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Comparison of self-consistent and crystal plasticity FE approaches for modelling the high-temperature deformation of 316H austenitic stainless steel

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ABSTRACT

The present article examines the predictive capabilities of a crystal plasticity model for inelastic deformation which captures the evolution of dislocation structure, precipitates and solute atom distributions at the microscale, recently developed by Hu and Cocks [1,2]. The model is implemented within a self-consistent framework and a crystal plasticity finite element (CPFE) scheme. Through direct comparison between the two CP schemes and with an extensive material database for Type 316H stainless steel, the different types of information and the degree to which the models are consistent with experimental observations are assessed. The study demonstrates an agreement between the SCM and the CPFE schemes, providing confidence in the micromechanical deformation model employed. The multi-scale approach also allows the effects of micro-scale deformation processes, related to dislocation-obstacle interactions, on the global deformation response to be captured. Modelling results from this study and their comparison to experimental observations show that deformation of polycrystalline materials, such as 316H stainless steel, is controlled by the evolution of microstructural state of the material and the redistribution of stress between individual grains. The study suggests that the SCM is a feasible tool to simulate and explain the deformation behaviour of complex alloys under industrially-relevant thermo-mechanical operating histories. The CPFE framework captures the effects of the variation in grain geometry and provides more detailed information about the variation of stress and strain within the individual grains, particularly their distribution near grain boundaries and triple points – which are important to understand in the context of damage development and failure. The SCM predicts a “stiffer”, more creep-resistant response than a CPFE model for a given set of material parameters due to the more highly-constrained deformation modes allowed in the model. As a result, material parameters calibrated using one modelling approach are not necessarily suitable for use in another approach – although parameters obtained when fitting the different models should not vary significantly.

NOMENCLATURE

a_c	Dislocation core area
b	Burger's vector

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c	Concentration of solute atoms
$\mathbf{C}, \mathbf{C}^{rot}$	Stiffness matrix – single crystal coordinates and rotated
$\mathbf{D}$	Rate of deformation
D_p, D_c	Core diffusion
$E, E_{ij,m}$	Young's modulus; Macroscopic strain tensor
$\mathbf{F}$	Total deformation gradient
$\dot{\mathbf{F}}$	Rate form of deformation gradient
F_{sol}	Strength of solute drag
ΔF_0	Activation energy for bypassing
G	Shear modulus
$\mathbf{G}_{ori}$	Matrix – rotation (global to lattice)
ΔG^*	Thermal activation energy
j_s, j	Fitting parameters - hardening
$\mathbf{J}$	Jacobian matrix
k	Boltzmann constant
$\mathbf{L}, \mathbf{L}^p$	Velocity gradient; plastic part of velocity gradient
L_d, L_p	Spacing of dislocation junctions and precipitates
ΔL_r	Annihilated dislocation segment length
N_d, N_0	Current and initial number density of dislocation junctions
p, q	Flow rule exponents
$\mathbf{R}$	Matrix – rotation (lattice to global)
$\mathbf{R}_2$	Reuter matrix
t	Time
T, T_m	Temperature, melting temperature
$\mathbf{T}_k$	Transformation matrix
ν	Poisson's ratio
V	Volume
W_c	Fitting parameter – static recovery
$\alpha_0, \alpha_d, \alpha_s$	Obstacle bypassing, dislocation junction, solute strength
$\gamma, \dot{\gamma}, \dot{\gamma}_0$	Resolved shear strain, strain rate and reference shear strain rate
$\varepsilon, \varepsilon_{el}, \varepsilon_{pl}$	Total, elastic, plastic strain
$\sigma, \Sigma, \sigma_{trial}$	Stress tensor; macroscopic stress tensor; trial stress tensor
$\tau, \tau_{cr}, \bar{\tau}_m^r$	Resolved and critical resolved shear stress; Type III residual stress
τ_d, τ_p, τ_s	Internal resistance - dislocation, precipitates, solutes
Ψ	Residual vector
Ω	Rate of continuum spin

1. INTRODUCTION

The macroscopic deformation of polycrystalline metallic materials is determined by the anisotropic deformation of the individual grains and how they interact with their neighbours. The intrinsic elastic and plastic deformation of a grain depends on its crystallographic orientation, local stress state and internal state (such as its microstructure and dislocation structure). The variation of crystallographic orientation and evolving dislocation structure from one grain to another results in inhomogeneous stress and strain fields within the polycrystalline aggregate. The way in which this internal stress state evolves during mechanical loading plays an important role in determining the macroscopic material response and needs to be adequately modelled in any constitutive description of the material behaviour.

The plastic anisotropy of the grains arises from the evolution of slip on different slip systems and hardening and recovery of the dislocation network. In complex engineering alloys second-phase particles and solute atom atmospheres play important roles determining the yield strength and the way in which the dislocation network evolves. In this paper we consider the behaviour of one such complex engineering alloy for which extensive material data is available over a range of loading histories and temperature; namely, type 316H austenitic stainless steel, which is used extensively in the boiler sections of Advanced Gas-Cooled (AGR) nuclear power plants, with the majority of the components operating at temperatures in the range 470-650°C and stresses of the order 100-300 MPa. The current Type II AGR nuclear reactors operated by EDF Energy in the UK are approaching the end of their design life. However, life extension of such power plants is desired to maximize the economic benefits of continually running existing plant, coupled with the environmental benefits of reducing our reliance on the use of fossil fuels. This necessitates a more detailed understanding of the deformation and failure behaviour in components which experience complex thermo-mechanical histories during operation of the plant [1]. At elevated temperatures, the life-limiting issues become the time-dependent inelastic deformation of components, such as creep, together with subsequent creep fracture due to steady accumulation of damage. Difficulties arise in predicting the deformation behaviour of the alloy at elevated temperatures during complex loading histories due to the heterogeneities in the intragranular residual stress field [2], the evolution of microstructural phases [3] and the way in which these influence the dislocation-obstacle interactions [4]. There is an extensive literature on the development of empirical and phenomenological models for creep deformation based on continuum plasticity theory [5,6]. However, these models may require a large number of fitting parameters to produce accurate predictions, especially under complex loading histories, see e.g. [7]. In addition, the

vast majority of such models are motivated by phenomenological observations, predicting general trends in response, but do not capture the detailed physics of the deformation behaviour. Continuum plasticity is also unable to capture the local interactions between individual crystals within a polycrystalline aggregate, which has been observed to play a major role in determining the macroscopic response [8,9]. In order to understand better the deformation and failure of complex alloys, such as 316H, and provide guidelines for improvement of existing models and assessment procedures, more sophisticated physical models are required. One of the candidates is the crystal plasticity (CP) framework [10,11], which allows mechanistic models and physically based constitutive laws to be applied at the scale of the slip systems, allowing the effects of microscopic physical deformation processes on the global material response to be assessed.

Recently, Hu and Cocks [3,12] developed a CP model for the inelastic behaviour of FCC alloys, which takes into account the role of evolving precipitate structure and solute distribution, as well as dislocation structure on the crystal constitutive response. They employed this model in the self-consistent framework of Budiansky and Wu [13] to determine the macroscopic response and development of internal residual stress state in a polycrystal containing grains with a random array of orientations. The model was employed to evaluate the behaviour of 316H stainless steel, with the intragranular residual stress state compared with experimental states obtained from neutron diffraction studies. Here, we employ the same model within a crystal plasticity finite element (CPFE) framework, explore the different types of information provided by the two approaches and evaluate the degree to which the results are consistent with each other. It is demonstrated that the global material response obtained from the different models are fully consistent with each other, providing confidence in the use of the simpler self-consistent model (SCM) in predicting the global deformation response under complex loading histories. The CPFE framework, however, provides more detailed information about the evolving internal stress state, which is important in the assessment of failure. In comparison with the phenomenological models described earlier, the CP model, because of its physical basis, contains four parameters which need to be fit to experimental data; all other parameters in the model are specified on the basis of their physical origin.

In the remainder of this section we provide more detailed overviews of the SCM and CPFE modelling approaches. In Section 2 the CP model developed by Hu and Cocks [14], which was employed in their SCM model, is presented; the implementation of this model within a large deformation 3-D CPFE framework is described in Appendix A. Predictions of the CPFE and SCM modelling approaches are compared in Section 3 for different idealized grain shapes and arrangements and selection of

representative volume elements. General trends and observations from these studies are discussed in Section 4.

THE SELF-CONSISTENT AND CRYSTAL PLASTICITY APPROACH

Self-consistent modelling (SCM) [15,16] and crystal plasticity (CP) [8,17] approaches have been developed for modelling polycrystalline aggregate deformation, which enable predictions of both macroscopic deformation and lattice strains at the grain scale. Extensive reviews of self-consistent modelling approaches and the integration of CP theory into these frameworks can be found in Lebensohn et al. [18] and Hu and Cocks [14], hence only a brief overview of such modelling approaches will be presented here. The first model of this type is probably the model developed by Lin [19] who assumed that the sum of the elastic and plastic strains in each grain is the same, similar to the concept introduced by Taylor [20]. Budiansky and Wu [13] and Kroner [21] subsequently made use of Eshelby's solution for a transforming inclusion in an infinite elastic matrix, which allows the elastic-plastic global response to be captured together with the grain-matrix interactions due to a uniform misfit strain field in a grain. In an alternative self-consistent approach described by Hutchinson [15], the problem of an inclusion in an elastic-viscoplastic medium is solved incrementally. More sophisticated large-deformation self-consistent approaches have been developed, see e.g. [22], which allow the effects of both elastic and plastic anisotropy on texture development and evolution of internal stresses to be assessed. Studies by Lebensohn et al. [18] and Wang et al. [23] employ the concept proposed by Hutchinson [15] in order to develop an elastic-viscoplastic large-deformation CP self-consistent model for polycrystalline aggregates. The model developed in [18,23] was successfully employed to describe elastic-plastic monotonic, creep and stress relaxation in a range of polycrystalline materials, particularly austenitic stainless steels [9]. The CP self-consistent model developed by Hu and Cocks [3,12,14] and extended by Petkov et al. [4] uses a physically-rich mechanistic deformation model compared with [9] to better capture the monotonic, creep, relaxation and cyclic deformation behavior of austenitic 316H stainless steel through the evolution of the dislocation structure within the grains.

Although predictions via CP first-order self-consistent models of the macroscopic response and lattice strains in grain families agree reasonably well with experimental results, local grain-to-grain interactions and strain incompatibilities are not explicitly captured due to the assumption of uniform stress and strain fields within the inclusion (grain) in the self-consistent schemes [24]. To capture the field variation in intragranular stress and lattice rotations in polycrystalline averaging schemes, novel

second-order homogenization schemes have been developed and employed recently in [25–32]. Bornert et al. [31] produced estimates for the effective deformation behaviour of non-linear materials and demonstrated that the predictions via their second-order (SO) homogenization model were more accurate than first-order (FO) self-consistent schemes. In [32], a comparison is made between full-field solutions via fast Fourier transform (FFT) algorithm and first- and second-order homogenization schemes within a 2D power-law continuum plasticity formalism. The study demonstrated the predictions of the statistical variations in stress and strain field via the SO framework agreed better with the full-field FFT solutions, even in cases with higher grain anisotropies for which fluctuations in strain rate increase. The study by Lebensohn et al. [32] was extended in [27] to examine the predictive capabilities of the SO homogenization schemes for deformation of FCC materials. A better agreement with experimental results and full-field solutions on texture development and strain rate variations was established via the SO homogenization framework, over the FO self-consistent models. A recent fully-optimized SO homogenization model developed by Ponte Castañeda [28] was employed in [25,26] to describe the deformation behaviour of porous viscoplastic FCC and HCP single crystals. It was determined that the predictions via the novel SO scheme agree well with full-field FE results, demonstrating the broad predictive capabilities of the proposed SO homogenization framework. It should be noted, however, that implementation of the higher-order homogenization schemes appears to depend on the constitutive model and loading history employed, with the majority of studies reviewed in this paragraph applying the SO homogenization scheme to time-independent monotonic loading scenarios. A study by Dohgri et al. [33] demonstrated a limitation of one such higher-order homogenization scheme in capturing the Bauschinger effect in a two-phase steel, for which the model otherwise yielded good agreement with full-field solutions and experimental data under monotonic loading.

The present study is part of a wider project to study the response of Type 316H stainless steel under complex thermal-mechanical loading histories typical of those experienced in industrial power generating plant, which can result in material elements being subjected to cyclic loading histories with stress or strain-controlled dwells, during which the material creeps or the stress relaxes. In these situations, evolution of the internal residual stress state due to the interaction between the elastic and inelastic responses of the individual grains plays an important role in determining the overall material response [4]. First order Budiansky and Wu [13] model captures the main features of the stress redistribution process during this important class of loading history. The ability of SO modelling approaches to deal with this type of loading history for general constitutive laws is yet to be established.

Hence, we employ a first-order self-consistent homogenization scheme here. Further consideration of the higher-order homogenization schemes is outside the scope of this paper. We do however employ approaches used in SO models [25,34] to evaluate the way in which the stress state and parameters representing the dislocation structure vary within individual grains and how this changes for the different realisations of polycrystalline structure studied in this paper. This provides a basis for explaining any differences between the predictions of the different models.

