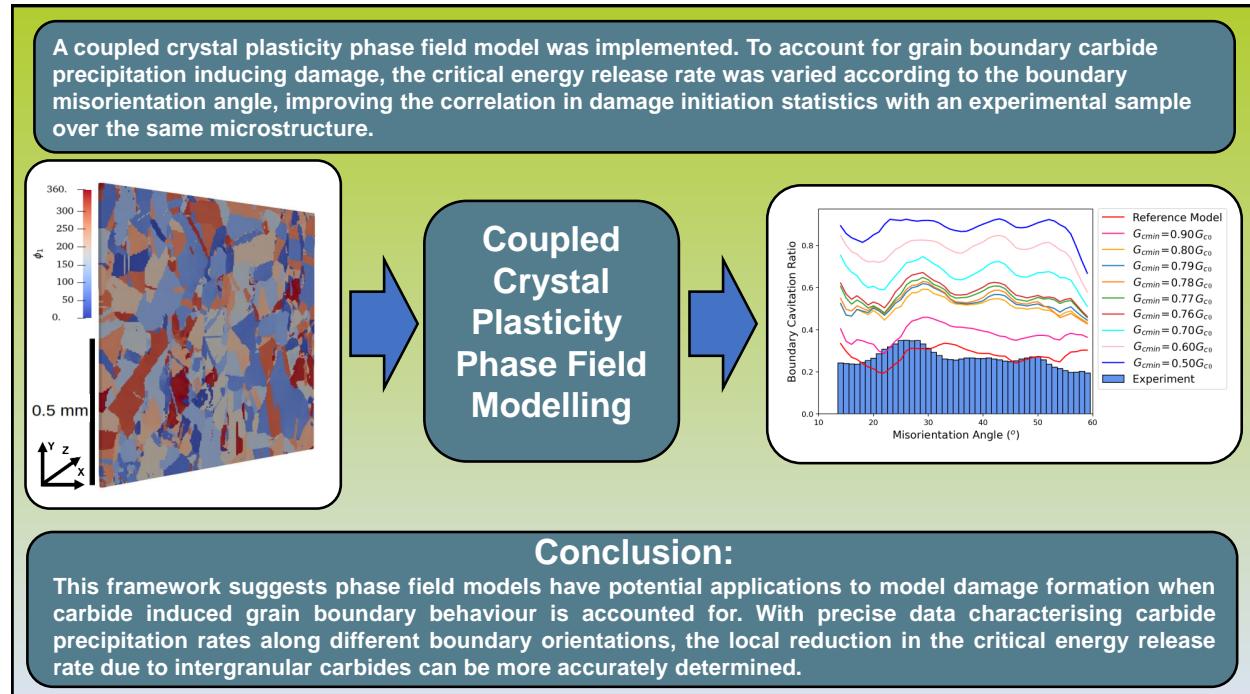


Graphical Abstract

Effect of grain boundary misorientation and carbide precipitation on damage initiation: a coupled crystal plasticity and phase field study

Michael Salvini, Nicolò Grilli, Eralp Demir, Siqi He, Tomas Martin, Peter Flewitt, Mahmoud Mostafavi, Christopher Truman, David Knowles



Highlights

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- Grain boundary misorientation angles affect the precipitation rate of intergranular carbides in 316H stainless steel
- A novel implementation of a misorientation dependent critical energy release rate was used to model their effect on damage
- A coupled crystal plasticity phase field finite element modelling framework was developed for early damage formation
- A strong correlation in damage initiation trends with experimental data was obtained over the same microstructure

Effect of grain boundary misorientation and carbide precipitation on damage initiation: a coupled crystal plasticity and phase field study

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Abstract

A coupled crystal plasticity phase field damage framework has been developed and applied to modelling damage initiation. A novel implementation of a grain misorientation angle dependent critical energy release rate has been used to determine a reduction in the local critical energy release rate resulting from the effects of intergranular carbide precipitates and grain boundary misorientation. When applied to a notched high temperature 316H austenitic stainless steel specimen, a good correlation between experimental results and void nucleation statistics for a misorientation dependent critical energy release rate was obtained. This has been evaluated through comparison with correlative electron microscopy experimental results, showing the potential of phase field models in the area of early damage formation. Additions to include plastic strain and creep deformation effects, with comparisons to experimental data for microstructural geometry properties such as the difference and actual values of Schmid factors at grain boundaries as well as the loading direction stress and dislocation densities. The limitations to this approach and opportunities for further work in this area are discussed, with specific interest in the need for additional literature data characterising grain boundary carbide precipitation and cavity nucleation analysis.

Keywords: Crystal plasticity, phase-field damage, plasticity, 316H austenitic stainless steel, damage, electron backscatter diffraction, electron microscopy, cavity nucleation, damage initiation, grain boundary misorientation

1. Introduction

A key target for improving the economics of existing nuclear fission reactor power station projects is extending their operational lifetime. The 60-year design of the next generation

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of electrical power generation nuclear power plants will integrate predictive modelling techniques combined with targeted in-service testing, monitoring, and maintenance to reduce operational outages [1, 2, 3]. Headers, boiler tubes, welded joints, and other structural components in the primary and secondary circuits are made of stainless steel and are subjected to high temperatures and pressures over a prolonged period of time [4]. As such, they exhibit degradation because of the interplay between various mechanisms including plastic deformation and fracture [5].

Material creep deformation is characterised by the strain rate, which dominates the overall response [6]. The creep strain rate is typically described using a modified Arrhenius power law [7, 8]. For temperatures of 550°C, components made from austenitic stainless steel such as 316H grade are expected to exhibit inelastic time dependent deformation through dislocation creep [9]. This process occurs through the glide of dislocations through a polycrystalline material to cause deformation of individual grains when the applied stress is in the range 10 – 200 MPa [10], which is below the yield stress for an austenitic stainless steel, ie 205 MPa for 316H stainless steel.

Ductile fracture in metals typically occurs through the nucleation, growth, and the intergranular interlinking of voids [11]. Similarly, creep cavity initiation is seen at grain boundaries during creep [12], and the average growth rate can be estimated using the macroscopic stress [13], while the final rupture is in the nature of a intergranular process. Lenticular cavities have been observed during creep at the grain boundaries in both 304 and 316 stainless steels, induced by a combination of high temperature void diffusion and dislocation climb [14, 15]. Factors including the temperature, local stresses and accumulated local strain are typically thought to contribute most to creep cavity nucleation and growth, but many of these mechanisms are accommodated and strongly influenced by the effect of the microstructure, such as grain orientations and carbide precipitates [16, 17, 18, 19]. At high stress, both plastic deformation and creep take place, with plastic strain induced void initiation dominating the formation of damage. Although creep cavities can form in these conditions at grain boundaries, overall failure occurs due to ductile failure resulting from creep cavities and other features found at grain boundaries.

Understanding the deformation mechanisms at the grain length-scale that contribute towards the nucleation of voids and creep cavities that can lead to ductile failure is key to understanding fracture behaviour [20]. It is known through measurements performed with electron microscopy techniques that cavitation is more pronounced in boundaries with second phases and precipitates than in higher purity materials as observed in high purity aluminium by Yavari et al. [21]. Hard second phases such as martensite as well as $M_{23}C_6$ carbide precipitates containing elements such as chromium and molybdenum between 1 nm and 5 nm diameter can increase cavity nucleation [22]. Carbides more readily precipitate in samples aged at higher temperatures, accumulate in higher concentrations at grain boundaries, and influence plastic deformation [23]. Certain grain boundary orientations will lead to higher levels of precipitation and carbide density [24, 25], and are thought to cavitate earlier [26, 27, 28, 29]. However, carbide precipitates are too small in size to be explicitly modelled using micron scale crystal plasticity simulations.

The misorientation between neighbouring grains is also a key factor in fracture nucleation.

The effect of the Taylor factor, which quantifies the average orientation and size of grains on fracture nucleation, has been investigated in ferritic steel [30]. It was found that damage tends to nucleate at the interface between high and low deformation zones, constituted of smaller grains and martensitic regions. Intergranular fracture in 316L stainless steel has been observed at the shorter grain boundaries between sets of elongated columnar grains, showing that grain morphology and length-scale effects also play an important role [31]. Moreover, the effect of strain incompatibility measures, such as the density of geometrically necessary dislocations (GND), on fracture nucleation is not widely studied [32]. The effects of grain misorientation and carbides on fracture are intimately related because the grain boundary misorientation angle partly determines the carbide density. This in turn decreases the grain boundary critical energy release rate, as well as affecting the strain incompatibility and the local stress state during load. The combined effect of these two intrinsic mechanisms cannot be easily studied without a combined computational and experimental study. The effect that $M_{23}C_6$ carbides have on local strain fields has been studied in 420 stainless steel using crystal plasticity [33].

Microscale modelling is an invaluable tool to characterise the plastic deformation and fracture at the length-scale of the individual grains [34]. The crystal plasticity finite element method (CPFEM) can model the incompatibility of the plastic deformation near the interface of grain pairs [35], while dislocation-based constitutive laws can reproduce the effect of slip gradients on the local slip resistance [36, 37]. Phase field fracture (PFF) models consist of a continuum scalar phase field across the simulated microstructure that describes a phase change. In PFF models, the field value varies between 0 for undamaged material, to 1 for completely damaged material. This approach has been applied to both brittle and ductile fracture at varying length-scales from component level simulations with continuum finite element approaches [38, 39], to crystal plasticity mesoscale damage modelling of grain microstructures [40, 41, 42].

The identification and description of influencing factors on damage initiation on the microstructural scale remains an open problem within the literature. The use of computational modelling techniques compared to experimental data to understand the influencing factors has been applied to fatigue crack initiation, [43, 44], with accumulated local plastic deformation and inclusions attributed. The use of microscopy techniques has been used to identify damage features [45, 46], however, a comprehensive approach encompassing the interplay between microstructural features, plastic strain localisation, and precipitates and second phases has been developed thus far. The effect of evolving microstructural texture under cyclic loading conditions has also been explored [47].

Borden et al. developed a model incorporating a degradation function to account for plastic softening after crack initiation [48], a feature of particular interest when applied to microstructural modelling, due to the effect local damage can have on surrounding regions and grains. To better correlate with experimental results, many approaches, including a set of threshold conditions to prevent damage nucleation before high elastic or plastic deformation, have been attempted. Energy based damage criterion have been implemented utilising an additive split of elastic and plastic strain energy by Amor et al. [49]. These include thresholds in energy and strain like that of Miehe et al. [50], or plastic work thresholds

implemented by Borden et al. [48], in which a threshold is applied to control the point at which plastic deformation can contribute to failure initiation. PFF has been used for both crack nucleation and propagation, reproducing stress, transition flaw size and toughness criteria for fracture [51, 52]. Although phenomenological from the modelling perspective, the introduction of thresholds and specific strain-based contributions to the fracture driving force has been used in many cases to more accurately capture nuanced, condition dependent behaviour observed in experiments and in-service material samples [53]. Other fracture models, such as the cohesive zone model [54, 55], element elimination [56] and Beremin model [57] can be used to predict damage formation surrounding micro-structural defects such as carbide precipitates. However, in the present work, PFF is used because of the large area analysed and the ability to use a structured mesh.

The following scientific questions remain unanswered: how much damage is induced by plastic and creep deformation respectively in 316H stainless steel depending on the applied stress? What is the interplay between grain boundary misorientation and carbides, and how can their effect on damage initiation be quantified? How much does the grain boundary critical energy release rate decrease in the presence of a specific carbide density or grain boundary orientation? Which is the most accurate indicator of damage across a microstructural region, in terms of dislocation density, elastic strain energy, or plastic work done? Are microstructural models for plasticity and fracture capable of predicting the cavity nucleation on individual grain boundaries? How effectively can continuous phase field models in conjunction with crystal plasticity, which have previously been mostly used in modelling crack propagation, be applied to early damage formation? In this article, a combination of coupled crystal plasticity-fracture simulations and electron microscopy experiments are used to consider and address these questions, in order to present a comprehensive model that accounts for the combined effect of grain misorientations and intergranular carbides reducing the local fracture at grain boundaries. Understanding the interplay between different mechanisms at the microscale in the formation and propagation of damage resulting from deformation is a key focus [58], particularly for the experimental reported by He et al., [45], and the modelling work shown here.

Electron microscopy techniques such as scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) allow for imaging and grain microstructure characterisation at up to nanometre resolution. The high resolution of SEM allows for voids, cavities, and other features of damage formation to be resolved and identified [59]. EBSD measurements allow for the orientations of grains to be determined which when combined and correlated with identified voids and damage features allow for significant insight into the underlying mechanisms of damage formation, as done by He et al. [29, 60, 45]. The combination of high throughput microscope detectors and interrupted mechanical tests allows damage nucleation over large areas, with the size of several square millimetres, to be investigated [61, 62, 45].

This article is organised as follows. Section 2 explains the computational method, including the crystal plasticity finite element method (CPFEM) framework in section 2.1 and the phase field fracture (PFF) formulation in section 2.2. Section 3 contains the experimental characterisation of the 316H stainless steel sample, with 4 and 5 detailing how the simulation parameters were calibrated and analysed. The final results are outlined in section 6, which

is split into sections 6.1, 6.3, 6.2, and 6.4 to detail results and analysis from the various crystal plasticity phase field models that have been implemented including the reference elastic strain energy damage model, a misorientation dependent critical energy release rate, an elastoplastic damage model, and a plastic-creep deformation crystal plasticity model respectively. Results are discussed and evaluated in the context of the outlined objectives and questions in section 7, with concluding statements in section 8, and a supplementary appendix in section 8.

2. Computational method

In this section, the coupled CPFE-PFF methodology used in the simulations is presented. The computational method solves for the three components of the displacement vector \mathbf{u} and for the scalar damage phase field variable c . The Cauchy stress tensor $\boldsymbol{\sigma}$ is calculated from the deformation gradient \mathbf{F} , as described in section 2.1. The local form of the quasi-static equilibrium problem neglecting body forces reads:

$$\nabla \cdot \boldsymbol{\sigma} = 0 , \quad (1)$$

is solved, together with the evolution equation for the damage phase field, as detailed in section 2.2. The model is implemented in the MOOSE multiphysics finite element framework [63] through a Fortran-based UMAT material subroutine.

