> ferrite grain, leading to accentuated micro-stress concentrations factors of $\sim$1.8 (relative to the global stress of Fig. 8). This type of micro-stress ‘hot-spot’ at a grain boundary is potentially detrimental with respect to fatigue crack nucleation. Figure 11(d) shows the peak $\varepsilon_{eq}^{pl}$ localisation in the martensite packet-block is adjacent to the ferrite grain (region B). For the ferrite with <110> orientation case, the peak strain is significantly higher than that in the martensite-only and <100> ferrite cases. Note that this is the location of predicted failure for the martensite-only and the <110> cases; the latter is shown below to have a lower ductility than the former, which is consistent with the relative strain localisations, viz. the higher localisation in the <110> case gives lower ductility. It may be noted that the value of peak strain at the failure location for the <100> case (not shown here in the interest of space) is
~0.13 which is lower than the martensite-only and <110> cases, as highlighted in Fig. 11(b) and (d), resulting in higher predicted ductility.

4.3 Prediction of micro-crack initiation of IC-HAZ

The preceding analyses have been for strain levels up to 5% with the damage model inactive. Figure 12(a) shows a comparison of the CPFE-predicted tensile stress-strain response to failure, for the single-phase martensite (assuming no ferrite in the IC-HAZ), with the measured IC-HAZ response [44]. The predicted response shown is for a range of critical strain values, \( \varepsilon_c \), in the damage model of Eq. (10) up to \( \varepsilon_c = 0.3 \). For critical strain values above 0.3 it was found that a converged solution was not obtained in the finite element analysis, and therefore the critical strain value of \( \varepsilon_c \), which is closest to the measured value for the IC-HAZ has been used in the subsequent analysis. The value of the damage transition parameter \( d \) is fixed at 0.1. Figure 12(b) shows the predicted damage distribution at failure. Intergranular cracking is predicted generally, i.e. along PAGB boundaries and block boundaries.

Figure 13 shows a comparison of the CPFE-predicted tensile stress-strain responses for the two-phase martensite-ferrite IC-HAZ microstructures with ‘soft’ and ‘hard’ ferrite grains with the measured IC-HAZ response from [44] and the corresponding damage distributions at failure. It can be seen from Fig. 13(a) that the effect of the ‘soft’ <100> ferrite grain is to cause a softer overall response with reduced hardening, leading to a discernible reduction in tensile strength and marginal effect on ductility for \( \varepsilon_c = 0.3 \) (see Table 5). In contrast, the most significant effect of the ‘hard’ <110> ferrite grain is to reduce predicted ductility with negligible effect on hardening response (up to the maximum stress). Although the single-phase martensite model has been calibrated (in Figure 12) to correlate closely to the measured IC-HAZ stress-strain response, on the assumption of no ferrite phase, the purpose of the mixed-phase models is to investigate the global (tensile stress-strain) and local
(inhomogeneity of local stress-strain distributions and cracking-fracture behaviour) effects of inclusion of such a ferritic phase (material imperfection), specifically, in the context of premature creep or creep-fatigue failure of P91 weldments. Small amounts of ferrite can be seen in the IC-HAZ region after welding.

Figures 13(b) and (c) show the predicted micro-cracking patterns for the ‘soft’ and ‘hard’ ferrite cases, respectively. It can be clearly observed that the ferrite grain can strongly influence the location of crack initiation with the ‘soft’ <100> ferrite grain causing a significant change in micro-cracking pattern, i.e. transgranular, relative to the single-phase martensite case (Fig. 12b). Figure 13(c) shows that the damage distribution for the ‘hard’ <110> is more consistent with that for the single-phase martensite, i.e. intergranular, though with increased damage at the same level of macroscopic strain (see also Figs. 10a and 10c).

Some additional observations are as follows:

Although the present quasi-2D modelling approach can match the overall stress-strain response, the predicted local (detailed) fracture morphology and fracture characteristics will undoubtedly be different to what would be predicted by a full 3D microstructure model (with microstructure variation in the out-of-plane direction, as opposed to the columnar assumption of the present approach). Specifically, 3D aspects of the fracture surfaces and crack morphology will not be captured in the quasi-2D approach. A 3D RVE model equivalent to the present quasi-2D RVE would contain about 7,525,000 elements, as opposed to the 30,100 required here. With damage and large-deformation effects, this would require prohibitively enormous run-times, particularly for the range of sensitivity analyses presented. Nonetheless, the present quasi-2D approach has provided a key first step in crystal plasticity modelling of IC-HAZ failure under tensile loading. It is argued that this simplification allows more accessible interpretation of the trends in terms of predicted inter- and intra-granular cracking vis-à-vis in-plane grain-block-packet and ferrite-martensite phase interactions.
5. Conclusions

A micro-mechanical modelling methodology is presented for tensile damage and crack initiation in the inter-critical heat-affected zone in 9Cr steels, due to the ferrite-martensite inhomogeneity. A damage model based on accumulated plastic strain, but independent of stress history has been examined. The key conclusions are as follows:

1. The predicted ductility and strength are shown to be in general agreement with previously-published measured test data for the IC-HAZ material.