CRYSTAL PLASTICITY FINITE ELEMENT APPROACHES

With advances in computational power, crystal plasticity finite element (CPFE) methods are being used increasingly, since they provide extensive insight into the effects of grain morphology and relative crystallographic orientations on localized behaviour at grain boundaries, size effects, residual stress fields, etc., as noted by Cailletaud et al. [17] and Roters et al. [11]. Pierce et al. [35] studied the deformation of anisotropic single crystals and the formation of shear bands using a CPFE approach with only two slip systems in an idealized 2-D model. Asaro and Needleman [36] extended the concepts from [35] and investigated texture development within plastically-deforming polycrystalline aggregates of anisotropic grains using the same rate-dependent power law formulation for the inelastic strain rate. These two studies established robust numerical techniques in the context of CPFE theory which served as a basis and guideline for future studies, with further examples found in [37,38]. The hardening and softening models employed, however, were initially purely empirical or phenomenological, with the latter still widely used in crystal plasticity models resolved at the slip-system level, e.g. Erinoshio et al. [39]. Studies by Balke and Estrin [40] and Ma and Roters [41] introduced micromechanical deformation models based on the evolution of dislocation density with plastic straining in FCC metals. Model predictions by both studies agree well with experimental data at different temperatures. The model from [41] describes the evolution of several types of dislocation structures, but adds complexities due to the large number of free parameters. The model established in [40], which is a physically-rich version of the dislocation-density based models developed by Kocks and co-workers [42,43] applied within a crystal plasticity framework, has provided the physical basis and motivation for development of the multi-scale dislocation network based model developed by Hu and Cocks [3,14] within their self-consistent modelling framework (see Section 2). The Hu and Cocks micromechanical model, in which the state variable is the mean spacing between obstacles to dislocation motion, has been extended recently by Petkov et al. [4] and is also employed in the present study.

Since the seminal work of Fleck et al. [44,45] there has been extensive interest in the development of constitutive laws that take into account the effect of strain gradients on the constitutive response. Studies on the theory of strain gradient plasticity [44,46] demonstrate that hardening is dependent on both the accumulation of plastic strain and the gradient of the plastic strain, which gives rise to geometrically-necessary dislocations (GND). A variety of micromechanical models based on the evolution of geometrically-necessary dislocations (GNDs) have been employed successfully within crystal plasticity modelling frameworks, see e.g. Gao and Huang [47] and Dunne et al. [8], which capture the enhanced local hardening both due to localized plasticity at highly-heterogeneous regions and size effects associated with physically-shorter length scales (e.g. smaller grain sizes). Since the objective of the current study is to compare the predictions of a CPFE modelling approach with a first order self-consistent scheme, which does not contain information about strain gradients, we do not consider the effect of strain gradients on the constitutive response in the CPFE models described here. It should be noted, however, that the concept of GNDs has been used in the formulation of the CP model (see Section 2) to take into account the effect of prismatic dislocation loops that are punched out from precipitate particles as they are bypassed by dislocations – the characteristic length scales that come into play here are the size of the particles (that determines the size of the prismatic loops) and the particle spacing (that determines that the distance over which the loops are punched out).

Studies of the deformation of polycrystalline materials and the evolution of texture have mainly been biased towards understanding forming processes [48], such as rolling, forging, etc. CPFE approaches gained popularity in describing grain-to-grain interactions and the effects of the redistribution of the mesoscale residual stress field on global behaviour. Studies by Sarma and co-workers [49,50] show that high stored energies and accumulation of plastic strain near the grain boundary regions result from more significant misorientations between neighbouring grains. CPFE modelling of polycrystalline aggregates has also demonstrated that local interactions and stress redistribution between anisotropic grains have a significant effect on the global response [9,51,52]. Dunne et al. [8] investigated cold-dwells in Ti-alloys through a physically-based CPFE model noting the importance of local residual stress evolution in determining the macroscopic response during a strain-dwell and possible indications for formation of damage (e.g. nucleation of facet cracks). Venkatramani et al. [10] demonstrated the effects of load shedding during creep deformation in Ti-based alloys and its dependence on stress redistribution on neighbouring grain orientations. The observations made on “hard-soft” grain configurations and slip localization agree with those made in [8], indicating that locations associated with large plastic deformation near certain grain boundaries or within the grain are possible damage

nucleation sites. Understanding localized damage formation and evolution in real polycrystalline materials has been a long-standing problem, and crystal plasticity methods possibly provide a feasible approach to gain better understanding of the factors controlling microscopic and global failure processes. Studies by Srivastava and Needleman [53], Liu et al. [54], Wei and Anand [55] and Simonovski and Cizelj [56] showed through CPFE modelling the importance of stress triaxialities, lattice orientation, slip localization, grain size and shape on the development of trans- and intergranular damage during both long- and short-term plasticity in polycrystalline aggregates.

The present study evaluates the utility of SCM and CPFE modelling approaches for predicting polycrystalline material deformation, and for capturing the local deformation behaviour of individual grains and the interactions between them, taking austenitic stainless steel 316H as an example. Detailed physical micromechanical deformation models are employed for determining the local slip activity and resistance to dislocation motion along the slip systems within an anisotropic grain. These are implemented in the SCM and CPFE modelling approaches illustrated in Figure 1. We assess the practicality, suitability and level of information provided by the different computational frameworks in describing polycrystalline material deformation under a range of thermo-mechanical histories (e.g. monotonic elastic-plastic loading and short-term forward creep). Another major objective of this study is to verify further the validity of the self-consistent models reviewed in Section 2. This will be achieved comparing the model predictions using the SCM [3,14], with those obtained from the crystal plasticity finite element method described in Section 3 and results from experimental studies.

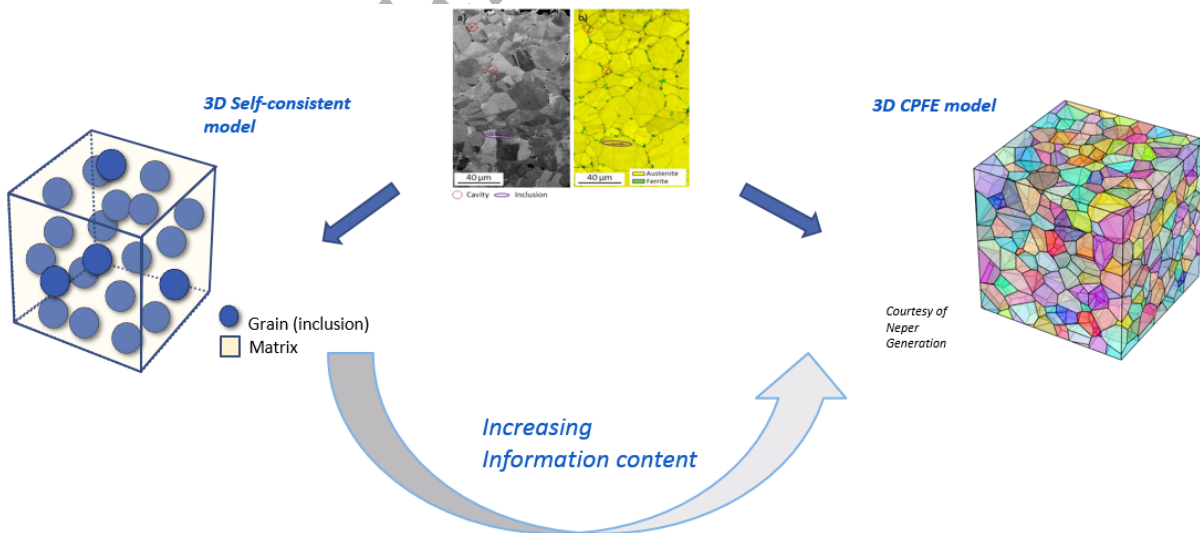


Figure 1. Overview of the two crystal plasticity modelling frameworks evaluated in this study. Left: 3D Multi-scale self-consistent model [14]. Right: 3D Crystal plasticity finite element framework. Tessellation image is courtesy of [57].

2. OVERVIEW OF MULTI-SCALE SELF-CONSISTENT CRYSTAL PLASTICITY MODEL

Recent studies undertaken by Hu and co-workers [3,14,52] have developed physical models of elastic-plastic deformation and forward creep of 316H under AGR power plant operating conditions, which have taken into account the detailed evolution of dominant microstructural elements (e.g. forest dislocation network, nature and distribution of precipitates, and concentration of solute elements in solid solution) and the evolution of the stress fields in a polycrystalline aggregate within a self-consistent crystal plasticity framework. The full scope of the micromechanical deformation mechanisms considered in the model is shown in Figure 2. Model predictions agree well with experiments on mesoscopic lattice strains and macroscopic deformation under short- and long-term plasticity and creep of ex-service (EX) and solution treated (ST) 316H samples [3,12,14].

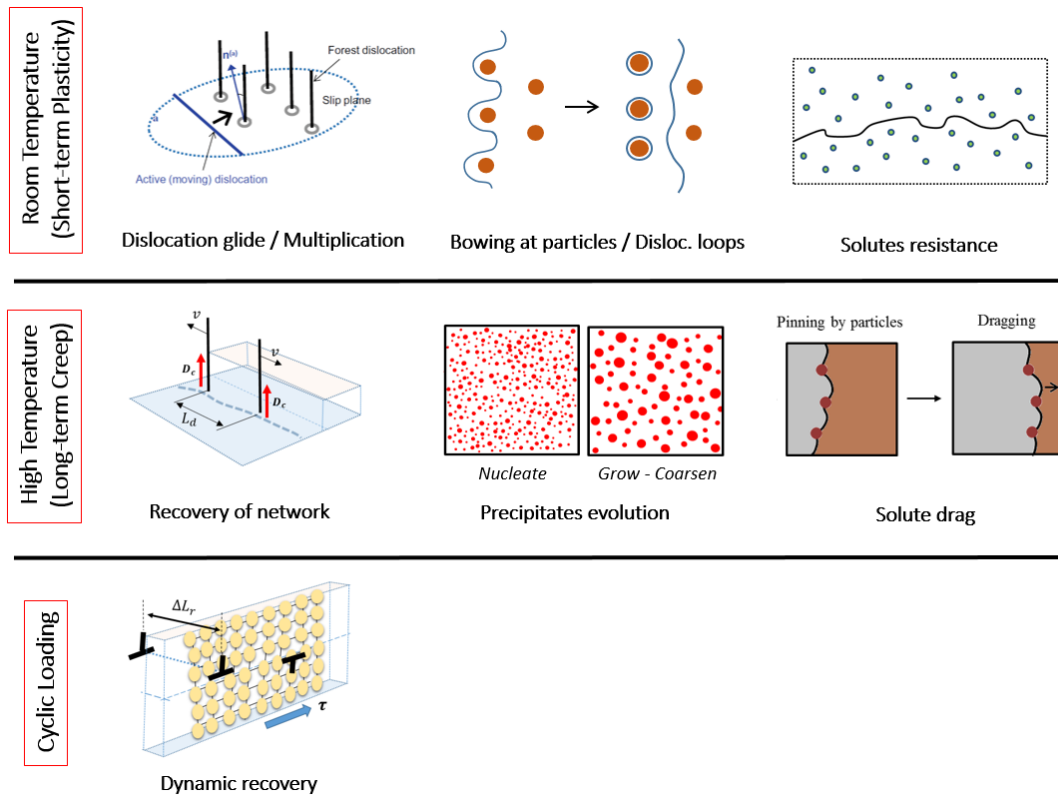


Figure 2. Schematic of the micromechanical deformation mechanisms considered in the model. The phenomena are related to the evolution of dislocation structures (left column), precipitates (middle column) and solute complexes (right column).

The model is based on three different scales – microscopic, mesoscopic and macroscopic – and captures the evolution of the mean spacing between individual types of obstacles to dislocation motion as the state variables. A brief introduction to the model is given here; a more detailed description can be found in [3,14,58,59]. A recent study [4] describes the enhancements of the existing models in predicting cyclic deformation and stress relaxation from forward creep through the incorporation of a dynamic recovery model [42] and modifications of the physical model describing the combined strength of obstacles to dislocation bypassing.

2.1. MICROSCOPIC DISLOCATION-BASED STATE VARIABLES

The microscopic part identifies the contributions of the three dominant obstacles to the internal resistance τ_{cr} on each crystallographic plane (see Figure 3), i.e. forest dislocation junctions (τ_d) with mean spacing L_d , intragranular precipitates (τ_p) with mean spacing L_p , which are typically $M_{23}C_6$ during the early stages of creep, and discrete solute atoms in the matrix (τ_s) with mean spacing L_s ,

$$\tau_{cr} = \left(\sqrt{\left(\frac{\alpha_d G b}{L_d} \right)^2 + \left(\frac{\alpha_p G b}{L_p} \right)^2} \right) + \alpha_s G b (c b)^{\frac{1}{2}} \quad (1)$$

where G is shear modulus, and b is the magnitude of Burger's vector [60]. The dimensionless obstacle strength parameters α_p , α_d and α_s are derived from geometrical considerations of the distribution of each type of obstacle and their effect on the pinned small segment of dislocation length attempting to bypass the obstacles [61]. L_s has been expressed as a function of the composition or solute concentration c of the discrete solute atoms in the alloy [14]. L_p is a function of the existing precipitate distribution (volume fraction and mean radius). L_d is a function of the dislocation junction obstacle density N_d . The evolution in dislocation junction obstacle density, ΔN_d , due to self- and latent-hardening results from dislocation multiplication related to the increment in the resolved shear strain $\Delta\gamma$ on the slip plane:

$$\Delta N_{self} = j \Delta\gamma \quad (2)$$

$$\Delta N_{latent} = j_s \Delta\gamma \quad (3)$$

where j_s and j are fitting parameters [14]. Evolution of the number density and spacing of precipitates and discrete solute atoms has been considered in [3,59] as a result of long term aging. However, this study is limited to short-term creep of ex-service material where evolution of precipitate phases and solid solution concentrations is negligible, and is therefore ignored here. Note that the three contributions in Eq. 1 scale with temperature through the variation of shear modulus, as noted by Ashby and Frost [62]. Beyond the internal resistance, τ_{cr} , the model also considers the contribution to internal resistance of prismatic dislocation loops which are punched out from the precipitates as the dislocations bow around them [63]. These loops also contribute to the internal stress in the lattice at the slip system level (Type III micro-scale residual stress).