2.1. Crystal Plasticity Formulation

A CPFE model, based on the integration scheme originally proposed by Kalidindi [64], is employed. The total deformation gradient can be decomposed into elastic and plastic components, denoted \mathbf{F}_e , and \mathbf{F}_p respectively, as shown below [65, 66]:

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p . \quad (2)$$

Simulations are conducted at constant temperature, 550°C, which is the same used in the experiment, and the model parameters reflect the material properties at that temperature. Therefore, no thermal expansion mechanism is included in this model. \mathbf{F}_p represents the plastic component of the deformation gradient, accounting for the plastic deformation contributions across all available slip systems in the crystal structure. The time evolution of \mathbf{F}_p is described by [67]:

$$\mathbf{L}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} = \sum_{\alpha=1}^{N_s} \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{n}^\alpha , \quad (3)$$

where \mathbf{L}_p is the plastic velocity gradient, α is the index characterising each slip system, whose unit vector for the slip direction is \mathbf{s}^α and slip plane normal is \mathbf{n}^α at the intermediate configuration. The slip rate of each slip system is represented by $\dot{\gamma}^\alpha$, which includes two contributions: plastic slip and creep. The number of slip systems in the crystal structure is given by $N_s = 12$ because 316H stainless steel consists of a dominant austenite phase with

| Type | Self-interaction | Co-planar | Cross-slip | Glissile | Hirth lock | Lomer-Cottrell lock |
|---------------------|------------------|-----------|------------|----------|------------|---------------------|
| χ_β^α | 0.1 | 0.22 | 0.3 | 0.38 | 0.16 | 0.45 |

Table 1: Slip interactions coefficients used for FCC crystal.

a face centred cubic (FCC) structure. Two power law terms, as proposed by Rice et al. [68], are used to calculate the plastic strain rate due to plastic slip and creep respectively:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0^s \left(\frac{|\tau^\alpha|}{\tau_c^\alpha} \right)^{1/m_s} \text{sign}(\tau^\alpha) + \dot{\gamma}_0^c \left(\frac{|\tau^\alpha|}{\tau_c^\alpha} \right)^{1/m_c} \text{sign}(\tau^\alpha), \quad (4)$$

where $\dot{\gamma}_0^s$ and $\dot{\gamma}_0^c$ are constant strain rate prefactors, m_s and m_c are constant exponents, which are the same for each slip system. These parameters are chosen in such a way that the plastic slip term is dominant compared to the creep deformation term during the initial load of the specimen up to 0.14%. The plastic slip term is then turned off for the following stage, allowing the creep deformation term to take over during subsequent loading, in which the stress is kept constant at 390 MPa, as detailed in section 4. τ^α is the resolved shear stress (RSS) in each slip system α , while the critical resolved shear stress (CRSS), τ_c^α , is given by [69, 70]:

$$\tau_c^\alpha = \tau_c^0 + \alpha_0 \mu b \sqrt{\sum_{\beta=1}^{N_s} \chi_\beta^\alpha \left(\rho_{\text{SSD}}^\beta + |\rho_{\text{eGND}}^\beta| + |\rho_{\text{sGND}}^\beta| \right)}, \quad (5)$$

where τ_c^0 is a constant Peierls stress, needed to move a dislocation within a plane of atoms, α_0 is the Taylor hardening prefactor, μ is the shear modulus, b the Burgers vector length. Each slip system is characterised by three state variables quantifying the dislocation density, these are: ρ_{SSD}^α , the statistically stored dislocation (SSD) density, $\rho_{\text{eGND}}^\alpha$ and $\rho_{\text{sGND}}^\alpha$, the density of geometrically necessary dislocations (GND) with edge and screw character respectively. This model choice is important to quantify the effect of slip gradients and of the grain size and morphology on the stress state. This is necessary because the stress state near grain boundaries determines intergranular fracture nucleation due to void formation [71]. χ_β^α is the latent hardening matrix that describes the interaction hardening effect induced by the slip system β on the slip system α . In FCC crystals, this is described using a symmetric 12×12 matrix whose entries represent different types of interactions between the slip systems, such as self-interaction, co-planar, cross-slip, glissile dislocations, Hirth and Lomer-Cottrell locks. The specific form of the matrix is report in Franciosi et al. [70], while the values of χ_β^α for the different types of interactions in 316H are given in table 1.

The evolution law for the SSD density ρ_{SSD}^α includes the dislocation multiplication and annihilation [72, 73]:

$$\dot{\rho}_{\text{SSD}}^\alpha = \left(k_m \sqrt{\rho_{\text{SSD}}^\alpha + |\rho_{\text{eGND}}^\alpha| + |\rho_{\text{sGND}}^\alpha|} - 2y_c \rho_{\text{SSD}}^\alpha \right) \frac{|\dot{\gamma}^\alpha|}{b}, \quad (6)$$

where k_m is the accumulation rate, y_c is the critical annihilation distance for adjacent dislocations, which has been measured accurately for 316 stainless steel [74]. The evolution law for ρ_{SSD}^α can reproduce hardening and saturation in FCC metals and the parameters will be calibrated by comparing the simulation results with experimental stress-strain curves. The evolution of the GND density is calculated using slip gradient [27], specifically their projections along the slip direction, \mathbf{s}^α and along the edge dislocation line direction, \mathbf{t}^α [75]:

$$\dot{\rho}_{eGND}^\alpha = -\frac{1}{b}\nabla\gamma^\alpha \cdot \mathbf{s}^\alpha , \quad (7)$$

$$\dot{\rho}_{sGND}^\alpha = -\frac{1}{b}\nabla\gamma^\alpha \cdot \mathbf{t}^\alpha . \quad (8)$$

These relationships incorporate a length-scale dependence of the CRSS in the model, which is essential to capture the stress state near grain boundaries [76]. The edge dislocation line direction, which is equivalent to the direction of motion of positive screw dislocations is calculated as:

$$\mathbf{t}^\alpha = \mathbf{s}^\alpha \times \mathbf{n}^\alpha . \quad (9)$$

The relationships (7) and (8) are calculated numerically by representing $\dot{\gamma}^\alpha$ with linear shape functions. The specific interpolation in each element is carried out by using the numerical values of $\dot{\gamma}^\alpha$ calculated from (4) at the integration points. In this section, the evolution laws of the plastic deformation gradient as a function of the stress state have been presented, while in the next section, the damage model, together with the stress calculation, will be shown. The equations of the CPFE model have been implemented into a UMAT subroutine, which can be utilized with different solvers.

2.2. Phase Field Damage Formulation

The phase field damage model is coupled with the crystal plasticity formulation in section 2.1 to describe damage nucleation and propagation during both plastic and creep deformation. It is based on a continuum damage variable c that can take any value between 0 and 1 [77]. Here, c indicates the damage level of the material where a value of 0 indicates undamaged material and 1 indicates entirely damaged material. This model is based on a free energy formulation, in which the free energy per unit volume includes the mechanical part Ψ_m and the energy released by fracture surfaces Ψ_f , which is regularised as an integral over the volume of the domain Ω [78]:

$$\Psi_f = \int_\Omega G_c \gamma(c, \nabla c) dV = \int_\Omega \frac{G_c}{2} \left(\frac{c^2}{l_0} + l_0 |\nabla c|^2 \right) dV , \quad (10)$$

where G_c is the critical energy release rate for fracture defined in Griffith's theory [79], $\gamma(c, \nabla c)$ is the regularised crack energy functional and l_0 is the characteristic regularisation length-scale, dictating the diffusiveness of the damage field. To incorporate the twist and tilt of a grain boundary, characterised by a misorientation angle $\Delta\theta$, G_c is set as a function of the coordinates. Specifically, it depends on the misorientation between neighbouring grains $\Delta\theta$ near a grain boundary, while it has a constant value in the inner part of grains, as detailed

in section 2.3. The mechanical free energy Ψ_m is decomposed into a part that drives the damage evolution, a^+ , and a part that is not affected by damage, a^- :

$$\Psi_m = \int_{\Omega} a \, dV = \int_{\Omega} [(1 - c)^2 + k_r] a^+ \, dV + \int_{\Omega} a^- \, dV , \quad (11)$$

where k_r is a small residual stiffness, which is necessary for convergence when parts of the representative volume are completely damaged. $a^+(\mathbf{F}_e)$ and $a^-(\mathbf{F}_e)$ are functions of the elastic deformation gradient \mathbf{F}_e . A dissipation function \mathcal{D} is introduced, which represents the plastic work rate \dot{W}_p , whose form follows that of Lee et al. [80, 81]:

$$\mathcal{D}(\mathbf{F}_e, \mathbf{F}_p, \dot{\mathbf{F}}_p) = \dot{W}_p = \int_V \text{tr}(\boldsymbol{\sigma} \mathbf{F}_e \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \mathbf{F}_e^{-1}) \det(\mathbf{F}_e) \, dV . \quad (12)$$

For the monotonic loads used in the present work, W_p is the total plastic work done, a monotonically increasing function. Since in a finite strain anisotropic medium the elastic energy cannot be decomposed into a part given by the volumetric strain only and a part given by the isochoric strain only, an effective bulk modulus K_0 will be used in the following:

$$K_0 = \frac{1}{9} \sum_{i,j=1}^3 \mathbb{C}_{iijj} , \quad (13)$$

where \mathbb{C} is the fourth-order stiffness tensor. The part of the mechanical Helmholtz free energy that drives damage is decomposed as follows:

$$a^+ = a_{\text{cpl}}^+ + a_{\text{vol}}^+ , \quad (14)$$

where a_{vol}^+ is the positive volumetric free energy, a_{cpl}^+ is the coupled free energy, which is defined as the difference between the total mechanical free energy of the anisotropic medium and the volumetric part of an equivalent isotropic linear elastic material with bulk modulus K_0 . The part of the mechanical Helmholtz free energy that is not affected by damage is equivalent to the negative volumetric free energy:

$$a^- = a_{\text{vol}}^- , \quad (15)$$

which represents the fact that, typically, volumetric compression does not induce damage in metals. The dissipation function in (12) depends on the damage phase field through the Cauchy stress $\boldsymbol{\sigma}$. The positive and negative volumetric free energies are calculated as:

$$a_{\text{vol}}^+ = \begin{cases} \frac{1}{2} K_0 \omega^2 , & \text{if } J_e \geq 1 , \\ 0 , & \text{if } J_e < 1 , \end{cases} \quad (16)$$

$$a_{\text{vol}}^- = \begin{cases} 0 , & \text{if } J_e \geq 1 , \\ \frac{1}{2} K_0 \omega^2 , & \text{if } J_e < 1 , \end{cases} \quad (17)$$

where:

$$\omega = \frac{3}{2} (J_e^{2/3} - 1) , \quad (18)$$

is the elastic volumetric expansion. The coupled free energy is given by:

$$a_{\text{cpl}}^+ = \frac{1}{2} \sum_{i,j=1}^3 \sum_{k,l=1}^3 \mathbb{C}_{ijkl} (\mathbf{E}_e)_{ij} (\mathbf{E}_e)_{kl} - \frac{1}{2} K_0 \omega^2 , \quad (19)$$

where the Green-Lagrange elastic strain tensor, \mathbf{E}_e , is given by:

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \mathbf{F}_e - \mathbf{I}) = \frac{1}{2} (\mathbf{C}_e - \mathbf{I}) , \quad (20)$$

where \mathbf{C}_e is the right elastic Cauchy-Green tensor and \mathbf{I} is the identity matrix. The coupled free energy a_{cpl} corresponds to the free energy given by the deviatoric strain in the small strain formulation. Overall, the second Piola-Kirchhoff stress tensor \mathbf{S} is derived by:

$$\mathbf{S}_{ij} = \frac{\partial a}{\partial (\mathbf{E}_e)_{ij}} = \begin{cases} [(1-c)^2 + k_r] \sum_{k,l=1}^3 \mathbb{C}_{ijkl} (\mathbf{E}_e)_{kl} , & \text{if } J_e \geq 1 , \\ [(1-c)^2 + k_r] \left(\sum_{k,l=1}^3 \mathbb{C}_{ijkl} (\mathbf{E}_e)_{kl} - J_e^{2/3} K_0 \omega \mathbf{C}_e^{-1} \right) + J_e^{2/3} K_0 \omega \mathbf{C}_e^{-1} , & \text{if } J_e < 1 . \end{cases} \quad (21)$$

Note that the dissipation function does not depend on the time derivative of \mathbf{E}_e , thus it does not contribute to the stress tensor [80]. However, it depends on the damage phase field, hence the plastic work affects the time evolution of c . Note that the stress degradation under a tensile load represents a loss of stiffness, which can be interpreted as the presence of voids in the system. The evolution of c is determined by the minimization of the sum of the free energies, Ψ_f , Ψ_m and of the dissipation function \mathcal{D} . However, in this work, a rate-dependent approach is adopted, based on an Allen-Cahn equation, which ensures the local growth of the fracture phase field [82, 83]:

$$\dot{c} = \frac{1}{\eta} \left\langle l_0 \Delta c - \frac{c}{l_0} + 2(1-c) \frac{(a^+ + \beta W_p)}{G_c} \right\rangle \quad (22)$$

where η is a kinetic coefficient, and $\langle \rangle$ indicate McCauley brackets, where $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = -x$ if $x < 0$. β is a prefactor of the plastic work contribution, taking values between 0 and 1. Even though, originally, the phase field fracture model was based on the elastic strain energy only [84, 85], a modification to include the plastic work into the damage evolution law is used in the present work. In the following, simulations are carried out with both $\beta = 0$ and $\beta = 1$; the comparison with experiments reveals the contribution of plastic work to local damage. Including the contribution to damage from both volumetric and isochoric strain is important for metals because the effect of stress triaxiality is required to characterise fracture nucleation in ductile materials [48]. For instance, both terms are included to predict the yield strength and void volume fraction in models such as the Gurson-Tvergaard-Needleman [86]. The hypothesis that is being tested in this work is that the damage phase field c is representative of the void nucleation, as compared to experimental

measurements of the void fraction. Details of the algorithm used for determining the plastic deformation gradient and the stress at each time step is presented in [Appendix A](#), in particular the Jacobian calculation that is required for the coupled plasticity-damage model, which has not been previously reported in the literature. The CPFE model is coupled with phase field fracture using the MOOSE multiphysics finite element framework [63]. A monolithic solver is used for the stress equilibrium (1) and for the damage evolution (22), which is based on the preconditioned Jacobian-free Newton-Krylov method, which provides an increased computational efficiency [87]. Specifically, the hypre BoomerAMG algebraic multigrid solver has been chosen, both as a solver and as a preconditioner, because of its speed [88].