2. The crystallographic orientation of ferrite grains significantly affects the localization of strain and the behaviour of crack initiation in the IC-HAZ.

3. Small volume fractions of softer ferrite are shown to have a detrimental effect on material strength, as expected. However, the effect on ductility can be detrimental or marginally beneficial, depending on ferrite grain orientation.

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References:


**Tables:**

Table 1: Slip systems of BCC structure.

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<td>{112}</td>
<td>{123}</td>
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<tr>
<td>Slip direction</td>
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<td>&lt;111&gt;</td>
<td>&lt;111&gt;</td>
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<td>Number of slip systems</td>
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Table 2: Elastic constants and flow rule parameters used in the poly-crystal model (Room temperature).

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<th>$C_{11}$ (GPa)</th>
<th>$C_{22}$ (GPa)</th>
<th>$C_{44}$$\mu$ (GPa)</th>
<th>$\gamma_0$ (s$^{-1}$)</th>
<th>$F_0$ (J)</th>
<th>$\tau_{0m}$ (MPa)</th>
<th>$\tau_{0f}$ (MPa)</th>
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<td>140.0</td>
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<td>1.25</td>
<td>0.43*10$^{-18}$</td>
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Table 3: Strain hardening and damage parameters used in the poly-crystal model.

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<th>$S_0$ (MPa)</th>
<th>$S_{\text{sat}}$ (MPa)</th>
<th>$h_s$ (MPa)</th>
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Table 4: 12 slip systems list used in the crystal plasticity model

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<th>System</th>
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Table 5: Comparison of CPFE results with measured IC-HAZ data.

<table>
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<th>Method</th>
<th>Tensile strength (MPa)</th>
<th>Ductility $\varepsilon_f$ (%)</th>
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<tr>
<td>Experiment [44]</td>
<td>665</td>
<td>10.2</td>
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<tr>
<td>CPFE-single phase</td>
<td>615</td>
<td>9.0</td>
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<tr>
<td>CPFE-mixed phase: &lt;100&gt; ferrite</td>
<td>590</td>
<td>9.3</td>
</tr>
<tr>
<td>CPFE-mixed phase: &lt;110&gt; ferrite</td>
<td>600</td>
<td>8.5</td>
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</table>
Figures:

Figure 1. A schematic of the weldment regions as corresponding to the equilibrium Fe-C binary phase diagram adapted from [6]. The dash line shows the carbon content of P91.

Figure 2. Examples of slip systems for BCC structure corresponding to each slip system family. In each figure the arrow and the blue lines indicate the slip plane and slip direction, respectively.
Figure 3. Schematic illustration of the hierarchical microstructure in P91 martensitic steel including PAG, packet, block and lath.
Figure 4. (a) IC-HAZ microstructure morphology measured by SEM [30]; (b) Distribution of Euler angle in a poly-crystal finite element model and the blue region indicate α-ferrite embedded in martensite matrix, (c) Illustration of quasi-2D (columnar microstructure) model with periodic boundary conditions.
Figure 5. Illustration of the micromechanical finite-element model for dual-phase constitutive parameter identification: (a) single-phase martensite model showing FE mesh (b) single-phase ferrite model (from [7]).
Figure 6. Identification of parameters for martensite by fitting the IC-HAZ data from ref [44]; The predicted ferrite response is also included.

Figure 7. (a) Isolated ferrite grain embedded within a martensite matrix; (b) Three typical ferrite orientations chosen for ferrite grain.
Figure 8. Comparisons of stress-strain responses for the ferrite with different orientations. (a) Global responses for the RVE including ferrite with different orientations; (b) single crystal response for the ferrite with different orientations.
Figure 9. Stress distribution ($\sigma_{yy}$) at 5% macroscopic tension for the ferrite with different orientations; (a) No ferrite; (b) ferrite with <100> orientation; (c) ferrite with <110> orientation; (d) ferrite with <111> orientation.
Figure 10. Accumulated equivalent plastic strain distribution (\( \varepsilon_{eq}^{pl} \)) at 5\% macroscopic tension for the ferrite with different orientations; (a) No ferrite; (b) ferrite with <100> orientation; (c) ferrite with <110> orientation; (d) ferrite with <111> orientation.
Figure 11. Effect of ferrite orientation on local stress and strain distributions at 5% global strain for path identified in Figure 7(a). (a) all-martensite analysis $\sigma_{yy}$ (b) all-martensite analysis $\varepsilon_{eq}^{pl}$ (c) mixed-phase analysis $\sigma_{yy}$ (d) mixed-phase analysis $\varepsilon_{eq}^{pl}$
Figure 12. Prediction of tensile damage and micro-crack initiation in tensile test for single-martensite phase RVE: (a) comparison of CPFE tensile stress-strain response with IC-HAZ data from [44] (b) CPFE-predicted damage distribution showing predicted failure locations.

Figure 13: Prediction of damage and micro-crack initiation for the mixed-phase martensite-ferrite RVE: (a) comparisons of predicted responses against measured IC-HAZ data [44]; (b) damage distribution for ‘soft’ <100> ferrite; (c) damage distribution at failure for ‘hard’ <110> ferrite.