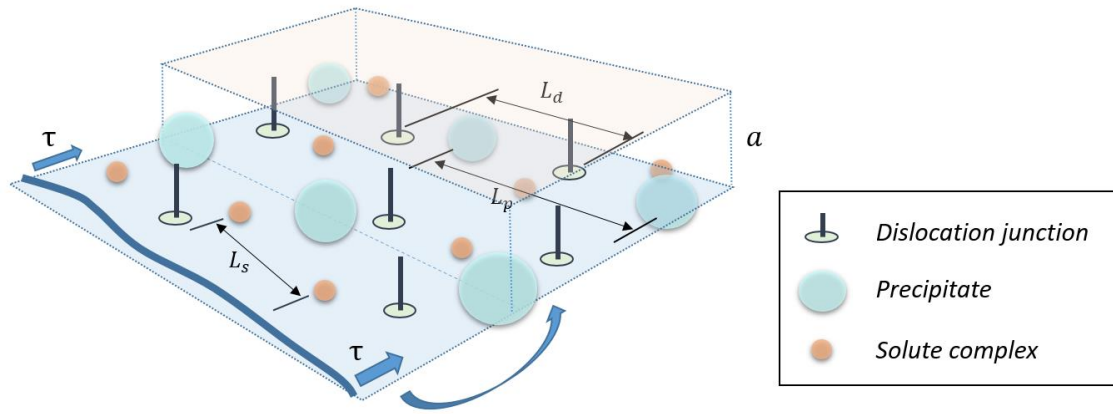


Figure 3. Schematic of the three dominant types of obstacles to dislocation motion along the slip plane. The resolved shear stress, τ , is acting upon the dislocation line represented by the thick solid line.

The phenomenon of dynamic recovery results from continuous annihilation of dislocation dipoles within the crystal through accumulation of plastic strain, particularly under cyclic loading [64]. The dislocation segment annihilation is captured within the multi-scale framework through a model, applied at the slip system level, introduced by Kocks [42] who suggests that the dynamic recovery process is based on the probability that a dislocation segment length (ΔL_r) is annihilated in a unit volume as a function of accumulated obstacle density given an increment of the resolved inelastic shear strain $\Delta\gamma$

$$\Delta N_d = -\frac{\Delta L_r}{b} N_d \Delta\gamma \quad (4)$$

Hu and Cocks [12] described the static recovery of the dislocation network assuming that at elevated temperatures long dislocation links grow at the expense of shorter ones. As a result, the full version of the evolution of the state variable (mean spacing between dislocation junction obstacles) can be expressed as

$$\dot{L}_{di} = -\frac{1}{2}L_{di}^3 \left(j_s \dot{\gamma}_i + \frac{j}{(m-1)} \sum_{j \neq i} \dot{\gamma}_j \right) + \frac{W_c D_c G b^5}{kT} \frac{1}{L_{di}^3} \quad (5)$$

where D_c is the core diffusivity and L_{di} is the dislocation junction obstacle mean spacing on the i th slip plane [59], and W_c is the free parameter controlling static recovery of the dislocation structure.

2.2. CRYSTAL PLASTICITY FRAMEWORK

The response of the individual anisotropic grains in the SCM is modelled using crystal plasticity (CP) theory, which is treated within a small-deformation framework [14]. The equivalent large-deformation description employed in the CPFE model is described in Appendix A. The CP theory allows for the determination of plastic strain rate in each crystal by considering the slip rate on individual slip systems within the crystal. In FCC materials such as 316H, 12 systems are formed from the four $\{111\}$ slip planes $\bar{n}^{(\alpha)}$ and three $\langle 110 \rangle$ slip directions $\bar{s}^{(\alpha)}$ [65]. The plastic strain increment in every grain can be obtained by summing the contributions from each slip system, α [36,66]:

$$\Delta \varepsilon^{pl} = \sum_{\alpha=1}^{12} \Delta \gamma^{(\alpha)} \text{sym}(\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)}) \quad (6)$$

The term $\text{sym}(\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)})$ represents the Schmid factor – the symmetric part of the direct vector product of the plane normal and slip direction of the system [67]. Physical models for the flow-rule describing the evolution of shear strain rate are selected, generally taking the form

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 g(\Delta F_0, T, \tau^{(\alpha)}, \tau_{cr}^{(\alpha)}) \quad (7)$$

Eq. 7 describes the shear strain rate $\dot{\gamma}$ as a function of ΔF_0 – the required thermal activation energy for plastic deformation – and $\tau^{(\alpha)}$ and $\tau_{cr}^{(\alpha)}$, being the resolved and critical resolved shear strength (CRSS) on a slip system [61]. The mechanistic rate-dependent formulation for resolved shear strain rate for the thermal activation of gliding dislocations follows the model proposed by Kocks et al. [68]. The model relates the shear strain rate to the required free activation energy ΔF_0 ($\alpha_0 G_0 b^3$, G_0 : shear modulus at 0 K) to allow the system to reach a new plastically-deformed state at a temperature T according to

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \exp \left(-\frac{\Delta F_0}{kT} \left(1 - \left| \frac{\tau^{(\alpha)} + (\bar{\tau}_m^r)}{(1 + F_{sol}) \tau_{cr}^{(\alpha)}} \right|^{\frac{3}{4}} \right)^{\frac{4}{3}} \right) \text{sgn}(\tau^{(\alpha)}) \quad (8)$$

where k is Boltzmann constant, $\overline{\tau}_m^r$ is the Type III (micro-) internal residual stress [52], $\dot{\gamma}_0$ the reference shear strain rate, and F_{sol} is a thermal solute strengthening term depicting the solute drag process (Figure 2), which results in an enhancement of the CRSS and is modelled via the theory suggested by Schmidt and Miller [69,70]. In this study of the ex-service 316H stainless steel with a pre-existing considerable population of precipitates, F_{sol} is simply set to be zero. For a detailed evaluation of the effect of F_{sol} in the self-consistent model (SCM), see [59]. Physically-motivated modifications of the model in predicting stress relaxation and understanding the relation between displacement-controlled deformation and forward creep have been introduced by Petkov et al. [4]. The parameter α_0 which determines the activation energy for bypassing (see ΔF_0 in Eq. 9), hence the overall effectiveness of obstacles within the thermally-activated glide rule, is found to control the deformation response. This enhancement of the model does not incorporate new equations into the framework, but adjusts α_0 as an additional free parameter whose value is within the physical range suggested by [62]; in this article we use the value of α_0 initially considered in [3].

At low stresses the model is essentially athermal, with plastic deformation only occurring when $[\tau^{(\alpha)} + (\overline{\tau}_m^r)]$ is of the order of $\tau_{cr}^{(\alpha)}$. Under these conditions it is computationally more efficient to employ a phenomenological power-law relationship [35]:

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left| \frac{\tau^{(\alpha)} + (\overline{\tau}_m^r)}{\tau_{cr}^{(\alpha)}} \right|^p \text{sgn}(\tau^{(\alpha)}) \quad (9)$$

where the exponent p is generally assigned a large positive value to provide a close approximation to time-independent plasticity. It should be noted that the power-law flow rule from Eq. 9 is used in the SCM only for simulation of room-temperature short-term plasticity.

The resolved shear stress on a system is obtained through the outer product of the Schmidt tensor and stress tensor as

$$\tau^{(\alpha)} = [\text{sym}(\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)})] : \bar{\sigma} \quad (10)$$

The polycrystalline aggregate is modelled via a SC scheme [14], similar to that proposed by Kroner [21] and Budiansky and Wu [13], capturing mesoscale residual stresses and macroscopic response by treating grains as anisotropic inclusions in an elastic matrix.

3. COMPARISON BETWEEN CPFE AND SCM FRAMEWORKS

In this section we evaluate and compare the predictive capability of the CPFE approach developed in Appendix A and the existing self-consistent model on which it is based [14], in terms of short-term plasticity and creep responses of EX 316H stainless steel. Under these conditions, compositional changes and changes of precipitate populations are minimal and these are assumed to remain constant in the simulations presented here. Experimental data for the EX 316H stainless steel for both monotonic elastic-plastic and forward creep has been provided by EDF Energy. The chemical composition of the material is shown in Table 1. The texture in 316H polycrystalline aggregates measured and employed in previous studies, e.g. [14,24], was found to be weak (approximately random, see Figure 4), hence the material here is treated as a globally-isotropic body.

Table 1. Chemical composition of 316H.

C	Si	Mn	P	S	Cr	Mo	Ni	Co	Fe
0.07	0.41	0.98	0.024	0.017	17.1	2.3	11.6	0.07	Bal.

Three geometries have been investigated using the CPFE approach: 1) a 3D aggregate of 216 grains, each of which is approximated as a cube to provide an “on-average” macroscopic response; 2) a realistic grain-shape quasi-3D thin polycrystal of 39 grains developed to assess localized deformation across grain boundaries; and 3) another aggregate of 216 grains generated as a tessellation in 3D, which was developed to provide an accurate description of the grain shape and arrangement in 3D space. The three configurations together with the employed boundary conditions are shown in Figure 5. The geometric size of the models, number of elements and average grain size are summarized in Table 2. The average grain size selected for the tessellation geometry follows the experimental observations from [71]. The polycrystalline models are treated as an isotropic material with a random texture, with the orientations of the grains represented by sets of three Euler angles (see Figure 4). Investigation of the size of representative volume element (RVE) used in the model predictions is presented in Section 3.4 in the context of geometries generated through 3D tessellations. Similar investigations of the RVE size were carried for the cubic grain polycrystalline aggregate (Figure 5) but are not shown here.

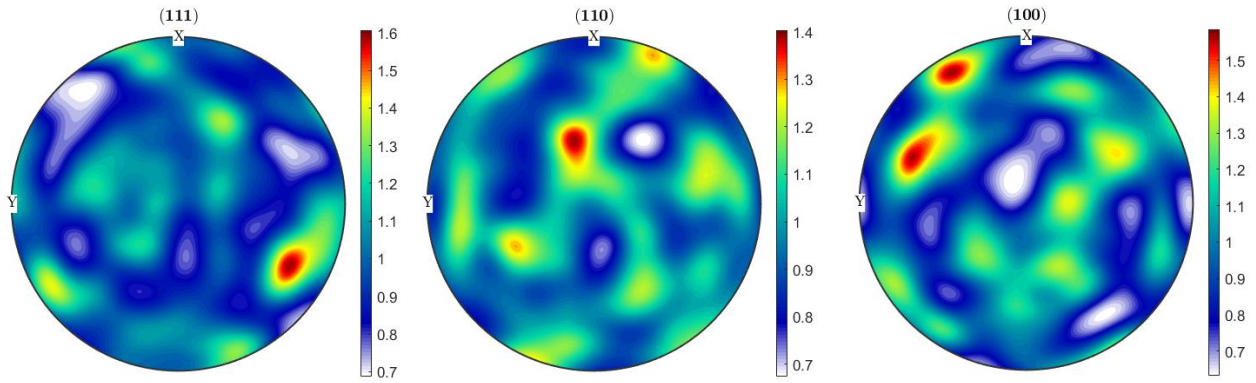


Figure 4. Pole figures of initial texture - ex-service 316H material considered (216 grains). Pole figures are generated using the MTEX open-source software [72].

Sections 3.1 to 3.3 review the CPFE model predictions using the 3D approximate cubic grain and thin quasi-3D geometries. Predictions using the more realistic grain aggregates in a full 3D formulation, developed through tessellations, are presented in Section 3.4.

Table 2. Model size, number of elements and average grain size for the three types of geometries considered.

Geometry	Size – $X \times Y \times Z$ (μm)	No. Elements	Average grain diameter (μm)
216 cubic grains	300 x 450 x 200	5832 (C3D20R)	50
39 grain thin slice	200 x 360 x 8	44296 (C3D8)	55
216 grains tessellation	300 x 450 x 200	60081 (C3D10)	60

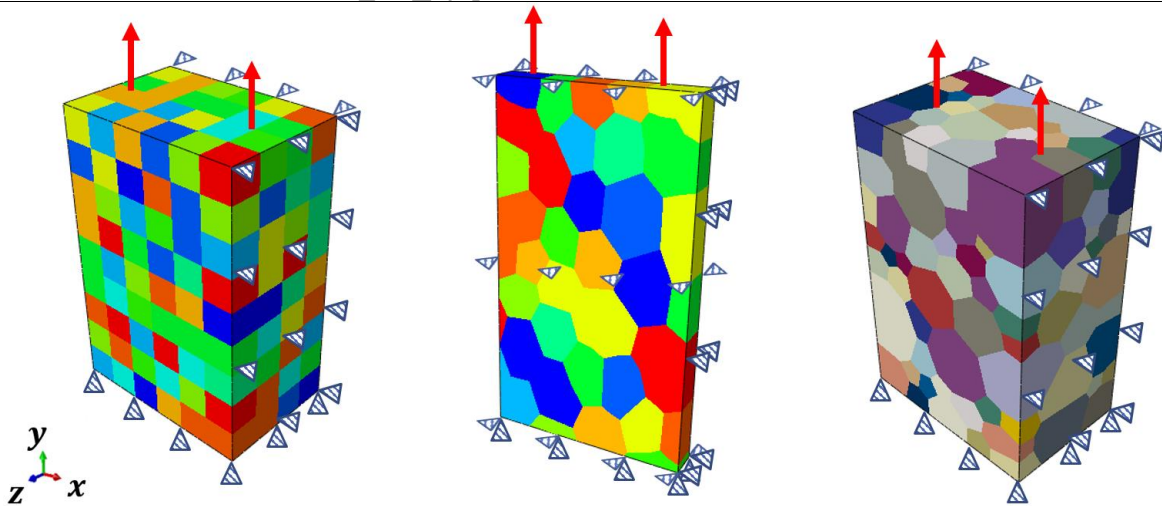


Figure 5. Polycrystalline aggregates approximated by cubic grains (left) and realistic grain-shape geometry (middle). 3D tessellation of 216 grains of realistic shapes, generated using Neper Generation software [57]. N.B. Images not presented to the same scale.