2.3. Misorientation dependent critical energy release rate

To characterise the strength of different types of grain boundaries, the local critical energy release rate G_c is set as a function of the local misorientation angle $\Delta\theta$. This is defined in each element of the mesh as the maximum misorientation between the element and its neighbours. The scalar misorientation $\Delta\theta$ between two neighbouring points A and B, whose orientation is described by rotation matrices \mathbf{R}_A and \mathbf{R}_B , is determined based on the misorientation matrix $\Delta\mathbf{R}_{AB} = \mathbf{R}_A^{-1}\mathbf{R}_B$, as detailed in [89]. Specifically, the rotation matrices are calculated in each element by considering the Euler angles obtained from EBSD measurements. 432 FCC crystal symmetry operation matrices \mathbf{G}_i (with $i = 1, \dots, 24$) must be accounted, which are explicitly reported in [Appendix B](#). This is because symmetry operations do not change the atomic arrangement in a grain, but they affect the misorientation calculation. Therefore, all possible combinations of symmetry operations are applied to the rotation matrices \mathbf{R}_A and \mathbf{R}_B before the scalar misorientation calculation is carried out; the minimum between all possible results is selected. Mathematically, $\Delta\theta$ can be defined as [90]:

$$\Delta\theta = \min_{i,j} \left(\arccos \left(\frac{\text{Tr}(\mathbf{G}_i^{-1}\mathbf{R}_A^{-1}\mathbf{R}_B\mathbf{G}_j) - 1}{2} \right) \right) \quad (23)$$

where i, j are pairs of indices with $i = 1, \dots, 24$ and $j = 1, \dots, 24$. This definition of scalar misorientation provides values in the interval from 0° to about 62° .

To understand the effect of the grain boundary carbides on grain boundary strength, different functions $G_c(\Delta\theta)$ are used in the simulations. The higher density of carbides observed in the microscopy experiments at $\Delta\theta = 27^\circ$, as detailed in section [6.2](#), has motivated the choice of trial functions $G_c(\Delta\theta)$ with a minimum value at that specific misorientation angle. Specifically, three different dependencies are used: linear, quadratic, and trapezoidal, as shown in figure [1\(a\)](#). Simulations using these functions will be used to find the best agreement with the misorientation dependence of damage nucleation in the high temperature mechanical test. The minimum and maximum values of $G_c(\Delta\theta)$ will be calibrated by comparing with the measured cavitation ratio during the experiment. Thus, the reduction of the grain boundary critical energy release rate due to the carbides can be determined. The interval of $(\Delta\theta)$ in figure [1\(a\)](#) starts from 10° because that is the smallest misorientation observed among the grain boundaries in the analysed polycrystal. An example of G_c as a function of the position in the analysed polycrystal structure is shown in figure [1\(b\)](#), where

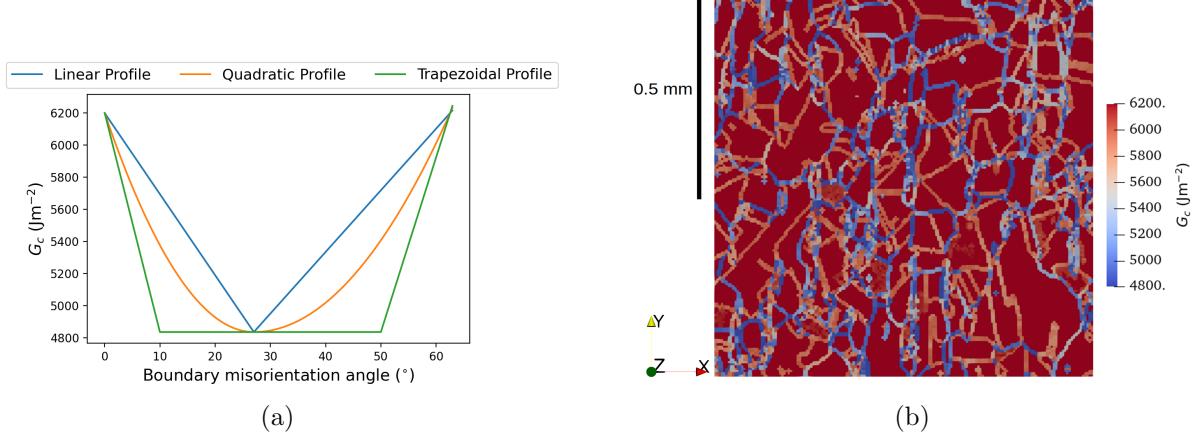


Figure 1: (a) Local critical energy release rate G_c as a function of the misorientation angle $\Delta\theta$ for the three analysed profiles. (b) The variation in G_c across differently oriented boundaries in the analysed polycrystalline structure for the trapezoidal profile.

the blue regions correspond to the grain boundaries with the lowest critical energy release rate.

The variation in the critical energy release rate is applied on an element by element basis. Since the misorientation angle is only calculated for two elements either side of a grain boundary, only these elements have the modified value of G_c . The characteristic length-scale of the phase field model was approximately half the element size at 3 μm .

3. Experimental Characterisation

He et al. [45] have recently investigated the use of correlative microstructural characterisation in creep cavitation in 316H stainless steel, but a systematic comparison with microstructural simulations was not carried out. The material studied was extracted from an ex-service boiler header made of type 316H austenitic stainless steel, whose chemical composition is given in table 2. The component was provided by EDF Energy Ltd. and it was first operated at a temperature between 490°C and 530°C for 65000 hours in a steam header.

Electron microscopy characterisation of a 316H stainless steel sample after high temperature deformation was carried out, the aim of which was to test the CPFE model to understand the contributions of different mechanisms to damage nucleation. A key component of this was to conduct direct comparisons to experimental samples over the same microstructure to identify which regions of high damage can be explained by certain mechanisms.

A uniaxial high temperature specimen with a double notch, each of 0.74 mm radius, and a notch diameter to notch root ratio of 10 was used. The longitudinal section is shown in figure 2(a). The sample was mechanically tested under strain control: first, the strain is increased linearly, until a far field stress value of 390 MPa is reached, leading to plastic

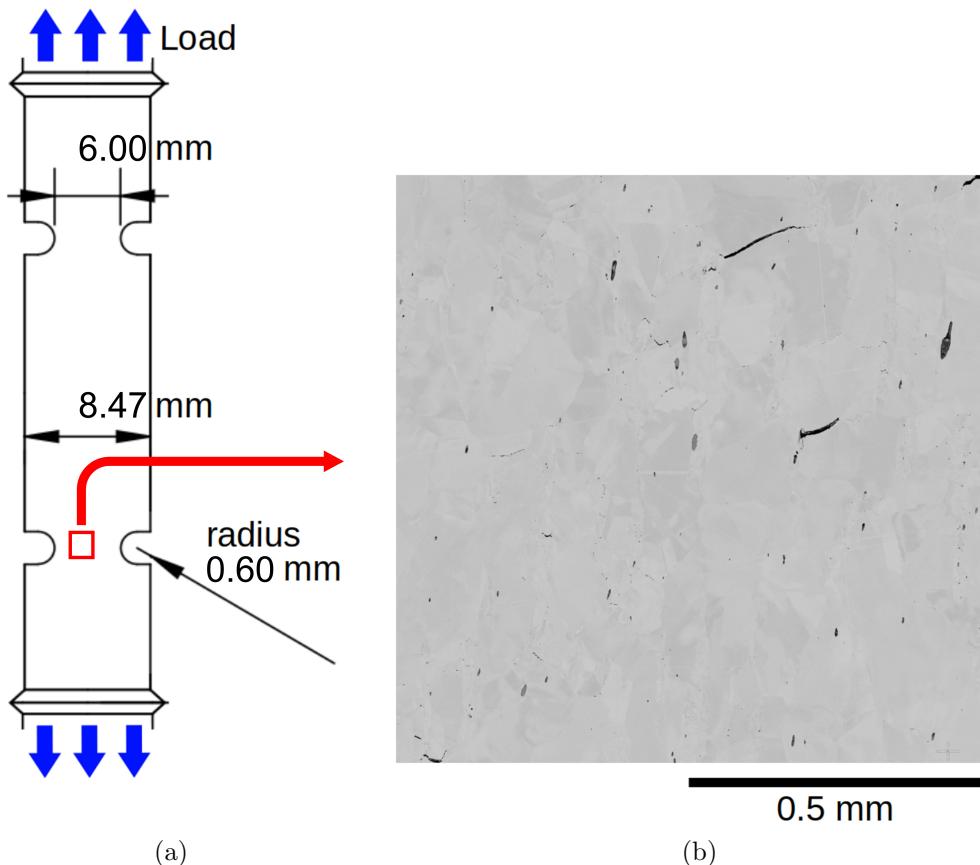


Figure 2: (a) Notched specimen and (b) An SEM image of the area of interest for the cavitation measurement; black spots indicate damaged regions.

deformation near the notch; second, stress relaxation due to creep deformation take place at constant strain for 500 hours; third, the strain is increased until 390 MPa is reached again. This procedure is repeated 25 times; thus the total dwell time is 25×500 hours.

| C | Si | Mn | P | S | Cr | Mo | Ni | B | Co | Fe |
|-------|-------|-------|-------|-------|--------|-------|--------|-------|-------|--------|
| 0.060 | 0.400 | 1.980 | 0.021 | 0.014 | 17.170 | 2.190 | 11.830 | 0.005 | 0.100 | 66.230 |

Table 2: The nominal composition of the ex-service 316H stainless steel header material (mass %).

The tested specimen was cut axially across the centre of the notch for correlative microstructural characterisation. Correlative Electron Backscatter Diffraction (EBSD) and Scanning Electron Microscopy (SEM) microstructural characterisation was performed by scanning across the notch section with both techniques and correlated in spatial coordinates through post image processing. A Zeiss SigmaHD FEG-SEM equipped with a DigiView 3 EBSD detector was used for the EBSD and SEM characterisation. The EBSD data was obtained at a voltage of 25 kV and a step size of 3 μm , while the SEM at 20 kV voltage.

The image segmentation software Dragonfly (Object Research Systems [ORS] Inc., Canada) was then applied to segment creep cavities from the SEM image. The segmentation was performed with a deep-learning platform in the Dragonfly software which was trained with randomly selected SEM frames, followed by manual work to reduce errors of automatic segmentation. The EBSD data in this study was processed by MTEX toolbox [91], where grain boundaries were calculated. In-house MATLAB scripts were written to project the segmented creep cavity data from Dragonfly onto the grain boundary data from EBSD, using fiducial marks inserted onto the specimen every 1 mm by focused ion beam (FIB) to calibrate the images. The combined cavity and grain orientation data has been used to study correlations between local microstructure and damage initiation [62]. The competing processes acting for damage formation in such specimens will be plastic void initiation as well as creep cavitation. Due to the stress induced of 390 MPa being well above the yield stress of the material at 550°C, it is posited that plastic void initiation and growth is the dominant mechanism acting.

4. Simulation setup and model calibration

The effect of different damage criterion is investigated in sections 6.1 and 6.3. The reference elastic strain energy damage model in section 6.1 and the elastoplastic damage model in section 6.3 refer to the same phase field model only with β in equation 22 taking on a value of 0 or 1, respectively. In the reference elastic strain energy damage model, $\beta = 0$, meaning that only the Helmholtz free energy contribution to damage resulting from elastic strain is included. In the elastoplastic damage model, where $\beta = 1$, the Helmholtz free energy contributions from both elastic strain as well as permanent plastic deformation are included in the evolution of the damage field.

4.1. Material Parameters

Figure 3 shows the experimental and simulated stress-strain curves. Standard values were obtained from the literature for the elastic constants of 316H stainless steel [23]. The calibrated material parameters are shown in table 3. Some parameters such as the accumulation rate coefficient K , or the initial SSD density, ρ_{SSD} , were obtained using a `scipy.optimize` in-house tool, called PyDakota [92]. Initially, the residual between an output stress strain curve taken from the CPFE model and a stress strain curve on the same material at the same temperature is calculated. A non-gradient based Nelder-Mead algorithm was used to determine the next generation values of K and ρ_{SSD} , and this process was repeated until an agreement between the curves from the experiment and the CPFE model was achieved.

Initially in the plastic and creep plasticity deformation model simulations shown in section 6.4, plasticity and creep deformation terms were both included before the plasticity term is switched off and the creep term is allowed to continue until the matching experimental time had elapsed. The reasoning for this was twofold: to better match experimental conditions which consisted of an initial tensile straining before a lengthy dwell time at constant load, and that limitations on computational processing make crystal plasticity an unfavourable

approach for long simulations such as these. Input parameter calibration for the creep deformation term was done through a similar iterative process in comparing output data to reference experimental specimen data. Since the range over which the stress strain curve for input parameters lay within the same stress range as that of the experimental specimen, the parameter choice and calibration is justified. The calibrated value of the annihilation length ensured that the model maintains the saturation behaviour of dislocation densities after linear hardening.

4.2. Material Critical Energy Release Rate Calibration

G_c is the critical energy release rate of the material used in the phase field model. It describes the threshold energy that the Helmholtz free energy must exceed locally for the phase field to rapidly evolve at that point. It dictates both the early evolution behaviour of damage initiation as well as the final strain to fail when subjected to tensile conditions. Using an engineering strain to failure value of 35%, similar to those observed in the literature [93], a set of simulations were used with varying values of G_c over a sample section of the EBSD microstructure to the point of failure. A plot relating the strain for failure of the simulated material against the initial value of G_c was used to determine an appropriate value of G_c that would result in the expected strain to fail in the model.