3.1. SHORT-TERM PLASTICITY

Here we examine the short-term elastic-plastic behaviour of EX 316H at 550°C and compare the predictions to those given by the SCM. The fitting parameters – initial density of dislocation junctions on each slip plane N_0 , and hardening coefficient j, j_s – and physical properties of 316H – are the same for the SCM and CPFE models (see Table 3). The geometry of 216 cubic grains was loaded in simple tension with the bottom (y_0), right (x_{max}) and back (z_0) sides of the aggregate prevented from moving in the direction normal to the boundary (Figure 5). A multi-point constraint was imposed on the forward (z_{max}), left (x_0) and top (y_{max}) sides of the body such that their faces remain planar. The macroscopic stress (Σ) and strain rate ($\dot{E}_{ij,m}$) in the loading direction (y-axis) are obtained according to

$$\Sigma_{22} = \frac{1}{A_{top}} \int_0^A \sigma_{22}^i dA_i \quad (11)$$

where σ_{22} is the stress along the top surface in the loading direction, A is the area of the top surface (y_{max}) given in terms of deformed dimensions of the aggregate, and

$$\dot{E}_{22,m} = \dot{Y}/Y \quad (12)$$

where Y is the deformed dimension of a side of the aggregate in the y-direction, respectively.

Table 3. Material parameters for SCM and CPFE simulations for 316H ($T_m = 1810$ K). Values of N_0 , j and j_s in brackets are for loading at high temperature pre-loading (see Section 3.2).

Parameter	Value	Parameter	Value
C_{11}	198 GPa*	N_0	2.5×10^{13} (3×10^{13})
C_{12}	125 GPa*	j	1.75×10^{15} (7×10^{14})
C_{44}	122 GPa*	j_s	8.75×10^{15} (3.5×10^{15})
E	101.3 GPa	W_c	80
ν	0.39	D_c	6.47×10^{-15} m ² /s
G_0	139 GPa	Δ	15 **
b	2.5×10^{-10} m	τ_p	21 MPa
$\dot{\gamma}_0$ (Eq. 10)	1×10^{-6} 1/s	τ_s	37 MPa
$\dot{\gamma}_0$ (Eq. 11)	1 1/s	α_d	0.35
α_0	1		

* Data taken from Kamaya [73]. ** Value from [4].

The predictions of macroscopic deformation from the CPFE and SCM agree well with one another, with both results replicating the experiment (Figure 6). However, it is observed that the CPFE prediction lies below the SCM prediction (note that in these simulations the SCM and CPFE have used exactly the same constitutive laws and formulations of the flow rule). This behaviour is consistent with the general observation in mechanics that increasing the number of degrees of freedom (i.e. increasing the number of different ways that a body can deform) gives a more compliant and softer predicted macroscopic response. In the CPFE model the strain is inhomogeneous within the grains, with stress and strain concentrations developing in the vicinity of triple lines, while in the SCM a uniform state of stress and strain is assumed within each grain, which is surrounded by a homogeneous material [14].

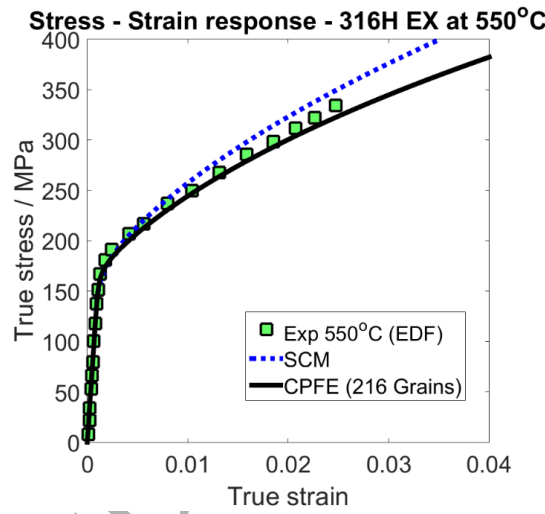


Figure 6. Stress-strain response of 316H at 550°C. Predictions from SCM and CPFE (cubic grains) are compared to experimental data.

An example of localized deformation patterns is shown in Figure 7 – the fields of effective plastic strain accumulated and average dislocation junction density are compared at $\varepsilon = 5.0\%$. The distributions of these quantities are virtually identical, as might be expected due to the relationship between dislocation junction density and local shear strain (Eqs. 2 and 3). Note that the order of magnitude of the dislocation obstacle density is in general agreement with values recorded experimentally, e.g. [74]. The variation of axial stress σ_{yy} , the von Mises effective stress σ_e and $N_{d,tot}$ for 10 selected grains within the CPFE scheme with cubic grains as compared to the SCM results is shown in Figure 8, making use of statistical parameters that have been employed to assess higher order self-consistent models [34]. For the CPFE model this plot shows the grain average stress ($\bar{\sigma}_{yy}^{(gr)}$ and $\bar{\sigma}_e^{(gr)}$) and obstacle density ($\bar{N}_d^{(gr)}$) plus and minus the standard deviation, e.g. $SD^{(gr)}(\sigma_{yy}) =$

$\sqrt{\langle \sigma_{yy}^2 - \bar{\sigma}_{yy}^2 \rangle^{(gr)}}$. The averaged values of stress and dislocation obstacle density predicted by the CPFE model differ by 8% and 11.5% from those predicted by the SCM. It proves convenient to examine the standard deviation of these quantities for the entire polycrystalline aggregate, e.g. $SD^{(poly)}(\sigma_{yy}) = \sqrt{\langle \sigma_{yy}^2 - \bar{\sigma}_{yy}^2 \rangle}$ and normalise these with respect to the average values for the polycrystal, i.e. $SD(\sigma_{yy})^* = \overline{SD^{(poly)}(\sigma_{yy})} / \sigma_{yy}^\infty$, $SD(\sigma_e)^* = \overline{SD^{poly}(\sigma_e)} / \sigma_e^{(poly)}$ and $SD(N_d)^* = \overline{SD^{(poly)}(N_d)} / \overline{N_d^{(poly)}}$, where σ_{yy}^∞ is the remote applied stress. After monotonic time-independent loading to 5% true strain these take values of 0.27, 0.14 and 0.186, respectively; the SD for σ_e is about 25% of that obtained in [34] for the fcc material model considered in that paper, indicating that the variation of stress within a grain is less than for their model and the role of second order effects is less important. It is these variations, however, that are responsible for the slightly different monotonic responses observed in Figure 6. The difference is a result of the local field variations arising from geometric constraints, grain heterogeneity and local variation in the constitutive response. In the following sections we employ the same method to further characterise and explain the relation between such local processes and changes in the observed macroscopic response, particularly during creep deformation (see Sections 3.3. and 3.4).

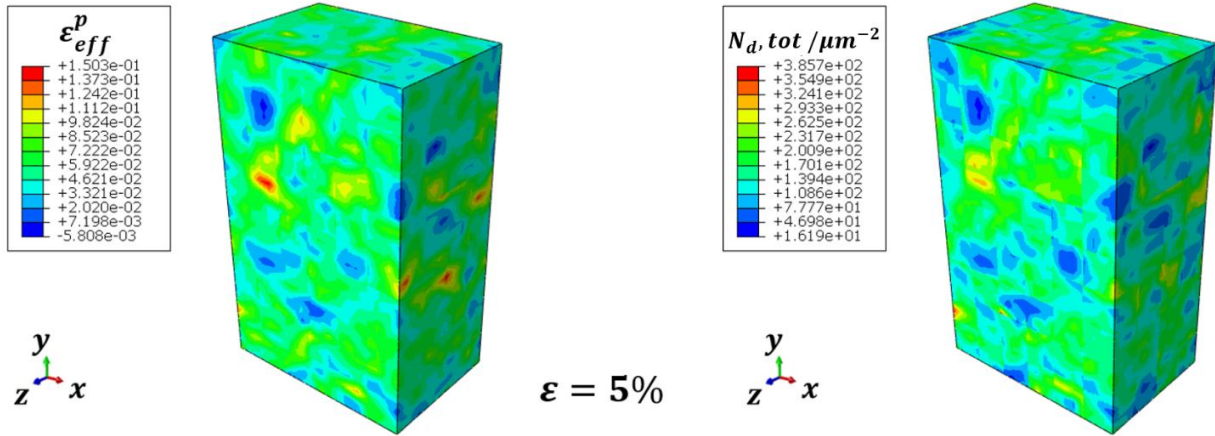


Figure 7. Contour plots of effective plastic strain (left) and average dislocation junction density (in $1/\mu\text{m}^2$) (right).

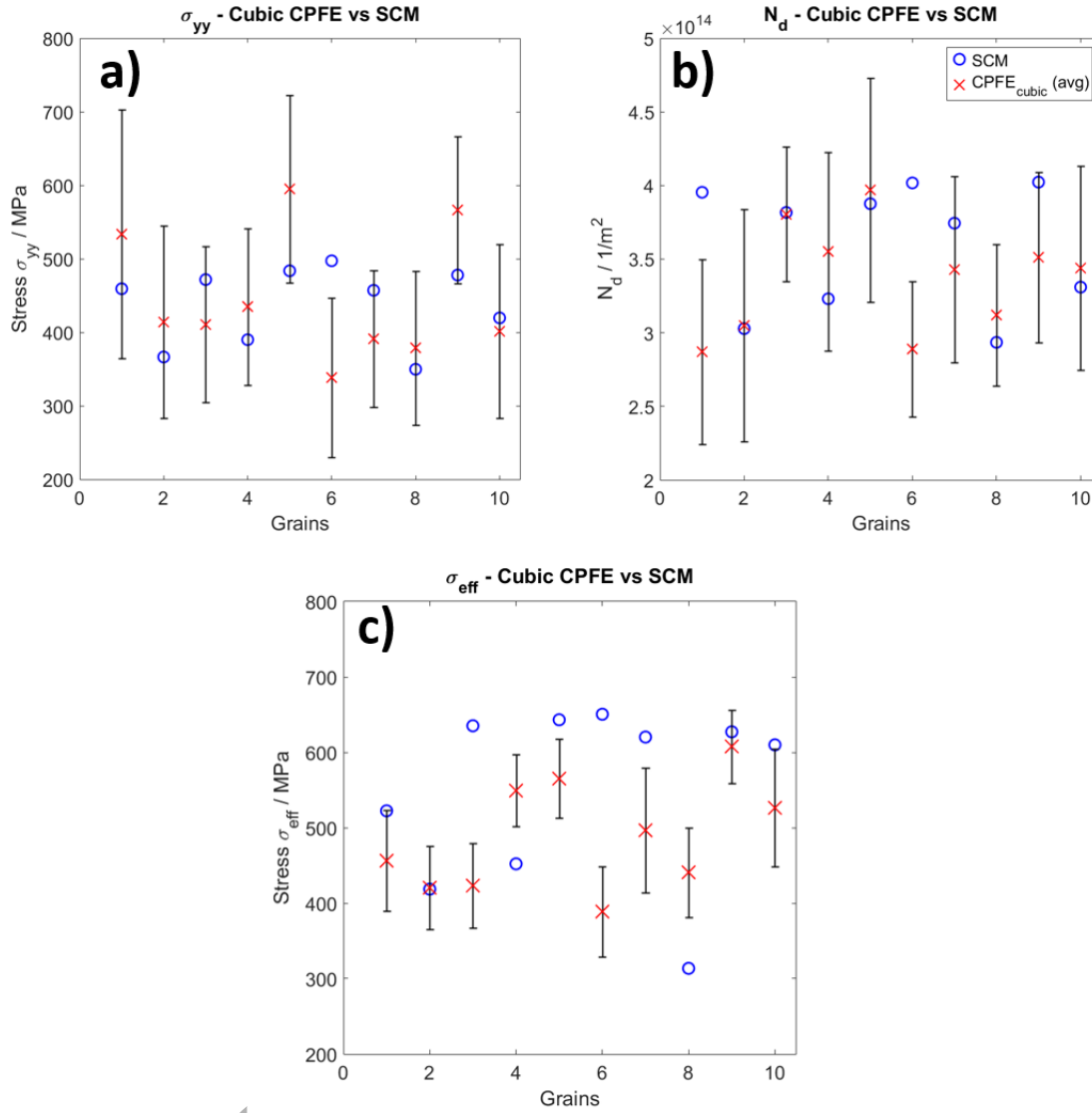


Figure 8. The average values and variation within grains, represented via the standard deviation of quantities within a given grain $SD^{(gr)}(\sigma_{yy})$ and $SD^{(gr)}(N_d)$, of σ_{yy} (a), $N_{d,tot}$ (b) and σ_{eff} (c) for 10 selected grains within the CPFE model (with cubic grains), compared to the SCM results, at 5% true strain.

Further, thin slice geometries of a polycrystalline material using the same fitting parameters were also investigated. Two simple tessellations of a thin 3D section of a polycrystal (Figure 9) were constructed. Gill and Cocks [75] suggested that the formed quadruple grain junctions in Geometry 1, constructed using a straightforward Voronoi approach, are unstable; more realistic grain shapes are formed in Geometry 2 [75] and this architecture is used hereafter. The relaxation of Geometry 1 towards Geometry 2 is obtained by moving quadruple and triple points according to out of balance grain-

boundary tensions, until they are in equilibrium, which is when there are only triple grain junctions and the intersecting boundaries are at approximately 120° with respect to one another [75]. As a result of this, some grain boundaries are slightly curved, which is closer to a real-life grain structure. The samples were loaded in tension under quasi-3D plane-strain (generalized plane strain along the z-direction) with the left-hand side of the thin slice (x_0) free to deform.

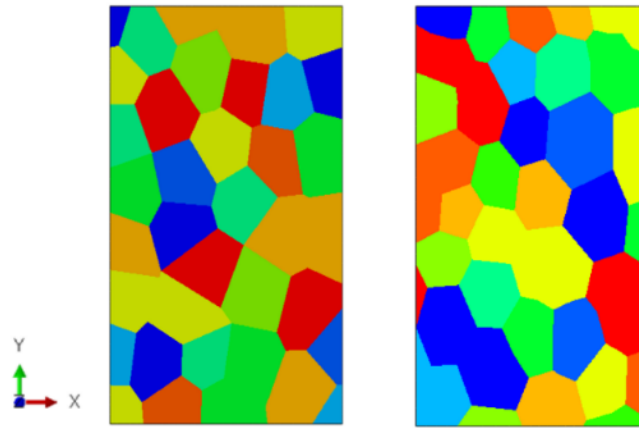


Figure 9. Geometry 1 (left) and Geometry 2 (right) developed.

Predictions of macroscopic response agree reasonably well with experimental data (Figure 10) and with the 3D simulations of Fig 6. A mesh sensitivity study using two model configurations of Geometry 2 consisting of 5424 and 44296 elements was also conducted only to find no significant variation in the result (see Figure 10).

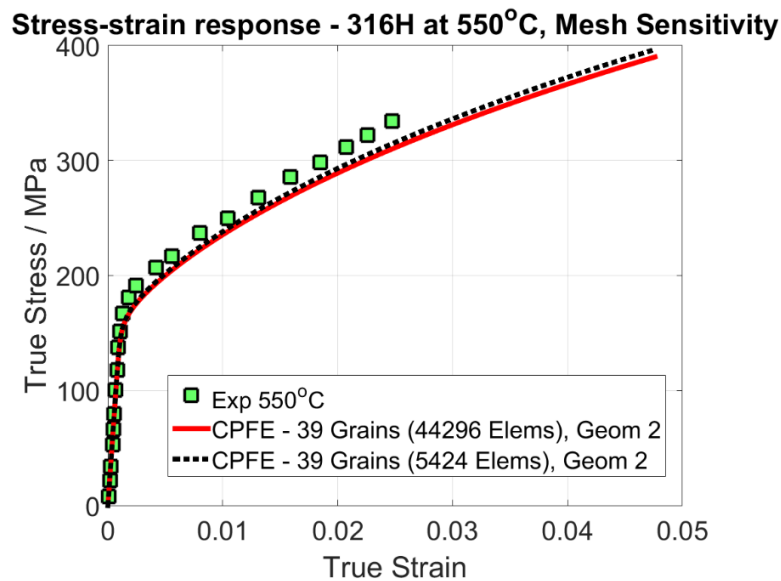


Figure 10. Stress-strain response of 316H at 550°C for Geometry 2.

Distributions of the accumulated effective plastic strain, the average junction density as well as the stress along the loading direction at $\varepsilon = 5.0\%$ are shown in Figure 11. Some concentrations can be seen near grain boundaries. The variation of σ_{yy} across multiple grains with different orientations is demonstrated through the line plots along several paths in Figure 12. It is clear from Figure 12 that stress concentrations are localized in the grain boundary regions. High local values of stress along the loading direction are observed near grain boundaries adjacent to crystals with a more significant mismatch in orientations, agreeing with [76]. Comparison between the stresses in the sampled neighbouring grains show that the effects of elastic anisotropy appear to be significant at the grain scale, which agrees with observations made by Dunne et al. [8].

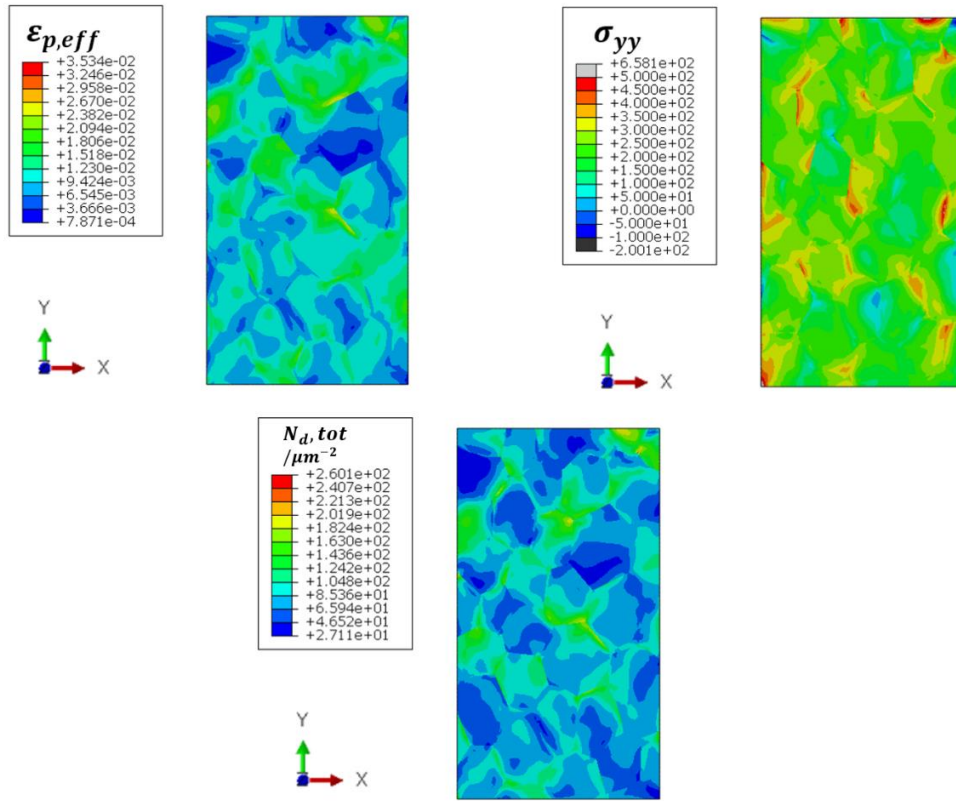


Figure 11. Contour plots of effective plastic strain (top left), average dislocation obstacle density in $1/\mu m^2$ (bottom) and stress in the loading direction (top right).

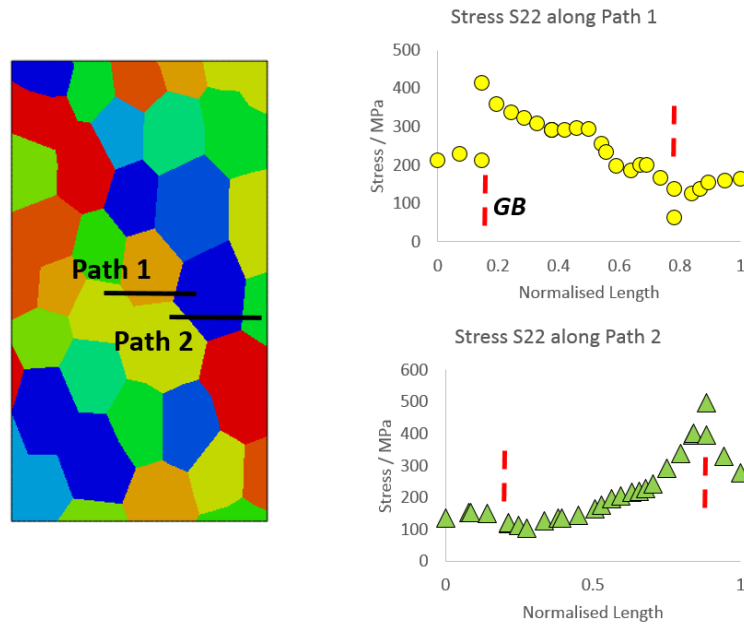


Figure 12. Line plots of σ_{yy} along paths crossing grains of different orientations.

3.2. BAUSCHINGER EFFECT IN 316H

Here, the Bauschinger effect in EX 316H at 550°C is examined and the result is compared to the predictions using the SCM obtained by Hu et al. [52]. The loading history comprises of high temperature (HT) tensile preloading and unloading at 550°C, followed by cooling and re-loading in either tension or compression at room temperature (RT). The free parameters in the model were calibrated to capture only the HT pre-load stress-strain response and these parameters were used to predict the subsequent response during the RT experiments. The boundary conditions of the 216 cubic grain aggregate was the same as those in employed in Section 3.1. The thermally-activated glide rule of Eq. 8 is chosen for the HT pre-loading, while the flow rule employed at RT is that given by Eq. 9 with the rate-sensitivity exponent $p = 600$ [52] to mimic a rate insensitive response.

The Bauschinger effect, which results in a sharp change in response at RT tensile re-loading compared to the gradual smooth change in response at RT during compressive re-loading, is captured well by both models (Figure 13). Figure 14 gives a clear example of the change in localized stress field during RT compression at different strain levels. Predictions by both models show that this complex response is a result of the evolution in both the internal microstructural state of the material and the generated residual stress field. As expected, the residual stress state at the end of the compression loading cycle is a “mirror image” of the stress field after the tension cycle, as observed in Figure 14 – differences in

macroscopic response depend on how the stresses redistribute from the initial pre-loaded stress state towards the end of the RT re-loading step, agreeing with Hu et al. [52]. The sharp change in the stress-strain behaviour after yielding given by the CPFE model appears to be slightly more gradual than that predicted from SCM. This is possibly related to relaxation of the localized residual stress field during HT unloading, which is captured by the 3D FE scheme but not by the SCM, causing localized plastic deformation earlier upon subsequent re-loading.

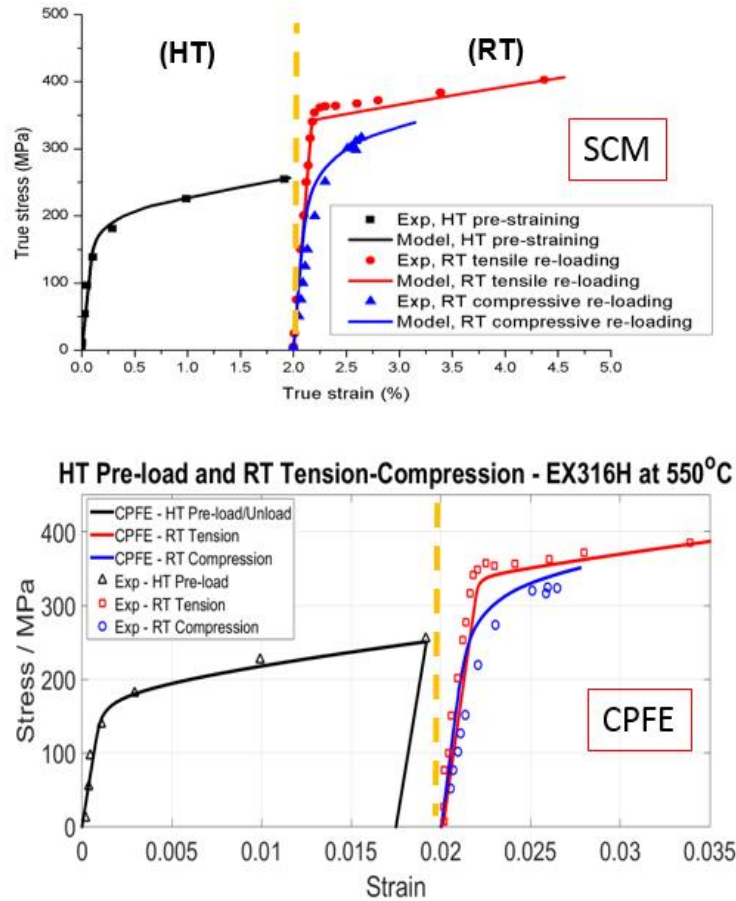


Figure 13. Stress-strain response of high temperature (HT) pre-loading and room temperature (RT) re-loading – SCM [52] (left) and CPFE (right).