From the graph shown in figure 3, the initial value of G_c was determined using the phase field model based on the elastic strain energy to damage to be 6200 Jm^{-2} . A similar procedure was followed with the amended phase field model containing a formulation to include both the elastic and plastic strain energy and G_c was determined to have a value of approximately 10500 Jm^{-2} . The EBSD microstructure displaying the phase field value once crack propagation was achieved is shown within figure 3(b).

5. Simulation Analysis Procedure

The simulation output data visualisation and analysis was done using a combination of ParaView and Python. An algorithm was designed to determine whether any element lay on a boundary to analyse the initiation of grain boundary damage. Each element orientation was compared to that of the adjacent elements. If any of the orientation Euler angles differed by a misorientation angle of more than ten degrees both the element and the adjacent were logged. Specific element data could then be picked out and analysed. A series of microstructural factors were investigated. Firstly, He et al. [45], found little correlation between boundary Schmid factor difference and average boundary Schmid factor with grain boundary damage. The Schmid factor, m , of each slip system, α , for each grain was calculated using the rotation matrix \mathbf{R}_{ij} , based on Euler angle orientations and the slip plane normals and directions, \vec{n} and \vec{s} respectively:

$$m = (\mathbf{R}_{ij}^a \cdot \vec{s}_\alpha) \cdot (\mathbf{R}_{ij}^a \cdot \vec{n}_\alpha) . \quad (24)$$

The slip system resulting in the greatest value of m for a particular grain orientation was used moving forward to calculate the arithmetic mean Schmid factor across a grain boundary and the difference in Schmid factor across a grain boundary. It should be noted

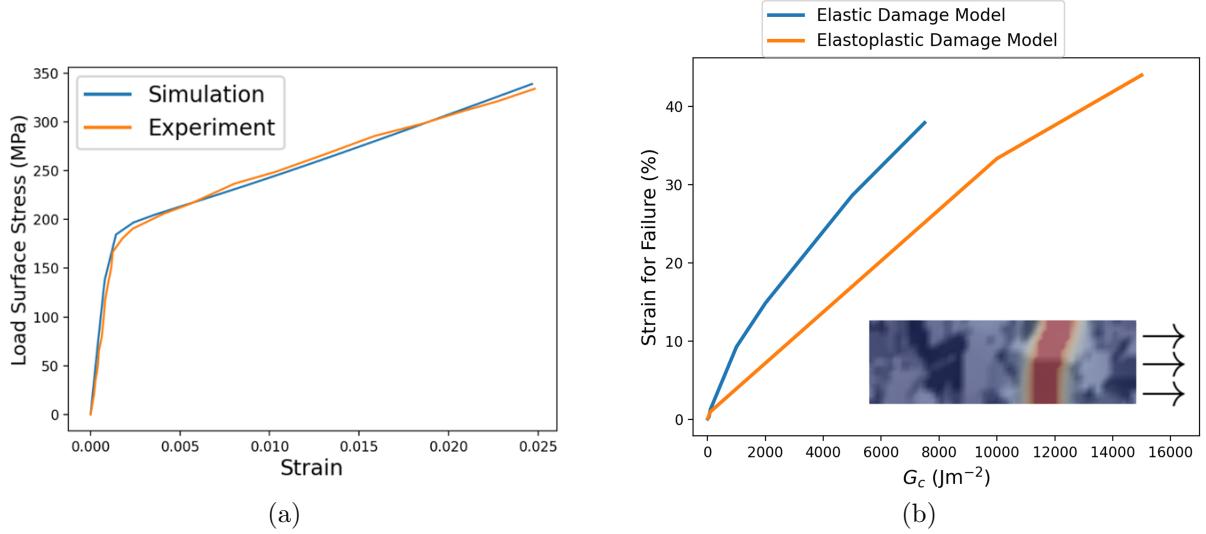


Figure 3: (a) The calibrated crystal plasticity output stress strain curve for 316H stainless steel under uniaxial tension at 550°C with the literature data for calibration using a `scipy.optimize` procedure [94]. (b) Calibration of the critical energy release rate using the strain to failure. The value of G_c determined for the reference elastic strain energy damage model was 6200 Jm^{-2} . For the elastoplastic damage model, the value of G_c determined was 10500 Jm^{-2} . The bottom left displays the output microstructure at failure, with red showing the crack path defined by the phase field and black showing the grain structure.

that the Schmid factor does not necessarily indicate which specific slip system is primarily active. For example, this can occur in the presence of obstructions such as second phases, inclusions, precipitates, or other obstructions to slip.

Secondly, a question to be addressed by the analysis here was to determine the magnitude of the influence of grain boundary misorientations on the formation of intergranular damage within a structure. The grain misorientation angle as determined by the relative orientations of two adjacent grains and the underlying crystal structure of both grains was calculated using the methodology described in section 2.3.

To draw a correlation between cavities in experimental samples and the continuous phase field damage variable within the simulated microstructure, there is no accepted standard on how this should be done. For the purposes of this work, a threshold damage value, c_0 , was determined relative to the maximum damage observed within the microstructure for a given simulation, c_{\max} using a threshold prefactor, λ , which could take a value between 0 and 1.

$$c_o = \lambda \cdot c_{\max} \quad (25)$$

If a grain boundary element, i , had a phase field damage value, c_i greater than or equal to this threshold $c_0 = \lambda \cdot c_{\max}$, then cavitation was said to have occurred. Therefore, the cavitation condition is $c_i \geq c_o$.

Each grain boundary element pair was categorised in this way, before being sorted by their misorientation angle into bins of 1° width. The proportion of elements that met the threshold condition $c_i \geq c_o$ was defined as the cavitation ratio. To determine the value of

λ to be used, the average cavitation ratio found by He et al. was 0.27, with a value of λ found that resulted in the same average cavitation ratio in the simulated microstructure. The Pearson product moment correlation coefficient was calculated to assess the relationship between microstructural and model parameters with the simulated phase field.

Finally, the applicability of the phase field model in predicting which individual grain boundaries were most susceptible to cavitation was assessed. The set of grain boundary elements was sorted by the value of the phase field, with the location of the two hundred points with the highest damage within the simulation marked on the EBSD image alongside points of high damage determined by He et al. [45], which are plotted in figure 10 as red scatter points.

6. Results

The objective of the following analysis detailed below was to assess the applicability of the implemented crystal plasticity phase field approach to predicting damage initiation. Comparisons were drawn between experimental results of He et al., [45], on a sample of 316H stainless steel with the reference elastic strain energy damage crystal plasticity phase field model, an elastoplastic strain energy based damage model, a combined creep plasticity deformation model, and a phase field model with a grain misorientation dependent critical energy release rate. Correlations between output model parameters and input microstructural parameters with the phase field damage value at grain boundary elements were determined and compared to those determined experimentally.

In section 6.1, the reference elastic strain energy damage model was used to find the correlation between the phase field value at grain boundary elements with the Schmid factors of adjacent grains, as well as the loading direction stress, and local densities of statistically stored and geometrically necessary dislocations. Afterwards, the cavitation ratio against boundary misorientation angle is compared with the equivalent experimental analysis alongside a comparison of individual grain boundaries most susceptible to cavitation. Section 6.2 presents analysis of the cavitation ratio and specific grain boundaries including the implementation of a misorientation dependent critical energy release rate, G_c . Finally, sections 6.3 and 6.4 detail similar analysis for the elastoplastic damage model and creep plasticity deformation model, respectively.

6.1. Reference Elastic Strain Energy Damage Model

In this section, the reference elastic strain energy damage model, with $\beta = 0$ in (22), is used. The EBSD microstructure determined by He et al. [62] for 316H austenitic stainless steel was recreated based on the Euler angles using MOOSE, shown in figure 4. The model had tensile boundary conditions applied to simulate uniaxial tensile loading up to 1.5% strain in the positive Y direction, with free boundary conditions applied to positive faces in X and Z. The negative faces in X, Y, and Z were held fixed at zero displacement. The strain amplitude in the region of interest, which was located close to the notch in the specimen, has been determined using macroscopic finite element simulations in previous works [95, 45]. The reference simulation used the coupled crystal plasticity phase field fracture model considering

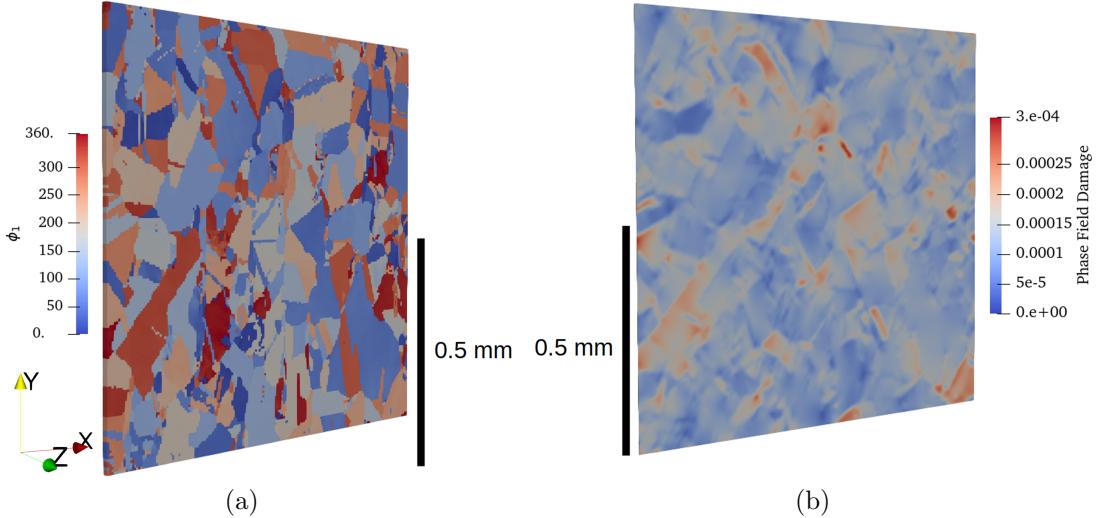


Figure 4: (a) The experimentally determined EBSD microstructure simulated of 316H stainless steel, upon which cavitation analysis statistics. (b) The resulting phase field across the microstructure using the reference elastic strain energy damage model.

only the elastic strain energy contributing to damage evolution. This was implemented by setting the plastic work inclusion factor $\beta = 0$. The model and material parameters used are shown in Table 3, including the elastic constants of 316H stainless steel in Voigt notation.

In figure 5(a), the relationship between the average between the Schmid factors (maximum among the slip systems) at pairs of elements across grain boundaries is compared to the phase field damage. In figure 5(b), the same is done for the difference between the Schmid factors (maximum among the slip systems). A very weak correlation was found between the phase field damage at grain boundary elements with the average boundary Schmid factor and difference in boundary Schmid factor, in agreement with experimental observations from He et al. [45]. However, it is evident that the range of the damage increases with the average Schmid factor, while it decreases with the difference in Schmid factor, indicating that more plastic activity in the pair of grains is more likely to induce more damage.

A linear regression has been used to provide bounds in each plot for the range within which 95% of the data sits, denoted by the area highlighted in red in figures 5, 6, and 7. A simulation including the effect of geometrically necessary dislocations (GNDs) was also run using the reference elastic strain energy damage model to detail the relation to the phase field damage as well as that from statistically stored dislocations (SSDs). Figure 6 details the relation between SSDs and GNDs at grain boundary elements with the phase field damage value. A strong correlation with the total SSD density and microstructural damage with a coefficient of 0.90 was determined. GNDs were found to have a weaker correlation with a coefficient of 0.46. Figure 7 shows how grain boundary element stress in the loading direction induces damage. As would be expected, higher stress elements are more susceptible to damage initiation, with a correlation coefficient of 0.47 determined.

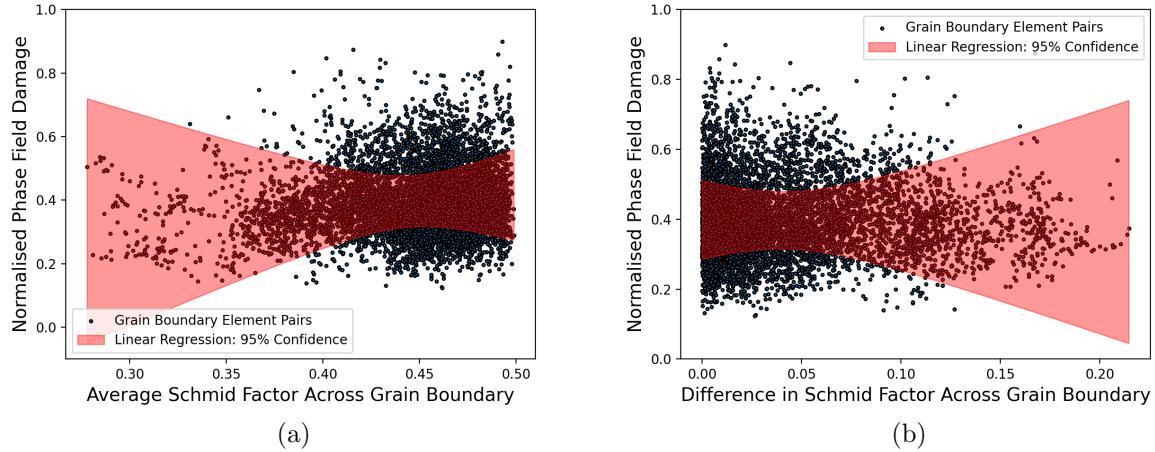


Figure 5: (a) The average between the Schmid factor (maximum among the slip systems) across a grain boundary against grain boundary phase field damage for a number of element pairs. (b) The difference in Schmid factor (maximum among slip systems) across a grain boundary against grain boundary phase field damage for a number of element pairs.