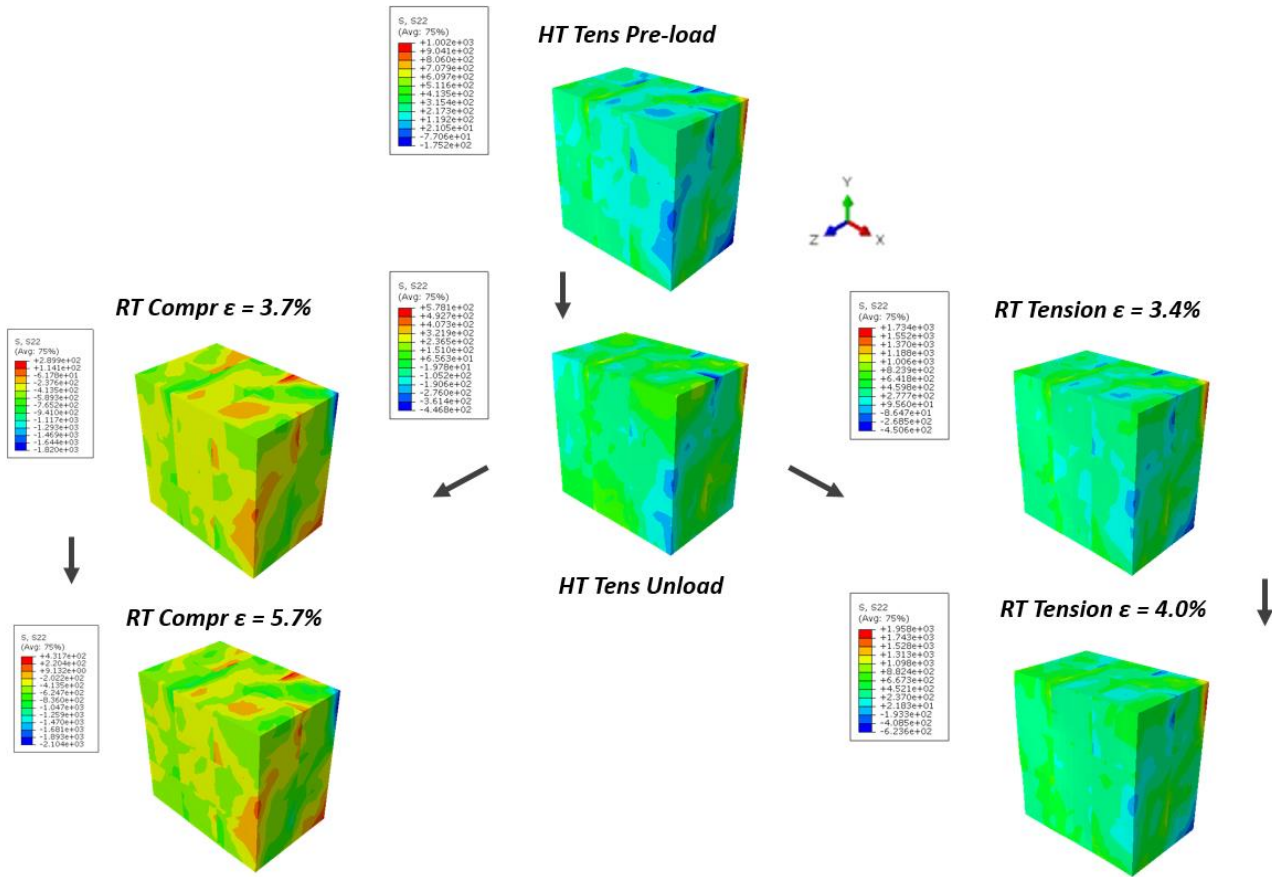


Figure 14. Contour plots of the stress field σ_{yy} developed in several sampled cubic grains for HT-RT Tension and HT-RT Compression loading paths.

3.3. SHORT-TERM CREEP RESPONSE

The short-term creep response of EX 316H was also predicted using the CPFE model and the results compared to SCM predictions obtained by Hu et al. [12]. The test conditions were rapid loading at 550°C up to a stress of 250 MPa, 280 MPa or 320 MPa, which was then maintained constant for the remainder of the experiment/simulation. The additional fitting parameter W_c is used to define the extent of the static recovery of the dislocation network (Eq. 5). The same two-step loading history as that in Section 3.2 was used here. Model predictions of the macroscopic creep curves are shown in Figure 15. It is found that the CPFE over-predicts the inelastic strain compared with SCM, suggesting that the extent of static recovery is overestimated. This is again consistent with the general observation that a softer, less creep resistant response is obtained with an increase in the number of degrees of freedom (i.e. reduction of internal constraint). A better match is achieved by recalibrating the fitting parameter W_c with a reduced value ($W_c = 19$), compared to that employed in the SCM. The resulting variations of

stress in the loading direction, effective stress and dislocation obstacle density predicted via the SCM and CPFE are illustrated in Figure 16, demonstrating the large difference between the average obstacle densities for the polycrystalline array predicted via the two frameworks with mean differences of 33% ($W_c = 19$) and 29% ($W_c = 80$). Note that the averages of the axial stress for each grain show a mean difference of 3% between the two schemes. Further, we determine the overall normalised standard deviations within the whole polycrystalline aggregate after creep for 555 hours at 550°C (using the same approach as that of Section 3.1) to be different to those for time-independent monotonic loading. For the cubic grain geometry and $W_c = 19$ it is found that $\overline{SD(\sigma_{yy})}^*$ increases from 0.27 to 0.288 while $\overline{SD(\sigma_e)}^*$ and $\overline{SD(N_d)}^*$ decrease from 0.14 to 0.114 and from 0.186 to 0.069, respectively, compared to the time-independent results from Section 3.1. While for $W_c = 80$, the difference in axial stress is even more pronounced with $\overline{SD(\sigma_{yy})}^* = 0.349$, $\overline{SD(\sigma_e)}^*$ and $\overline{SD(N_d)}^*$ decrease further from 0.14 to 0.109 and from 0.114 to 0.0643, respectively. This result illustrates an important point. Creep is a balance between two highly non-linear processes – thermally activated glide and climb controlled recovery of the dislocation structure. Small variations of deviatoric stress (which we use σ_e to provide a measure of) and N_d can have a significant effect on the deformation rate, so the stress and material state tend towards a more uniform state. Increasing the characteristic rate of recovery tends to further promote a more uniform state (i.e. residual effective stress and critically resolved shear stress – which depends on N_d). The increase of the variation of axial stress, however, indicates that during creep there is a more significant variation of hydrostatic stress σ_H within the polycrystalline body as compared to the variation of hydrostatic stress after monotonic short-term plasticity loading to the same stress, which is illustrated in Figure 17. This result illustrates that parameters employed in any model need to take into account the fidelity of the model and how the average macroscopic response is determined, as well as the details of the physical processes that give rise to the macroscopic response. We discuss this further in Section 4.

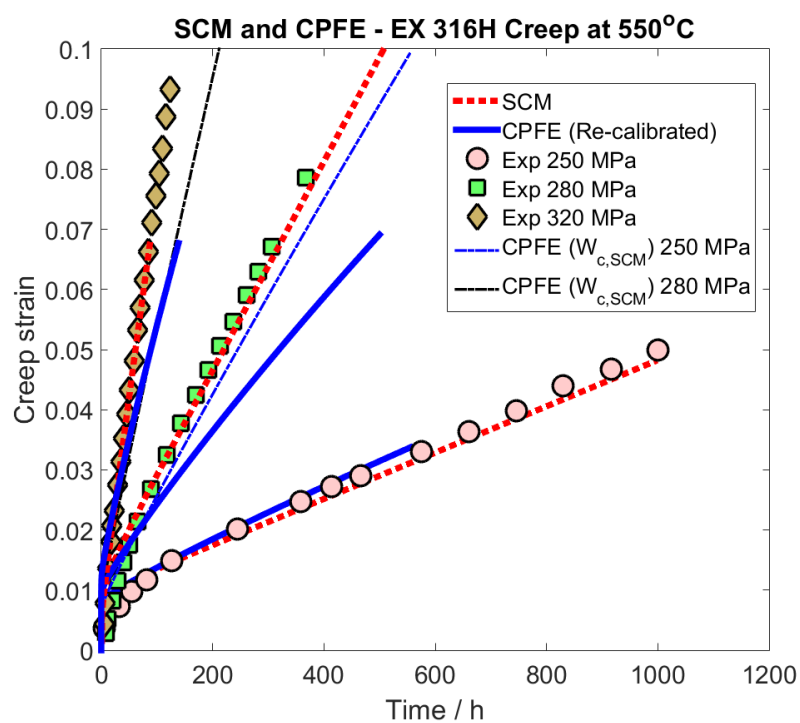


Figure 15. Creep response of EX 316H at 550°C at different stress levels – SCM and CPFE predictions. Initial CPFE predictions before calibration of the model, using the same parameters as those in the SCM, at 250 MPa and 280 MPa are shown.

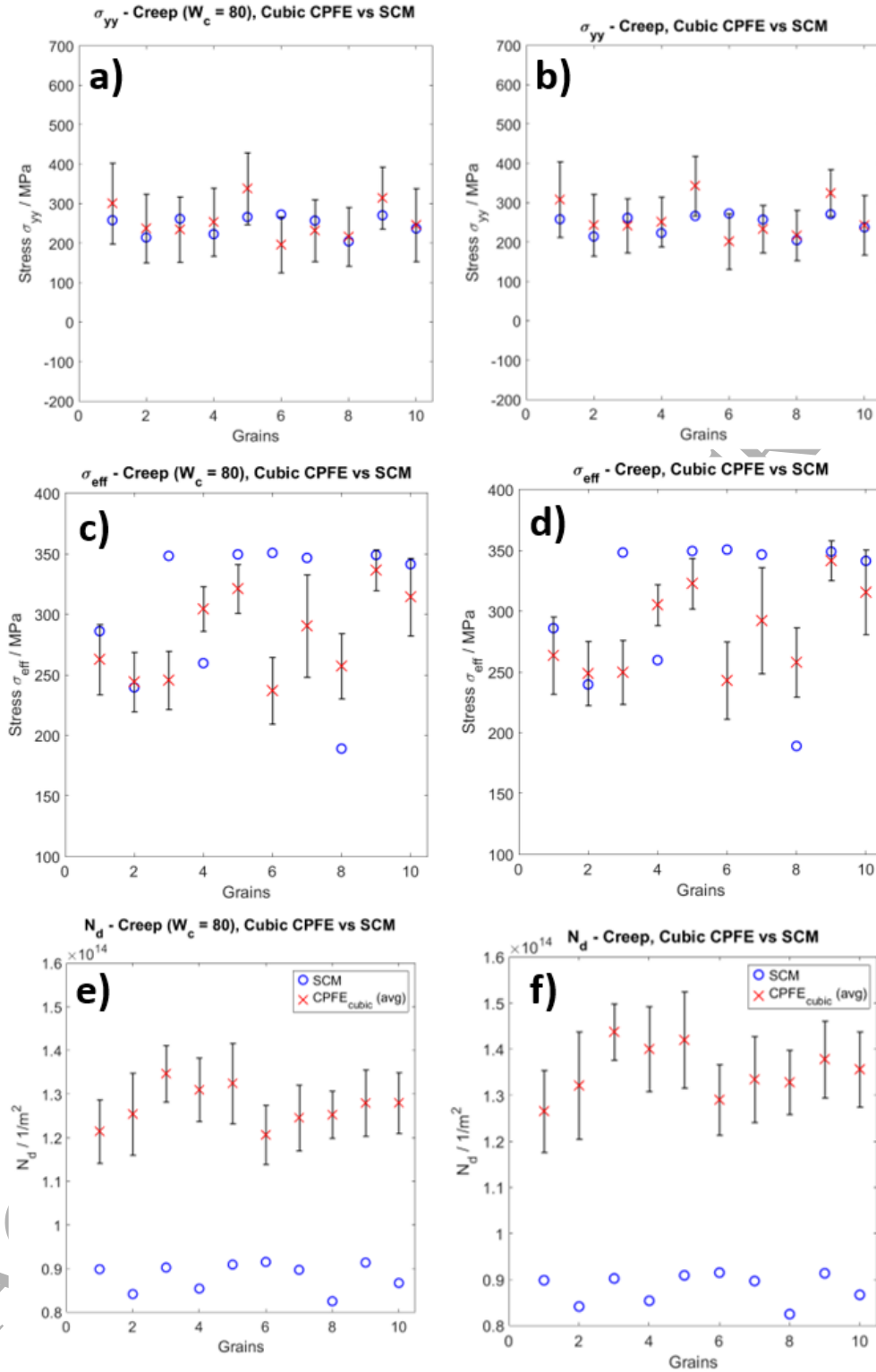


Figure 16. The average values and variation within 10 selected grains within the CPFE model, represented via the standard deviation of quantities within a given grain defined in Section 3.1, of σ_{yy} is shown in a) $W_c = 80$ and b) $W_c = 19$ compared to the SCM results after creep for 555 hours at 250 MPa – note that the average is not

affected greatly. In c) and d) the variation of σ_{eff} is presented. The average values and variation of $N_{d,tot}$ for e) $W_c = 80$ and f) $W_c = 19$, showing the increase in dislocation obstacle density with reduction in W_c by a factor of 4, responsible for the lower values in accumulated creep strain.

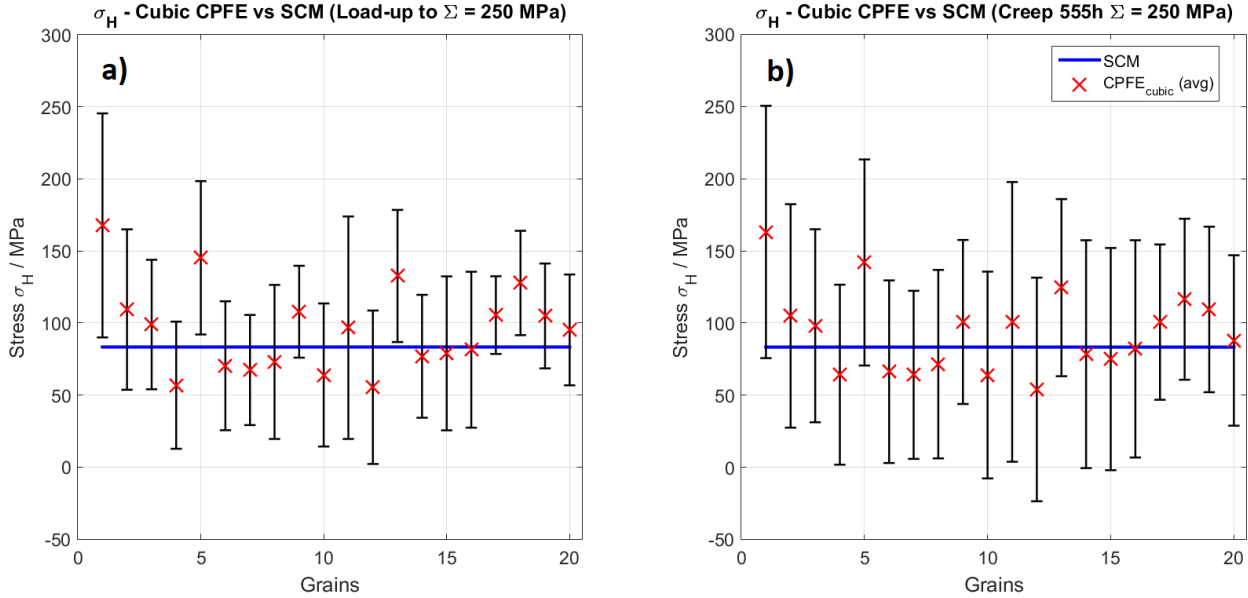


Figure 17. The average values and variation within 20 selected grains predicted via the CPFE model, represented via the standard deviation of quantities within a given grain, defined in Section 3.1, of the hydrostatic stress σ_H is shown in a) after short-term plasticity loading to 250 MPa prior to creep and b) after 555 hours of creep at 250 MPa. Comparison is also made with the SCM results. Note that the average of the hydrostatic stress is not affected greatly. The variation of the hydrostatic stress within grains, however, is greater in b) because of the increase in the variation in axial stress as a result of the stress redistribution process.

Short-term creep simulations of EX 316H were also conducted with the realistic grain geometry of Fig 5b under generalized plane strain at 550°C and 250 MPa; predictions of the macroscopic creep strain accumulation with time agree well with experimental data (not shown here for brevity). The stress redistribution between grains during creep due to compatibility and equilibrium requirements is shown at different creep times t_c in Figure 15. It is found that the stress redistribution evolves during primary creep but saturates when the secondary creep regime is reached. In the context of crystal plasticity, grains of “hard” orientations can be termed those in which inelastic shear strains do not develop readily, i.e. grains in which plastic deformation is difficult due to the orientation of their slip systems in three-dimensional space. Similar to observations made from Figures 10 and 11, during the stress-controlled creep loading, the stress concentrations are localized in grain boundary regions – more specifically near the triple grain junctions (see Figure 18). Larger local values of stress along the loading direction are

observed at grain boundaries between adjacent crystals with more significant mismatch in orientations, as seen in Figure 19. This observation can provide insight into primary locations of damage development during creep. We simply flag this up here; further consideration of damage development is beyond the scope of this paper. Modelling of long-term creep response using this quasi-3D geometry serves as an introduction to studies using the realistic 3D tessellation geometries of Fig 5c presented in the following section.

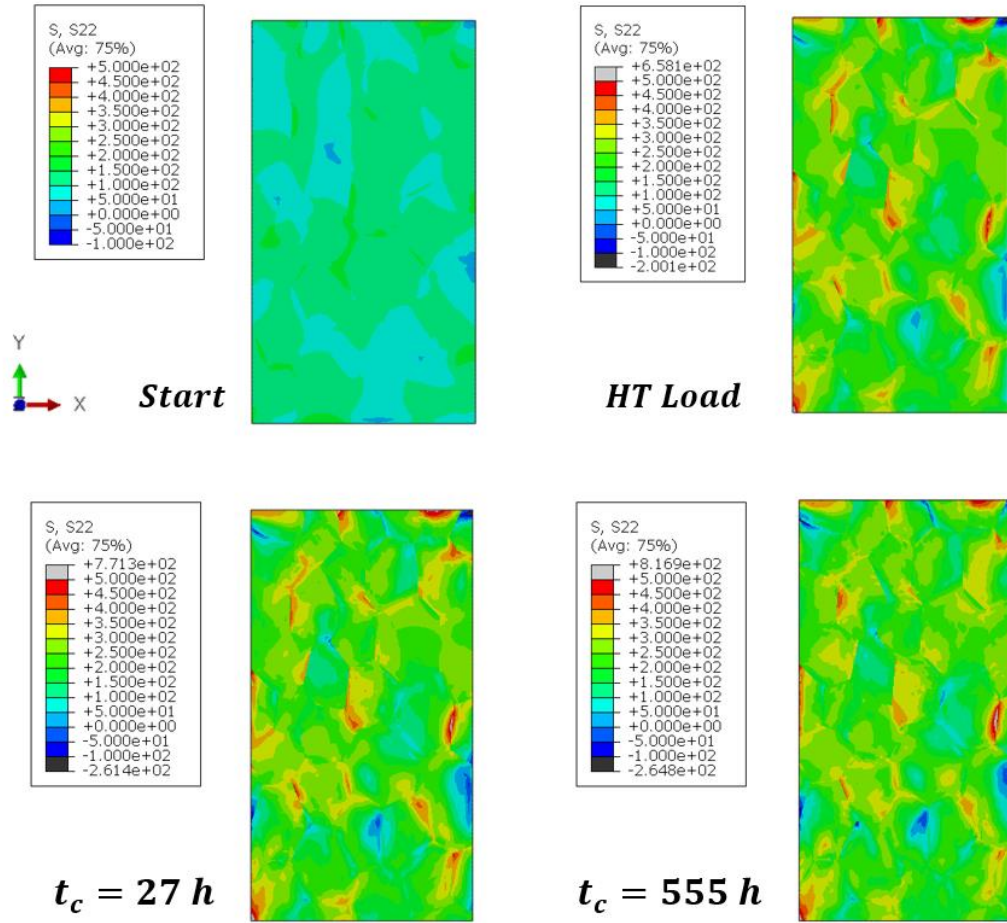


Figure 18. Contour plots of the evolution of σ_{yy} during the creep load history – 39 grains thin slice geometry. The stress field distribution shown at $t_c = 27 h$ is within the primary creep regime and that at $t_c = 555 h$ is within the secondary creep regime.

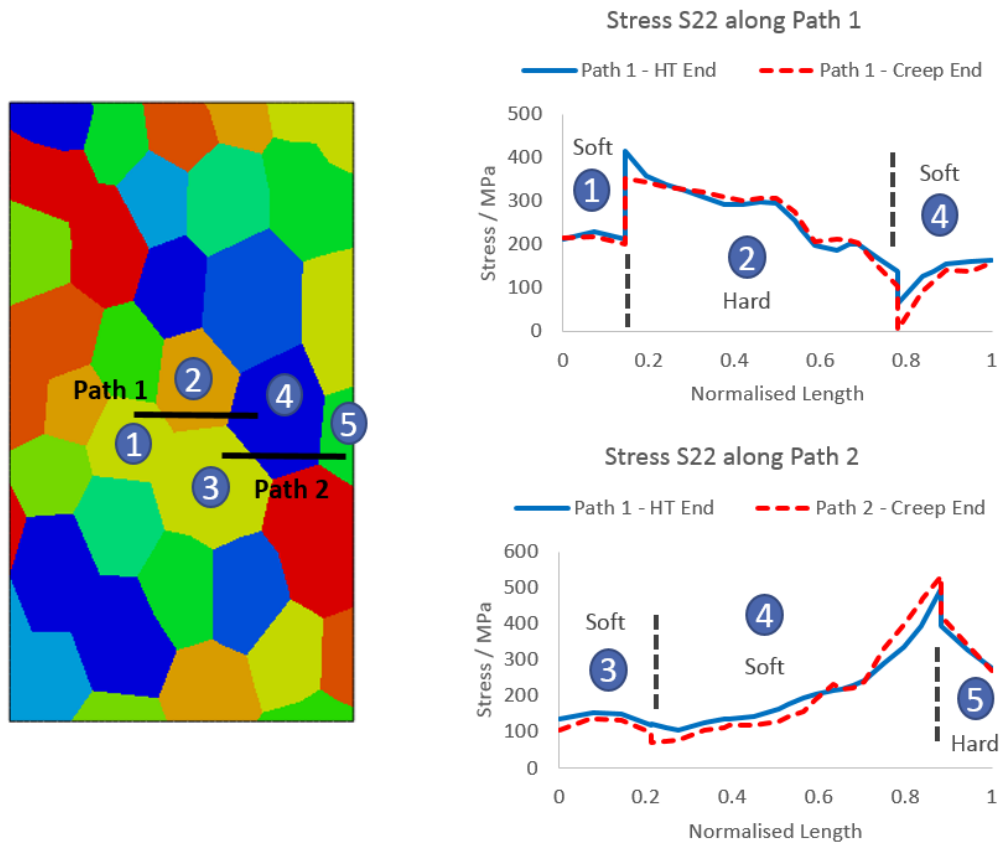


Figure 19. Line plots of σ_{yy} along paths crossing grains of softer and harder orientations showing the redistribution of stress fields, generated during the initial elastic-plastic loading step, during stress-controlled long-term creep after 555 h at 250 MPa. Grains examined along the paths are labelled 1-5; “harder” and “softer” grains are labelled.

3.4. PREDICTIONS USING REALISTIC 3D GEOMETRIES

Predictions using the more realistic grain aggregates in 3D, developed through tessellations, are presented in this section, which were constructed using the Neper Generation software [57]. The 3D tessellation geometry is more realistic than the quasi-3D geometry, due to the fact that grain boundaries are also inclined at an angle through the thickness of the aggregate which is observed in real microstructures. This idealisation is more representative of EX 316H stainless steel and allows us to gain a better understanding of the development of localised deformation fields in polycrystalline materials and how this influences the macroscopic response. A polycrystal consisting of 216 grains was constructed in order to allow for direct comparison with the original 216-cubic grain aggregate. The size of the model is given in Table 3 and Figure 20. In order to construct the cells of the tessellation a similar procedure to that suggested by Gill and Cocks [75] described in Section 3.1 was employed. This

is achieved using a regularization procedure as a standard option in Neper together with modification of the sphericity and centroid position of each cell to replicate experimentally-observed grain growth morphologies (“-morpho gg” option in Neper). The mesh is comprised of quadratic tetrahedral elements (C3D10) with a characteristic length of approx. $12\ \mu\text{m}$. The use of tetrahedral rather than brick elements for realistic grain structures allows the geometries to be more readily meshed without the need for highly distorted elements. The constructed tessellation and mesh are shown in Figure 20.

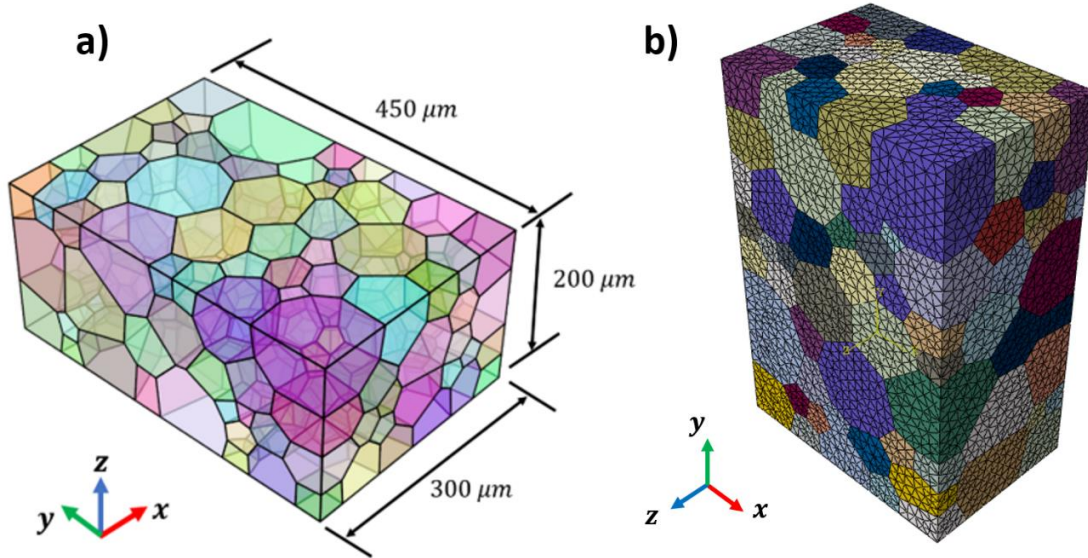


Figure 20. a) The 3D tessellation with 216 grains and b) the generated mesh.