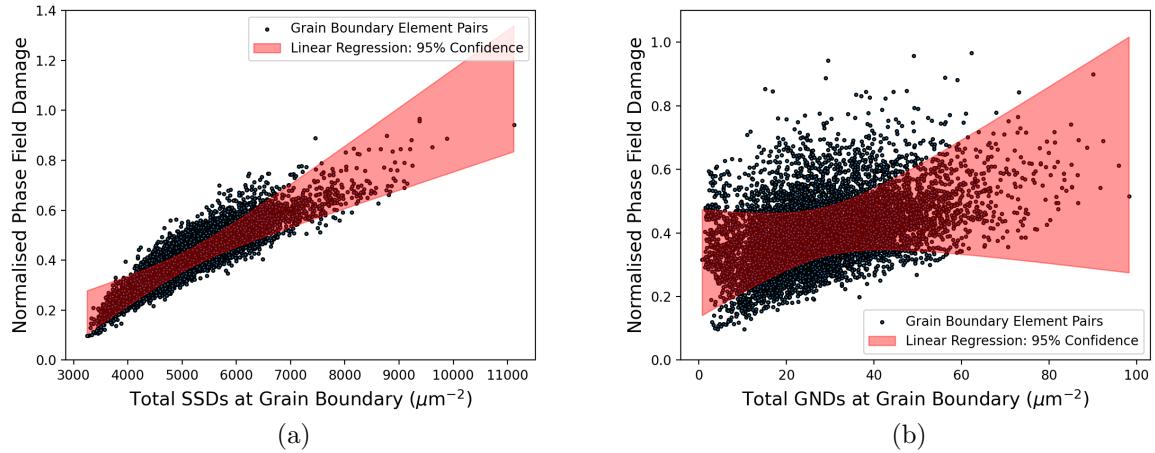


Figure 6: (a) A plot of phase field damage against the density of statistically stored dislocations across a grain boundary. The Pearson product moment correlation coefficient recorded was 0.90. (b) A plot of the normalised phase field damage against the total density of geometrically necessary dislocations (GNDs) across all slip systems at grain boundary elements. The Pearson product moment correlation coefficient calculated was 0.46.

Table 3: Calibrated material and model parameters.

| | |
|--|----------------------------------|
| Number of Elements | 28730 |
| Temperature (T) | 823 K |
| Elastic constant C_{11} at $T = 550^\circ\text{C}$ | 204.6 GPa |
| Elastic constant C_{12} at $T = 550^\circ\text{C}$ | 137.7 GPa |
| Elastic constant C_{44} at $T = 550^\circ\text{C}$ | 126.2 GPa |
| Shear modulus (μ) | 86 GPa |
| Initial SSD density (ρ_{SSD}^α) | 257.36 μm^{-2} |
| Initial GND Density - Edge ($\rho_{\text{eGND}}^\alpha(t=0)$) | 0.0 μm^{-2} |
| Initial GND Density - Screw ($\rho_{\text{sGND}}^\alpha(t=0)$) | 0.0 μm^{-2} |
| Reference Slip Rate ($\dot{\gamma}_0^s$) | 0.001 s^{-1} |
| Section 6.4 - Reference Creep Slip Rate ($\dot{\gamma}_0^c$) | $3 \cdot 10^{-8} \text{ s}^{-1}$ |
| Slip strain rate sensitivity exponent (m_s) | 0.1 |
| Section 6.4 - Creep strain rate sensitivity exponent (m_c) | 0.1 |
| Peierls stress (τ_c^0) | 0.112 MPa |
| Burgers vector (b) | 0.256 nm |
| Taylor hardening prefactor (α_0) | 0.3 |
| Dislocation accumulation rate (k_m) | 1.13 |
| Dislocation Capture Radius (y_c) | 1.3 nm |
| Room temperature (T_0) | 293 K |
| Characteristic Phase Field Model Length-scale (l_0) | 3.0 μm |
| Section 6.1 - Critical Energy Release Rate (G_c) | 6200 J m^{-2} |
| Reference Elastic Strain Energy Damage Model | |
| Section 6.3 - Critical Energy Release Rate (G_c) | 10500 J m^{-2} |
| Elastoplastic Damage Model | |
| Damage kinetic coefficient (η) | 0.001 sm^{-1} |

6.2. Grain Misorientation Dependent Critical Energy Release Rate

Carbide precipitates are known to exacerbate material degradation and intergranular cavitation [22]. It has been established that carbide precipitation density varies with the

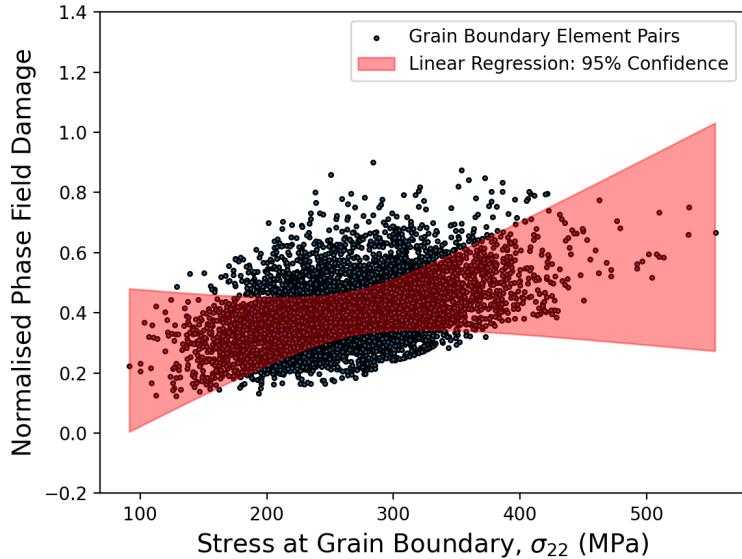


Figure 7: A plot of the phase field damage at grain boundary elements against the loading direction stress, σ_{22} , in MPa. The Pearson product moment correlation coefficient recorded was 0.47.

grain boundary misorientation angle, $\Delta\theta$, in various stainless steels experimentally [24, 25, 28, 29], with high angle boundaries of particular interest. By locally varying the value of G_c depending on the boundary misorientation angle, it is possible to model the effect of grain boundary misorientation and the presence of intergranular carbides in the aggregate to more accurately capture both large scale trends in damage initiation as well as predict boundaries and regions more susceptible to early damage formation.

Typically, grain boundary behaviour is separated into two categories, with mid angle boundaries separated from high and low angle boundaries. This was considered by using a simple model for a local reduction in G_c that varies with grain boundary misorientation angle. A transition point was selected as ten degrees from either end of the profile in figure 1, leaving the only free parameter to be varied as the size of the fractional reduction in G_c . By analysing the difference in overall damage trends and adjusting the scale of the reduction in G_c to maximise the Pearson product moment correlation coefficient between the cavitation ratio of the simulation and the experimental data, a quantitative estimate of the reduction in G_c caused by carbide precipitation and grain misorientation can be obtained through computational means. Additionally, linear, and parabolic profiles for G_c were simulated to assess the stability of results to profile shape as well as the minimum value of G_c . The profiles implemented can be seen in figure 1. In the following, the maximum and minimum values of $G_c(\Delta\theta)$ in figure 1(a) will be called G_{c0} and G_{cmin} . A range of simulations were run using the reference elastic strain energy damage model, with the minimum value of G_c given by:

$$G_{cmin} = \nu G_{c0}, \quad (26)$$

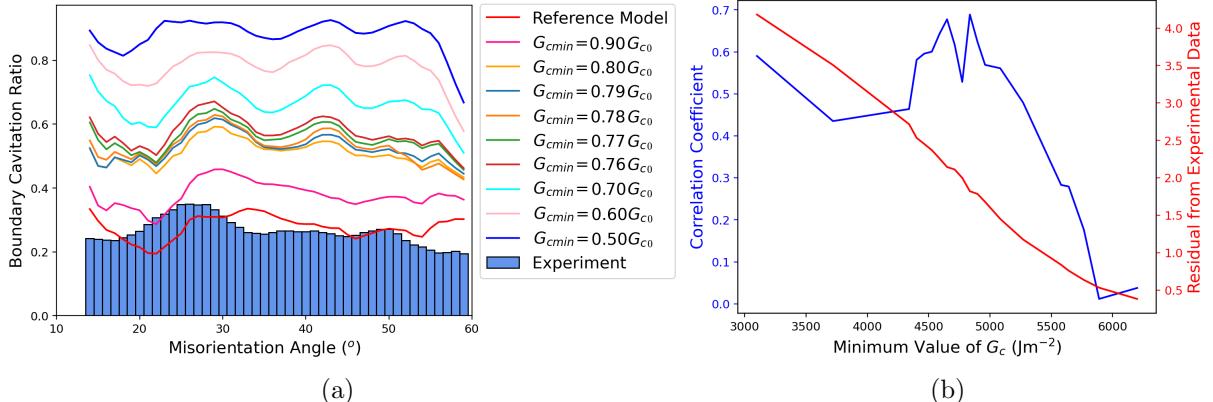


Figure 8: (a) A histogram of the experimentally determined cavitation ratio against boundary misorientation angle in 316H stainless steel compared with the simulated data with varying reductions in the critical energy release rate, G_c , for the trapezoidal profile from figure 1. (b) Plots of the correlation coefficient and the residual norm between the experimentally determined cavitation ratio and simulated data against the minimum critical energy release rate implemented. The optimal correlation was 0.69 for $G_c = 0.78G_{c0}$.

where ν is a scalar that was varied between 0.5 and 1 describing the fractional value of G_c . The model input parameters were otherwise identical to those used in section 6.1, which are reported in table 3.

Figure 8(a) shows the experimental and simulated grain boundary cavitation ratio as a function of the grain boundary misorientation angle $\Delta\theta$. Different curves represent simulations carried out with different values of G_{cmin} using the trapezoidal profile shown in figure 1. The Pearson product moment correlation coefficient between these two distributions is shown in figure 8(b) as a function of G_{cmin} . The threshold value, λ , used to determine cavitation was 0.45. For the analysis here, this value was taken using the uniform G_c model and was applied to subsequent simulations with varying G_c to reflect the increase in cavitation relative to the reference elastic strain energy damage model that occurs because of lowering the critical energy release rate. The same figure reports the residual as a function of G_{cmin} , which is the integral over $\Delta\theta$ of the absolute value of the difference between simulated and experimental data in figure 8(a). By varying the minimum value of G_c , the highest correlation of greater than 0.69 was found for $G_{cmin} = 0.78G_{c0}$. This is a substantial improvement in the correlation compared with the uniform G_c model, which has a correlation coefficient of 0.04 only. It corresponds to intergranular carbides and grain misorientation effects resulting in an approximate 22% local reduction in the critical energy release rate G_c . The optimum value of G_{cmin} found previously was then implemented using the linear and quadratic profiles shown in figure 1, with the boundary cavitation ratio shown for both alongside the trapezoidal model, experimental results, and the reference elastic strain energy damage model using an homogeneous G_c in figure 9. The highest correlation coefficient obtained was 0.71 using the quadratic profile, with the linear and trapezoidal profiles significantly more accurate than the reference elastic strain energy damage model with correlations of 0.53 and 0.69, respectively.

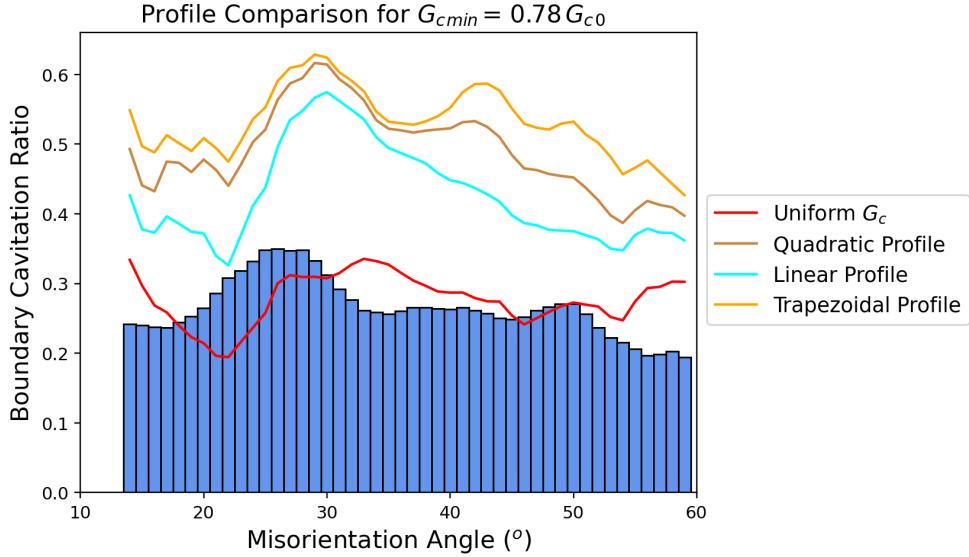


Figure 9: A histogram of the experimentally determined cavitation ratio against boundary misorientation angle in 316H stainless steel compared with the simulated data using the optimum fit value of $G_{c\min} = 0.78G_{c0}$ implemented using the linear, quadratic, and trapezoidal profiles from figure 1, as well as the reference homogeneous G_c model.

Using this misorientation dependent value of G_c , a comparison between damage initiation sites within the simulated microstructure was made to the same experimental sample. Figure 10 shows the EBSD microstructure used, with overlaid scatter plots detailing the two hundred highest damage points within the simulation and experimental structure. The objective of this analysis is to identify which grains and grain boundaries are susceptible to cavitation, not just matching specific elements. Out of eleven grain boundaries exhibiting the most significant cavitation experimentally, one was predicted by the reference elastic strain energy damage model seen in figure 10 as red scatter points. The implemented variation in G_c resulted in further two grain boundaries matching experimental cavitation data, seen as green scatter points.

6.3. Comparing the use of an Elastoplastic Strain Energy Damage Model

The reference elastic strain energy damage model was now used with the plastic work contribution to damage evolution implemented to produce an elastoplastic damage model, which was then applied over the same microstructure with identical input parameters except for $\beta = 1$, and the value of G_c , for which the calibrated value of 10500 Jm^{-2} was used. The boundary cavitation ratio across grain boundary elements was compared between the two damage models and that found from the experimental microstructure are shown below in figure 11.

The cavitation ratio as a function of misorientation angle was determined using a threshold value ν of 0.45 for both the reference elastic strain energy damage model and elastoplastic damage model was determined. A histogram below shows the same metric determined across the same microstructure using the correlative microscopy techniques described in section 3.

Grain Misorientation Dependent G_c , Damage Site Initiation

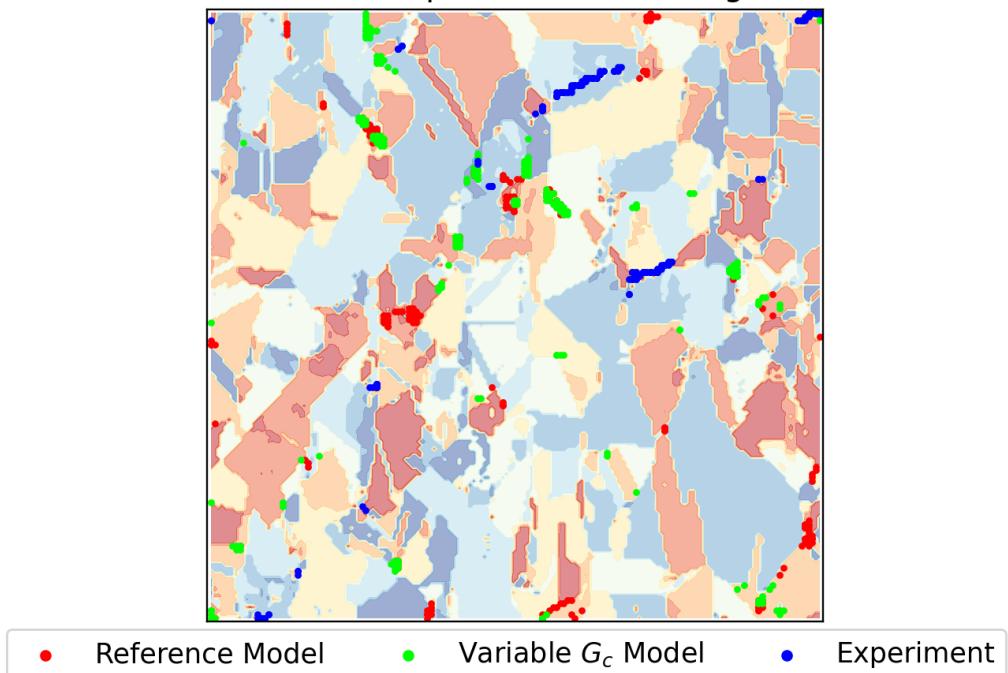


Figure 10: An EBSD microstructure overlaid with scatter plots of highly damaged regions within experimentally determined cavitation data as well a crystal plasticity simulation with the optimum misorientation dependent critical energy release rate implemented.

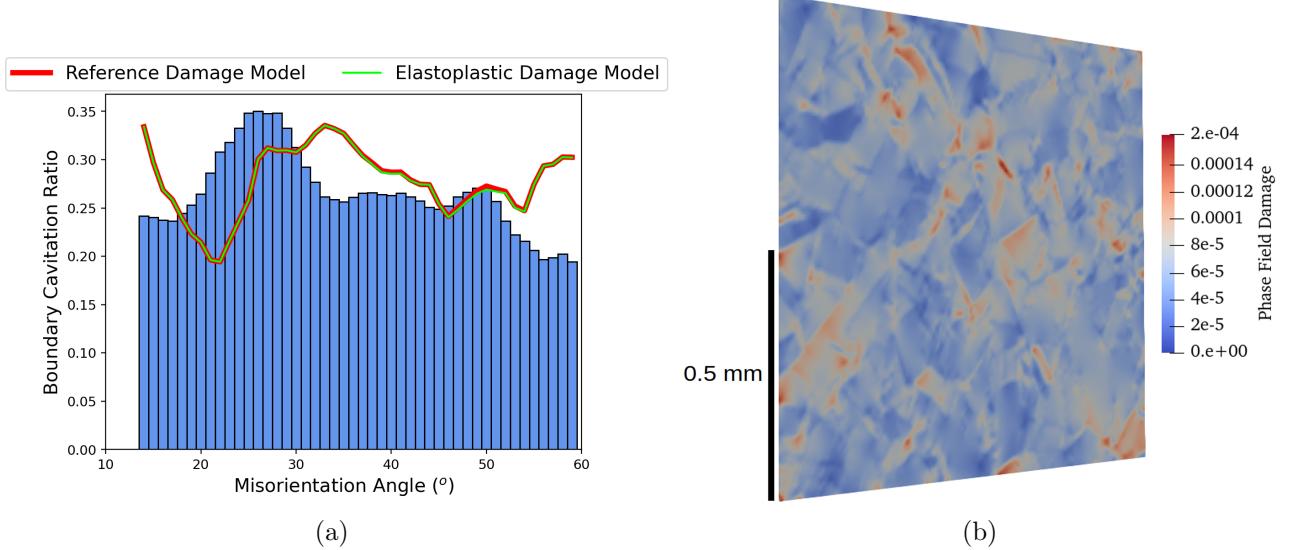


Figure 11: (a) Plots of the cavitation ratio against grain boundary misorientation for an experimental sample of 316H stainless steel, compared to the reference elastic strain energy damage model and elastoplastic damage model respectively with correlation coefficients of 0.04 and 0.03, respectively. (b) The damage field produced using the elastoplastic damage model over the microstructure shown in figure 4

The correlations found for the reference elastic strain energy damage model and elastoplastic damage model were 0.04 and 0.03, respectively. At the low strain levels imposed in these simulations, there is limited plastic deformation across the microstructure, meaning that the plastic work contribution term is small relative to that of elastic strain. Since both the reference elastic strain energy damage model and elastoplastic damage model had input values of G_c calibrated to ensure fracture at the same level of strain, the magnitude of the damage in figure 11(b) is lower, the pattern of damage initiation simulated in figure 11(a) and therefore the damage field obtained is almost identical, resulting in similar correlations with experimental analysis.

Finally, the positions and sites of cavity nucleation determined in an experimental sample were compared to those identified using both the reference elastic strain energy damage model and elastoplastic damage model. An image of the EBSD microstructure is shown in figure 12.

Within the EBSD microstructure, there were eleven grain boundaries that exhibited significant cavitation upon considering the two hundred highest points across the structure, seen as black scatter points in figure 12. The two hundred highest points within the reference elastic strain energy damage model and elastoplastic damage model are shown as green and red scatter points respectively in figure 12. The reference elastic strain energy damage model predicted only one of the eleven grain boundaries of interest, with the introduction of the plastic work contribution improving this to four of the eleven boundaries or grains of interest. It is suspected that large MnS inclusions which are not currently accounted for in the model are responsible for some of the significant cracks observed.

Effect of Plastic Work on Damage Site Initiation

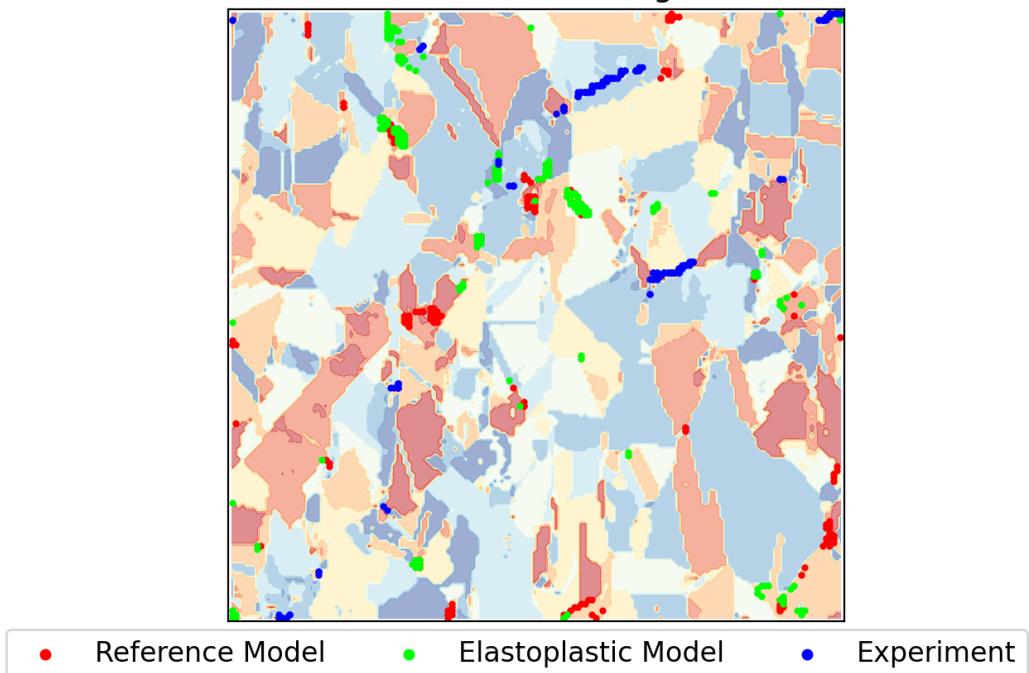


Figure 12: An EBSD image of the simulated microstructure, with scatter plots detailing grain boundaries meeting the damage threshold from the reference elastic strain energy damage model, the elastoplastic damage model, and experimentally determined cavitation data over the same microstructure.

6.4. Comparing Damage Initiation due to Plasticity and Creep Deformation

The additional creep deformation term outlined in equation 4 in section 2 was also applied to the same microstructure to examine the difference in damage initiation resulting from the addition of creep deformation alongside plasticity. The boundary conditions and level of total creep strain applied were determined using a component level continuum finite element model with an ABAQUS creep subroutine of the double notched specimen studied by He et al. [45]. This model was used to inform the crystal plasticity model of the average in-plane strain components which were extracted from a 1 mm^2 area from the region between the notch tip and the centre-line of the specimen. Figure 2 displays the location of the area stated. In the crystal plasticity model the plastic slip term, which is the first term in equation 4, is suppressed at a strain level of 0.15%, leaving only the creep deformation term in equation 4 active subsequently to reflect long term deformation. The creep deformation term has the same form as the plastic slip term, with different rate constants, see table 3.

A similar analysis to that of sections 6.3, 6.2, and 6.1 was carried out to determine the cavitation ratio for varying grain boundary misorientation angles. The threshold value in equation 26 used to decide if a grain boundary element was exhibiting damage, ν , had a value of 0.33. This resulted in a correlation of cavitation ratios between the experimental result and creep plasticity deformation model of 0.35, a significant increase on that of the reference elastic strain energy damage model which was 0.04. Finally, the grain boundaries most susceptible to damage within the simulated microstructure were compared to the experimental specimen using the two hundred most damaged points within the simulation and the specimen. Of the eleven boundaries outlined within the specimen, two were predicted by the creep plasticity deformation model. Not including creep diffusion effects for creep cavitation is justified here due to the stress induced during the experiment of 390 MPa. At this high stress, damage is likely to be dominated by plastic void initiation, making the crystal plasticity phase field approach suitable for this analysis.

7. Discussion

The applicability of a continuous damage variable such as a phase field to modelling the distribution of discrete voids is a matter of debate, with little precedent established within the literature, although this has been attempted for other modelling techniques [96]. The interpretation of the phase field as it pertains to void initiation was critical for the analysis presented here. As is commonly done with phase field formulations, the stiffness tensor is locally modified depending on the phase field value by applying a degradation function, usually of a quadratic form as in equation:

$$\mathbb{C}_{ijkl} \rightarrow (1 - c^2)\mathbb{C}_{ijkl} \quad (27)$$

This can be seen as analogous to a local loss in material or crystalline structure at this point, which causes the reduction in elastic constants and local stress, therefore allowing for correlation with void initiation within the mesoscale structure. Moreover, the point at which void initiation is said to have taken place was based on a cavitation damage threshold here,

but other approaches could also be used, again there is little work existing in the literature in this area. Furthermore, the evolution of the phase field is affected by interpretation. The characteristic length-scale in equation 22, l_0 , dictates the diffuseness of the phase field. A low l_0 results in point like damage formation of high intensity that could be seen as more accurately representing void initiation, without allowing the damage field to evolve and spread that is critical for void nucleation and growth when modelling ductile failure. Similarly, issues are associated with a large l_0 . Here, damage is too diffuse, facilitating void coalescence type behaviour at the cost of preventing discrete crack path definition and growth. The effect of varying the characteristic length-scale on damage initiation within the model framework presented here is shown in [Appendix C](#). While increasing the length-scale did increase the correlation in the cavitation ratio compared to the reference model from 0.04 to 0.24, the effect is significantly smaller than other effects such as grain misorientation and varying the critical energy release rate.

The goal of this work was to establish a framework in which by accounting for certain degradation mechanisms within a material, phase field models would be suitable to modelling early damage initiation. The growth and ductile failure of creep cavities formed as a result of intergranular carbides at grain boundaries, as well as the formation and failure due to plastic strain induced voids were accounted for using a grain boundary misorientation dependent value of the critical energy release rate. The application to an experimental 316H stainless steel sample was used to demonstrate the potential of this approach. Electron backscatter diffraction measurements were used to identify a grain microstructure in the experimental specimen. The microstructure was recreated in crystal plasticity and trends in damage initiation were directly compared between simulation and experiment. By implementing a misorientation dependent critical energy release rate, G_c , a much stronger correlation was found with the experimentally determined cavitation ratio of 0.67, compared with little to no correlation observed with the reference elastic strain energy damage model and elastoplastic damage model from sections [6.1](#) and [6.3](#), both of which used a constant value of G_c . This suggests that when local variation in G_c is introduced, CPFE approaches have significant potential to capturing plastic void initiation behaviour associated with grain boundaries observed experimentally. The sensitivity of the profile shape used for the critical energy release rate was examined. with the relation between the simulated and experimental cavitation ratio varying by up to 26% when comparing the trapezoidal, linear, and quadratic profiles exhibited in figure [9](#). This further outlines the importance of adding accurate experimental data characterising the precipitation rate of carbides along grain boundaries of different misorientation angles, which would allow for a more precise determination of the reduction in the critical energy release rate attributable to a specific carbide density. It should be noted that due to the large microstructural region with more than three thousand grain boundary elements, as well as the interlinking effects within the crystal plasticity model implemented, the likelihood of obtaining high Pearson product moment correlation coefficients between two model parameters is reduced. This is in a similar manner to that of Zhang et al., who applied machine learning techniques to determine grain boundary susceptibility to damage [\[97\]](#).

The correlation of SSD and GND density with simulated damage indicates that grain

boundary pile up and plasticity are key influencing factors on damage formation within the model framework presented here. As a means of identifying factors predictive of damage within the phase field model, it should be noted that figures 6 and 7 predict a minimum value of the phase field at a particular grain boundary element based on the value of SSD density, GND density, or loading direction stress. The effect microstructural factors such as the average value and difference in Schmid factors of adjacent grains on damage were also considered, with little correlation found. This matches the findings over the same microstructure in an experimental sample by He et al. [45], who observed no significant correlation between damage formation and Schmid factor values of adjacent grains.

Limitations in application of this framework to experimental results relate mostly to the availability of experimental data allowing for further inclusion of microstructural features and effects that contribute to damage formation. For example, elongated manganese sulphide (MnS) inclusions that can form across grains and grain boundaries in 316H stainless steel can cause stress concentrations leading to void nucleation in both grains and grain boundaries through local variations in elastic material properties. Such inclusions have not been accounted for in the crystal plasticity model outlined in this work. Including the effect of inclusions such as MnS could allow for more accurate prediction of grain boundaries particularly susceptible to damage initiation.

These features could be characterised through a scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDX) study before implementation into the initial starting microstructure for finite element analysis, but such data was not available for the work shown here. It is suspected that the limited accuracy of predicting specific grain boundaries that exhibited void initiation are possibly due to inclusions, but further testing would be required to examine exactly which voids within the real specimen had inclusions present using EDX analysis.

The subsurface microstructure and boundary conditions on a specimen have been discussed within the literature as an influencing factor in the surface stress field, with differing stress states known to have an impact upon damage initiation [46]. The effect of varying subsurface microstructure is explored in [Appendix C](#). The correlation in cavitation ratio with boundary misorientation increased from 0.04 to up to 0.78 depending on the substructure. This indicates that the effect of subsurface microstructure on damage initiation is as significant within the presented model framework as grain misorientation. What cannot be precisely recreated within the model framework at present is the effect of boundary conditions resulting from a large scale microstructure. Further experimental characterisation using successive EBSD and focused ion beam scans to produce a full 3D reconstruction of a target area within the specimen. This would not only for an accurate

One difficulty with the comparison of simulations with experimental data shown here was the loading history of the sample, resulting in significant complexity in active degradation mechanisms causing damage. Planned future work will include applying this model framework and similar experimental analysis on a specimen subjected only to tensile load, before then recreating a section of the microstructure for simulations using the same CPFE model. The goal of which is to examine a sample purely in tension, in which plasticity alone causes microstructural degradation. This study may also allow for the calibration of the

relative contribution to damage formation of plastic work compared to elastic strain energy. At present, the plastic work term included is given equal weighting to the elastic strain energy term in equation 22 with $\beta=1$, but a study to more accurately calibrate the value of β would be of interest. Furthermore, the relative contribution of creep deformation also requires further investigation to accurately calibrate the relative size of its contribution to damage initiation.

Further work can also include improvements to the existing model framework. Void nucleation is not typically seen until high levels of plastic strain are incurred in a specimen. The models here were run to low levels of strain of 0.15%. Typically, this mismatch in strain levels leading to damage initiation is addressed using a strain damage threshold to limit damage initiation until higher strains are reached. While a strain-based threshold was not included for the work shown here, it is something to be addressed for future applications to other materials and loading modes. Following on from this, variations in damage initiation resulting from specimen geometry and stress triaxiality also present avenues for further work. Moreover, there is evidence within the literature that the influence of carbides on damage nucleation can be exacerbated by intergranular residual stress fields [98], as well as affecting the formation of creep damage [99]. The determination and inclusion of grain to grain residual stresses and their effect on damage initiation within the existing model presents an additional avenue for further work.

8. Conclusions

A novel approach to apply crystal plasticity phase field modelling techniques to damage initiation has been implemented. To assess the applicability of this framework to modelling early damage formation, this approach has been applied and compared to experimental cavitation results across the same microstructure obtained with correlative electron microscopy techniques. Analysis correlating the damage field across a microstructure of 316H stainless steel has been done to identify correlations between the phase field damage value and microstructural and model characteristics including the Schmid factors, dislocation densities and loading direction stress at grain boundaries. A very strong correlation between the SSD density and phase field damage of 0.90 was found along these grain boundary elements, with GND density correlated to a lesser extent with 0.46. Correlations obtained for the Schmid factors for adjacent grains with the phase field damage returned no correlation, a result matching experimental observation.

A novel threshold was used to infer cavitation across a simulated microstructure damage field to calculate the proportion of grain boundaries that exhibited cavitation as a function of the grain boundary misorientation angle, known as the cavitation ratio. To model the effect of grain misorientation on damage, alongside intergranular carbides which are too small to be explicitly modelled using mesoscale crystal plasticity simulations, an aggregated approach was used. This was in the form of a misorientation dependent value of the critical energy release rate was able to greatly improve the correlation of this metric with experimental data from 0.04 to 0.71, suggesting that the effect of misorientations and carbide precipitation has a strong influence in early damage and cavity nucleation.

The size of the local variation in the energy release rate G_c was varied to find the value of G_c that returned the highest correlation against experimental data for the cavitation ratio as a function of the grain boundary misorientation angle. The local reduction in G_c along grain boundaries due to misorientation effects and carbide precipitation was up to 22%. Due to a lack of literature data detailing precipitation rates along grain boundaries of varying misorientation, the variable energy release rate was implemented using an assumed profile. The effect of changing the profile shape was investigated, and the correlation of the cavitation ratio to the misorientation angle was found to vary by up to 26% with different profile shapes. This underlines the need for further experimental investigation characterising intergranular precipitation behaviour of 316H stainless steel along grain boundaries of different misorientation angles.

Model variations such as those including the contribution to damage resulting from plastic deformation and a creep deformation term were also considered. The inclusion of creep deformation alongside plasticity improved the correlation of the cavitation ratio from 0.04 to 0.35, whereas the plastic work inclusion had no significant effect.

The grain boundaries most susceptible to cavitation within a real specimen of 316H were determined, and the ability of the phase field model variations to predict the same boundaries as high in damage was examined. From this, it can be suggested that elastic strain energy does not accurately map this behaviour, which is better described by plastic work contributing to damage as well as local reductions in G_c due to grain misorientation and carbide precipitation, although the improvement in the accuracy of the presented approach requires further investigation to incorporate additional microstructural defects and degradation mechanisms to the model.

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Appendix A. Jacobian calculation with damage

The Jacobian of the Newton-Raphson algorithm that determines the stress and plastic deformation at each time step is calculated by slightly modifying the method described in [100]. In this section, sum over repeated indices is assumed. The Cauchy stress $\boldsymbol{\sigma}$ is related to the 2nd Piola-Kirchhoff in (21) by:

$$\boldsymbol{\sigma} = \frac{1}{\det(\mathbf{F}_e)} \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T . \quad (\text{A.1})$$

The variable that is updated at each iteration step is the Cauchy stress and the material tangent, \mathbf{W} , which is a fourth rank tensor, is defined as the partial derivative of the Cauchy stress with respect to a relative strain increment or stretch increment tensor, $\Delta\mathbf{U}$, as in Eq. (A.2):

$$\mathbf{W} = \frac{\partial \boldsymbol{\sigma}}{\partial \Delta\mathbf{U}} \Rightarrow \partial \boldsymbol{\sigma}_{ij} = W_{ijkl} \partial \Delta U_{kl} \text{ in index notation.} \quad (\text{A.2})$$

The $\Delta\mathbf{U}$ is defined as the stretch increment in one time step in the co-rotational reference frame [101, 102]. It can be expressed mathematically by the relationship:

$$\Delta F_{ij} = \Delta R_{ik} \Delta U_{kj} , \quad (\text{A.3})$$

where ΔF_{ij} are the components of the increment of the deformation gradient and ΔR_{ij} is the relative rotation increment, determined using the polar decomposition.

The variation of the Cauchy tensor is given by (A.4):

$$\partial \boldsymbol{\sigma} = \frac{1}{\det \mathbf{F}_e} [\partial \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T + \mathbf{F}_e \partial \mathbf{S} \mathbf{F}_e^T + \mathbf{F}_e \mathbf{S} \partial \mathbf{F}_e^T - (\mathbf{F}_e \mathbf{S} \mathbf{F}_e^T) \partial \mathbf{F}_e : \mathbf{F}_e^{-1}] . \quad (\text{A.4})$$

It is useful to define two additional fourth rank tensors P_{ijkl} and Q_{ijkl} as in (A.5) and (A.6):

$$P_{ijkl} = \frac{\partial (F_e)_{ij}}{\partial \Delta U_{kl}} , \quad (\text{A.5})$$

$$Q_{ijkl} = \frac{\partial S_{ij}}{\partial \Delta U_{kl}} . \quad (\text{A.6})$$

Substituting (A.5) and (A.6) into (A.4), the Jacobian in index notation becomes as in (A.7):

$$W_{ijkl} = \frac{1}{\det \mathbf{F}_e} \left[P_{imkl} S_{mn} (F_e)_{jn} + (F_e)_{im} Q_{mnkl} (F_e)_{jn} + (F_e)_{im} S_{mn} P_{jnkl} - (F_e)_{im} S_{mn} (F_e)_{jn} P_{pqkl} (F_e^{-1})_{qp} \right] . \quad (\text{A.7})$$

i. Calculation of $P_{ijkl} = \partial (F_e)_{ij} / \partial \Delta U_{kl}$

To calculate P_{ijkl} , the elastic part of the deformation gradient is expressed in terms of the relative stretch as in (A.8), in which $(F_e)_{ij}(t)$, S_{ij}^β and $\Delta\gamma^\beta$ represent the elastic deformation

gradient at the former time step, the Schmid tensor and the slip increment of the slip system β respectively:

$$(F_e)_{ij} = \Delta R_{ik} \Delta U_{kl} (F_e)_{lm}(t) \left[\delta_{mj} - \sum_{\beta=1}^{N_s} \Delta \gamma^\beta S_{mj}^\beta \right]. \quad (\text{A.8})$$

Differentiation of (A.3) with respect to the relative stretch gives Eq. (A.9):

$$P_{ijkl} = \Delta R_{ik} (F_e)_{lj}(t) - \Delta R_{ik} (F_e)_{lp}(t) \sum_{\beta=1}^{N_s} \Delta \gamma^\beta S_{pj}^\beta - \Delta R_{im} \Delta U_{mn} (F_e)_{np}(t) \sum_{\beta=1}^{N_s} T_{kl}^\beta S_{pj}^\beta, \quad (\text{A.9})$$

in which T_{kl}^β is the differential expressed as in (A.10):

$$T_{kl}^\beta = \frac{\partial \Delta \gamma^\beta}{\partial \Delta U_{kl}}. \quad (\text{A.10})$$

ii. Calculation of $Q_{ijkl} = \partial S_{ij}/\partial \Delta U_{kl}$
First an additional second order tensor A_{ij} is defined:

$$A_{ij} = (F_e)_{mi}(t) \Delta U_{nm} \Delta U_{np} (F_e)_{pj}(t), \quad (\text{A.11})$$

together with the so-called coefficient matrix for corrector term C_{ij}^β , which is an extension for the phase field damage model of the corrector term presented in [64]:

$$C_{ij}^\beta = \begin{cases} \frac{1}{2} (1-c)^2 \mathbb{C}_{ijkl} \left(A_{km} S_{ml}^\beta + S_{nk}^\beta A_{nl} \right), & \text{if } J_e \geq 1, \\ \frac{1}{2} \mathbb{C}_{ijkl} \left(A_{km} S_{ml}^\beta + S_{nk}^\beta A_{nl} \right), & \text{if } J_e < 1, \end{cases} \quad (\text{A.12})$$

To find Q_{ijkl} , first the expression for the 2nd Piola-Kirchhoff stress is defined in (A.13), in which S_{ij}^{tr} and C_{ij}^α represent the trial stress and coefficient matrix for corrector term:

$$S_{ij} = S_{ij}^{\text{tr}} - \sum_{\beta=1}^{N_s} \Delta \gamma C_{ij}^\beta. \quad (\text{A.13})$$

After differentiating with respect to ΔU_{kl} , (A.14) is obtained in which Q_{ijkl} is expressed as:

$$Q_{ijkl} = D_{ijkl} - \sum_{\beta} C_{ij}^\beta T_{mn}^\beta \sum_{\beta=1}^{N_s} \Delta \gamma^\beta J_{mnkl}^\beta. \quad (\text{A.14})$$

where:

$$D_{ijkl} = \frac{\partial S_{ij}^{\text{tr}}}{\partial \Delta U_{kl}}, \quad (\text{A.15})$$

and:

$$J_{ijkl}^\beta = \frac{\partial C_{ij}^\beta}{\partial \Delta U_{kl}}, \quad (\text{A.16})$$

which represent differentials of the trial stress and corrector terms respectively.

iii. Calculation of $D_{ijkl} = \partial S_{ij}^{\text{tr}} / \partial \Delta U_{kl}$
 Trial stress is computed using the elasticity tensor and damage phase field:

$$S_{ij}^{\text{tr}} = \begin{cases} \frac{1}{2}(1-c)^2 \mathbb{C}_{ijkl} [A_{kl} - \delta_{kl}] , & \text{if } J_e \geq 1 , \\ \frac{1}{2} \mathbb{C}_{ijkl} [A_{kl} - \delta_{kl}] , & \text{if } J_e < 1 , \end{cases} \quad (\text{A.17})$$

where δ_{ij} is the identity matrix. Differentiating (A.17) with respect to the stretch increment reveals (A.18):

$$D_{ijkl} = \begin{cases} \frac{1}{2}(1-c)^2 \mathbb{C}_{ijmn} L_{mnkl} , & \text{if } J_e \geq 1 , \\ \frac{1}{2} \mathbb{C}_{ijmn} L_{mnkl} , & \text{if } J_e < 1 , \end{cases} \quad (\text{A.18})$$

in which L_{ijkl} is the differential shown in (A.19):

$$L_{ijkl} = \frac{\partial A_{ij}}{\partial \Delta U_{kl}} . \quad (\text{A.19})$$

iv. Calculation of $L_{ijkl} = \partial A_{ij} / \partial \Delta U_{kl}$
 A_{ij} is the same expression in [64] but written in terms of the relative stretch tensor and former elastic part of the deformation gradient as in Eq. (A.11). Its derivative gives:

$$L_{ijkl} = (F_e)_{ki}(t) \Delta U_{lm} (F_e)_{mj}(t) + (F_e)_{mi}(t) \Delta U_{mk} (F_e)_{lj}(t) . \quad (\text{A.20})$$

v. Calculation of $J_{ijkl}^{\beta} = \partial C_{ij}^{\beta} / \partial \Delta U_{kl}$
 Differentiating (A.12) gives:

$$J_{ijkl}^{\beta} = \begin{cases} \frac{1}{2}(1-c)^2 \mathbb{C}_{ijmn} (L_{mpkl} S_{pn}^{\beta} + S_{pm}^{\beta} L_{pnkl}) , & \text{if } J_e \geq 1 , \\ \frac{1}{2} \mathbb{C}_{ijmn} (L_{mpkl} S_{pn}^{\beta} + S_{pm}^{\beta} L_{pnkl}) , & \text{if } J_e < 1 . \end{cases} \quad (\text{A.21})$$

v. Calculation of $T_{ij}^{\beta} = \partial \Delta \gamma^{\beta} / \partial \Delta U_{ij}$
 Using chain rule, (A.22) is obtained:

$$T_{ij}^{\beta} = \frac{\partial \Delta \gamma^{\beta}}{\partial S_{kl}} \frac{\partial S_{kl}}{\partial \Delta U_{ij}} . \quad (\text{A.22})$$

giving Eqn. (A.23)

$$T_{ij}^{\beta} = B_{kl}^{\beta} Q_{kl}{}_{ij} , \quad (\text{A.23})$$

in which B_{kl}^{β} is given by (A.24):

$$B_{ij}^{\beta} = \frac{\partial \Delta \gamma^{\beta}}{\partial S_{ij}} = \frac{\partial \Delta \gamma^{\beta}}{\partial \tau^{\beta}} \frac{\partial \tau^{\beta}}{\partial S_{ij}} = \frac{1}{2} \frac{\partial \Delta \gamma^{\beta}}{\partial \tau^{\beta}} (S_{ij}^{\beta} + S_{ji}^{\beta}) , \quad (\text{A.24})$$

and:

$$Q_{kl}{}_{ij} = \frac{\partial S_{kl}}{\partial \Delta U_{ij}} . \quad (\text{A.25})$$

Note that $\partial\Delta\gamma^\beta/\partial\tau^\beta$ can be obtained from the slip constitutive law.

vi. Calculation of $Q_{ijkl} = \partial S_{ij}/\partial\Delta U_{kl}$
Substituting (A.23) for the expression of T_{kl}^β into (A.14) reveals (A.26):

$$Q_{ijkl} = D_{ijkl} - \sum_{\beta=1}^{N_s} C_{ij}^\beta B_{mn}^\beta Q_{mnpq} \sum_{\beta=1}^{N_s} \Delta\gamma^\beta J_{pqkl}^\beta. \quad (\text{A.26})$$

Re-arranging the terms to solve for Q_{ijkl} gives (A.27):

$$\left[\delta_{im}\delta_{jn} + \sum_{\beta=1}^{N_s} C_{ij}^\beta B_{mn}^\beta \right] Q_{mnkl} = \left(D_{ijkl} - \sum_{\beta=1}^{N_s} \Delta\gamma^\beta J_{ijkl}^\beta \right), \quad (\text{A.27})$$

in which an inversion of the first term on the left hand side can be carried out by first transforming the fourth rank tensor into a matrix by using Voigt notation convention, then applying an inversion operation. The tensors P_{ijkl} and Q_{ijkl} are then used to compute the Jacobian in Eq. (A.7). Note that the effect of the damage phase field appears in (A.12), (A.17), (A.18), (A.21).

Appendix B. FCC structure grain boundary misorientation symmetry

This appendix reports the symmetry matrices \mathbf{G}_i that are used to calculate the misorientation angle $\Delta\theta$ in section 2.3 [103]. They correspond to the 432 FCC crystal symmetries, i.e. they represent the complete set of rigid body motions that transform the crystal into itself. These 24 matrices represent the following operations: identity; inversion with respect to the centre of the cube; 180 degrees rotation around the 3 dyad axes perpendicular to the faces of the cube; 180 degrees rotation around the 3 dyad axes passing through the mid points of the edges of the cube; 120 degrees rotation around the 4 triad axes passing through pairs of vertices of the cube; 90 degrees rotation around the x, y, z axes; reflections with respect to the x, y, z axes; 6 diagonal planes of symmetry that pass through two opposite edges of the cube. They are given by:

$$\begin{aligned}
\mathbf{G}_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \mathbf{G}_2 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} & \mathbf{G}_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
\mathbf{G}_4 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} & \mathbf{G}_5 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \mathbf{G}_6 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
\mathbf{G}_7 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} & \mathbf{G}_8 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} & \mathbf{G}_9 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
\mathbf{G}_{10} &= \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} & \mathbf{G}_{11} &= \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} & \mathbf{G}_{12} &= \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \\
\mathbf{G}_{13} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} & \mathbf{G}_{14} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} & \mathbf{G}_{15} &= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
\mathbf{G}_{16} &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \mathbf{G}_{17} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \mathbf{G}_{18} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
\mathbf{G}_{19} &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} & \mathbf{G}_{20} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} & \mathbf{G}_{21} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \\
\mathbf{G}_{22} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} & \mathbf{G}_{23} &= \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \mathbf{G}_{24} &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{B.1}$$

Appendix C. Effect of the characteristic regularisation length-scale and subsurface microstructure

The characteristic length-scale, l_0 , of the phase field model in equation (22) determines the diffuseness of damage across the microstructure. To examine the effect that this length-scale has on results outlined within this paper, a parametric study was run to compare the effect of varying l_0 on the cavitation ratio. The results of which are shown in figure C.14(b).

Additionally, it is thought that the subsurface microstructure is a complicating factor in how damage initiates across a microstructure. This is not included in the reference simulation, where only the two dimensional EBSD data is used, which allows only for surface data to be reproduced within crystal plasticity. A series of 3D microstructures were generated by taking the original EBSD microstructure and layering a second layer of elements underneath as shown in figure C.13. The effect of the subsurface was varied by changing the texture of the bottom layer. One has the same microstructure added as an identical layer underneath,

another has a similarly textured microstructure, and the last was a layer consisting of randomly oriented elements with no grain morphology features. The modified microstructures were simulated under the same conditions as the reference model in section 6.1. The results are shown in figure C.14(a).

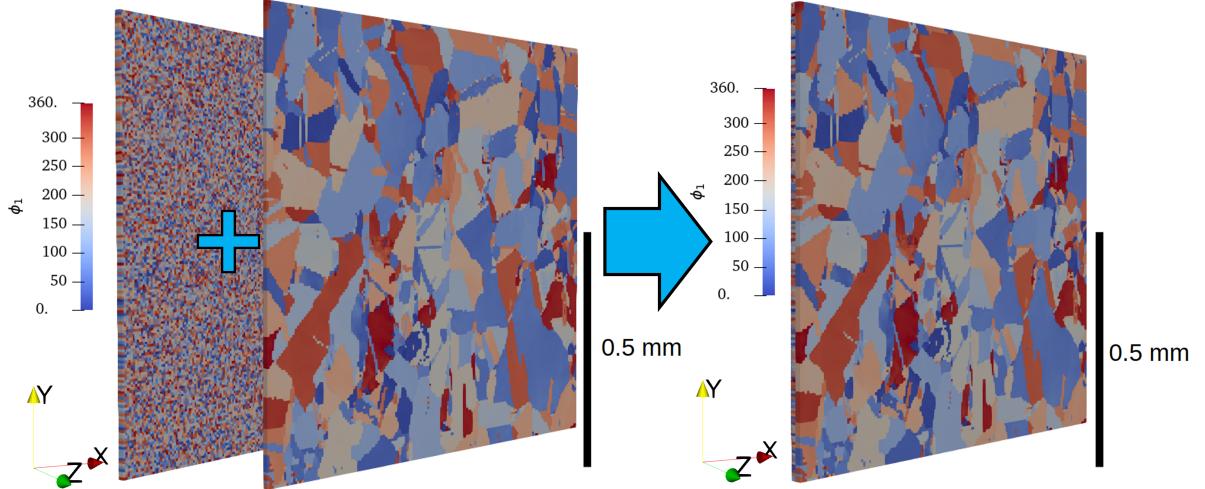


Figure C.13: An example of how a different substructure was implemented underneath the EBSD microstructure. The plus sign denotes how the subsurface is added to create a two element thick mesh. The random orientation substructure is shown here for reference.

Figure C.14 (a) shows the variation in the cavitation ratio with subsurface microstructure. The variation in correlation calculated was significant, ranging from 0.04 for the reference model from section 6.1 to an absolute value of 0.78 for the textured substructure. This result outlines the significance of the effect of subsurface microstructure on damage initiation. Through the combined use of successive EBSD scans on new layers of material that is exposed by removing the top surface with a controlled focused ion beam, a full 3D microstructure could be reconstructed within this crystal plasticity framework. This result also shows that grain boundary misorientation, which in turn increases rates of carbide precipitation carbide precipitation [24], can be seen as significant a factor in grain boundary damage initiation as the subsurface microstructure by comparison between the correlations in cavitation ratio. The stress strain response in each model was sufficiently similar to rule this out as a reason for differences in damage initiation, as well as the relation between grain boundary stress and phase field damage which was similar in each model.

The length-scale, l_0 , used within section 6.1 was 3 μm . Simulations were run over the reference simulation mesh with the same conditions other than varying length-scale. By increasing l_0 from 3 μm to up to 15 μm , the correlation in cavitation ratio against experimental data increased from 0.04 to up to 0.24. Upon comparison of the phase field across the microstructure, the increase in l_0 causes two main differences. The first is that the damage is higher across the entire microstructure, this is due to the terms in equation (22) dependent on the length-scale and the gradient of the damage parameter c . The second difference to note is that the phase field is more diffuse, with fewer distinguishable

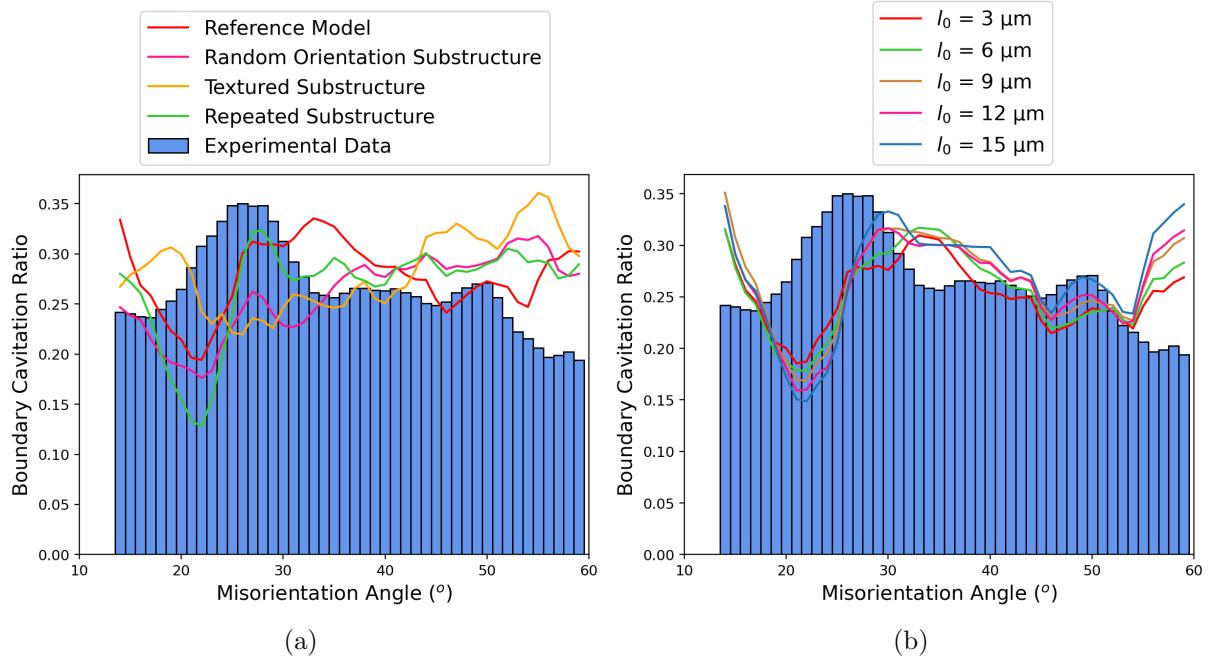


Figure C.14: (a) Comparing the experimentally determined cavitation ratio with boundary misorientation angle for a 316H specimen with both the single layer reference model and models with varying subsurface microstructures. (b) Comparing how the cavitation ratio varies with boundary misorientation angle against for varying values of the phase field model characteristic length-scale l_0 .

sharp features that can be mapped to the underlying grain boundaries within the starting microstructure. This result suggests that while changing the characteristic length-scale has an effect on the final phase field and the magnitude of the damage observed, the variation in damage initiation across the microstructure with grain boundaries of varying misorientation is not significantly changed.

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