3.4.1. Selection of representative volume element (RVE)

Complex statistical approaches for the determination of the representative volume element (RVE) have been described in the literature; a detailed review of such techniques can be found in Pelissou et al. [77]. In this study we adopt the simplistic approach employed by Simonovski and Cizelj [78] and modify it by including the statistical assessment on the standard deviation of predicted macroscopic behaviour through different cell morphologies and sizes, proposed by Mirkhalaf et al. [79] for geometries at finite strains. Sets of three Euler angles were selected for individual grains to give an approximately random texture (see Section 3). In order to determine the size and number of grains of the RVE, five tessellation geometries with 50, 100, 200, 216 and 300 grains, with the same grain-to-size ratio were established (examples are shown in Figure 21). The average number of elements per grain in the tessellation geometries is ~ 300 . The monotonic elastic-plastic and creep responses predicted for every geometry using the same fitting parameters and element size were compared and the standard deviation

of the responses was assessed. A brief summary of the mesh convergence results is given in Appendix B. Geometries for which the response falls within a prescribed bound of less than $\pm 5\%$ deviation from the mean, were treated as RVEs of appropriate size. The differences between the variation in response for monotonic loading and creep (Figure 21) was insignificant. The analysis indicates that adding more grains to the tessellation realisation of 200 grains does not result in significant changes in macroscopic response, agreeing with Cailletaud et al. [17]. Hence the geometry with 216 grains was selected, which provides a good balance between the accuracy in the resulting predictions and reasonable computational efficiency.

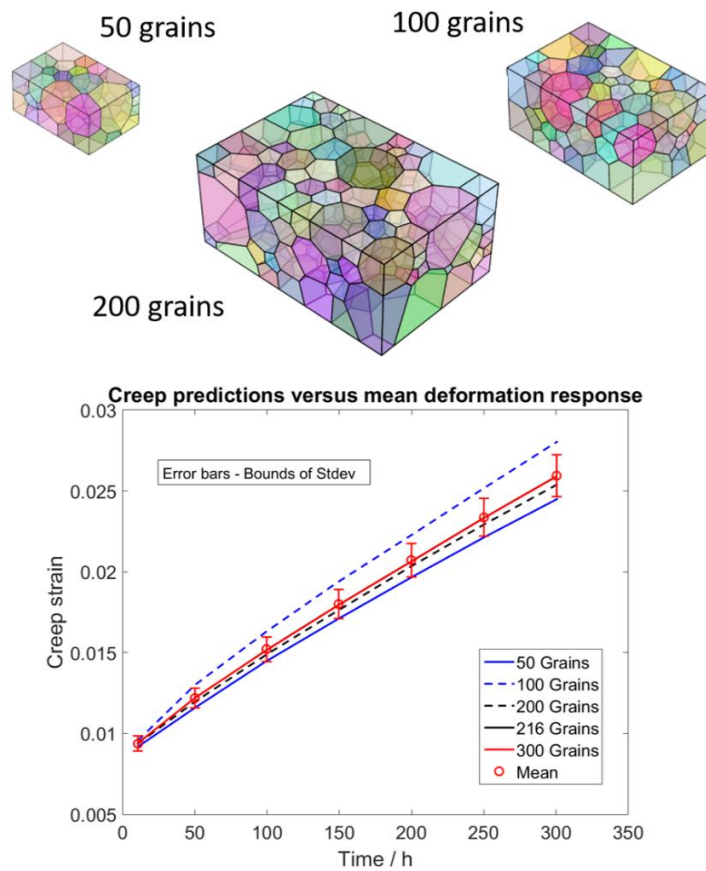


Figure 21. Top: Examples of grain configurations examined in the determination of RVE. Bottom: Comparison between predictions of creep response using the different cell geometries.

3.4.2. Monotonic elastic-plastic response

Monotonic elastic-plastic behaviour of EX 316H at 550°C is examined here for the realistic tessellation polycrystalline aggregate. All the settings are the same as those employed for the cubic grain geometry in Section 3.1, except the grain shape, thus allowing a direct comparison between the two FE

geometries. The predictions of the macroscopic stress-strain curves of the material by the two FE geometries agree well (Figure 22) which illustrates that usage of a polycrystalline geometry with cubic-shaped grains is appropriate to capture the monotonic elastic-plastic deformation response. The evolution of effective plastic strain with macroscopic strain during monotonic loading within the realistic grain aggregate is shown in Figure 23. Effective plastic strain accumulates near grain boundaries as a result of localised slip activity within grains favourably orientated for activation of slip on multiple slip systems.

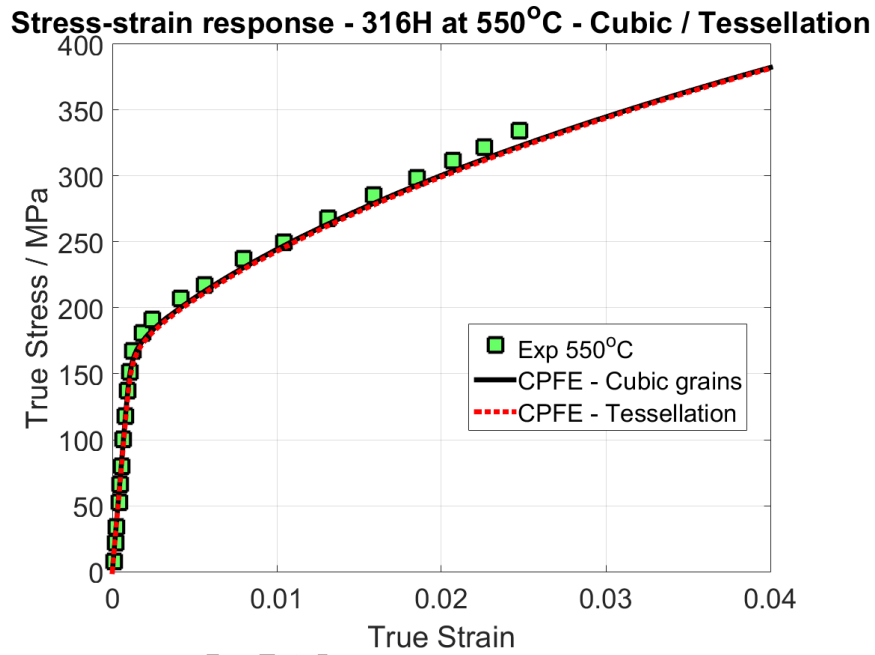


Figure 22. Stress-strain response of 316H at 550°C. Predictions via the CPFE model using cubic and realistic tessellation grain shapes compared to experimental data.

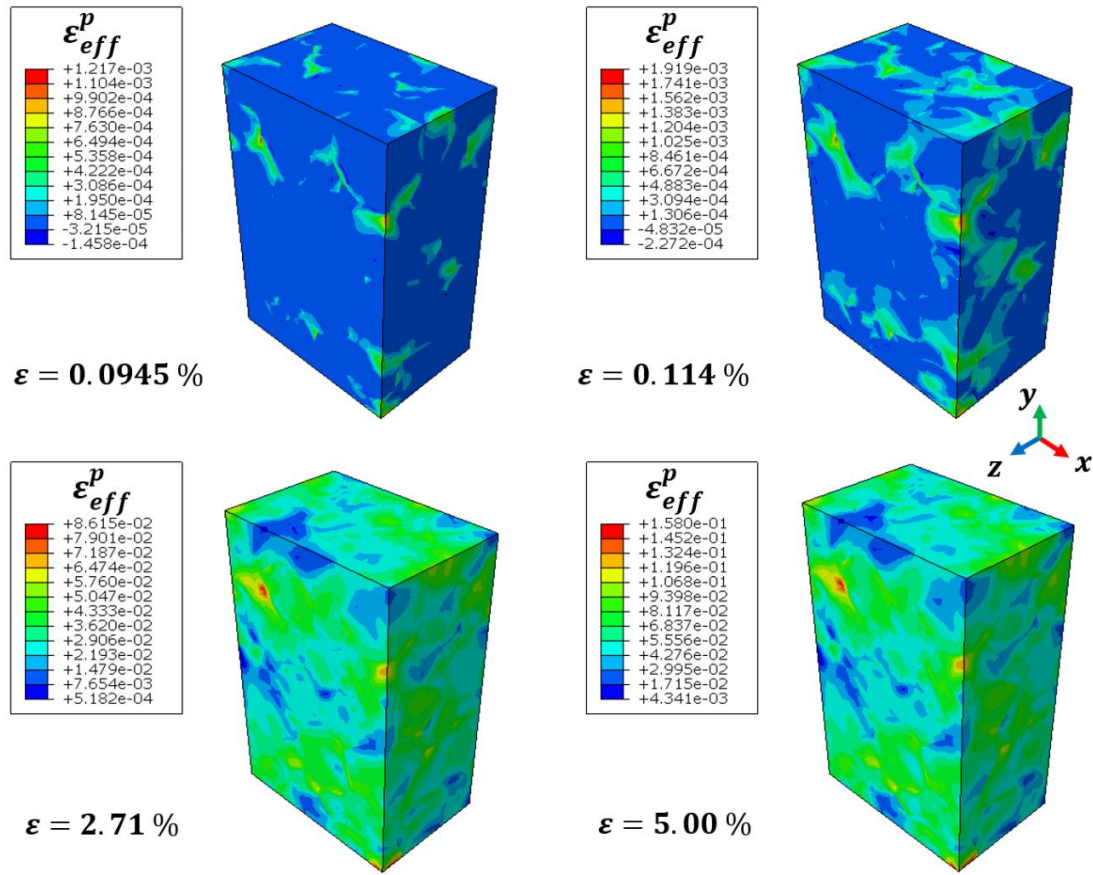


Figure 23. Contour plot of the evolution of effective plastic strain, ϵ_{eff}^p , with total macroscopic strain.

3.4.3. Short-term creep of ex-service 316H

Predictions of short-term creep of EX 316H at 550°C through the tessellation geometry were compared to those via the cubic grain geometry (Figure 24) at the same three test conditions (constant stresses of 250 MPa, 280 MPa and 320 MPa) using the same value (“Re-calibrated”, Figure 15) of W_c calculated in Section 3.3. The trend in stress dependence of the creep strain accumulation with time is captured by the CPFE model for both geometries. Note that the negligible difference in short-term monotonic loading in Figure 22 ($< 1\%$) between the two polycrystalline geometries does not become pronounced during short-term creep. The calibrated response of both geometries agrees well with experimental data, but at larger strains some discrepancies are observed again between the SCM and CPFE predictions which stems from the finite lattice rotations, captured via the CPFE framework, which affects the axial creep rate of the crystals. We do not further explore the calibration of the tessellation geometry to experimental data, but emphasize that the agreement can be improved by increasing the value of W_c .

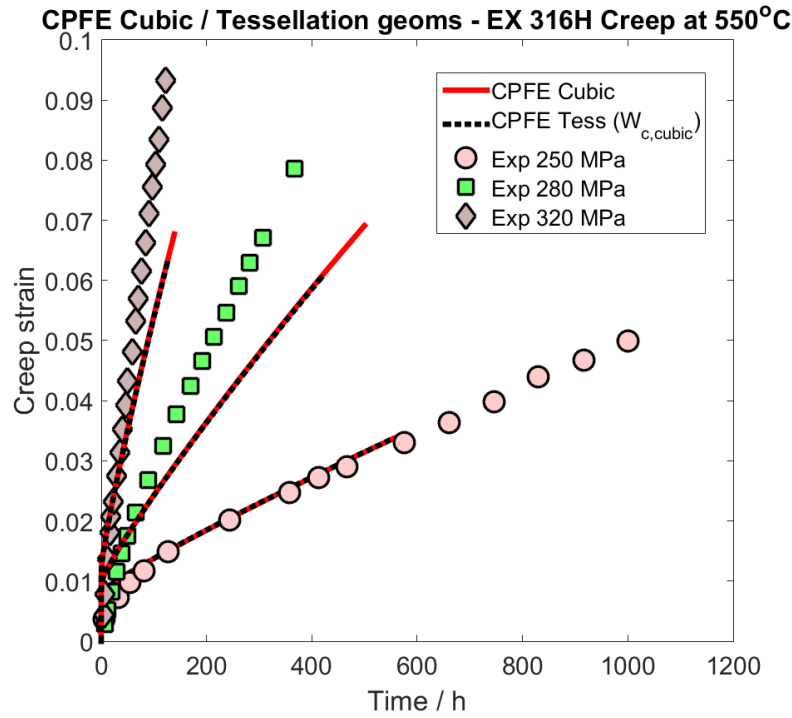


Figure 24. Creep response of EX 316H at 550°C at different stress levels – CPFE predictions through cubic grain and realistic tessellation geometries.

Although the employed micromechanical models in the CPFE framework are highly-nonlinear during creep, capturing the interactions between the glide activity of dislocations as well as thermal recovery and hardening of the microstructure, the present article demonstrates that sufficiently refined meshes with appropriately selected element types capture the macroscopic deformation response of the RVE, independent of the grain shapes used. The minor differences observed between the predicted macroscopic creep and monotonic elastic-plastic deformation responses via the cubic grain and tessellation geometries in the present study support the use of simplistic single crystal shapes, such as cubes, for modelling deformation of polycrystalline materials where the prime interest is the macroscopic response. Contour plots of the effective plastic strain and the accumulated forest dislocation junction obstacle density in the two geometries after creep into the primary and secondary stages at a constant stress of 250 MPa are shown and compared in Figure 25, which demonstrates minor differences supporting this argument.

However, the deformation of each individual grain will be affected by both its shape and neighbouring crystals which could affect the local distribution of stress, strain and obstacle density within the grain. Hence, the predictions via the two different polycrystalline realisations are examined further via

statistical analyses of the stress fields and the microstructural state development locally. The resulting variations of stress along the loading direction, the von Mises effective stress and dislocation obstacle density predicted from the SCM and CPFE at 250 MPa are illustrated in Figures 26 and 27, demonstrating the differences between the average obstacle densities predicted for the cubic-shaped grain and tessellation geometries, as compared to the SCM results, with means of 33% (cubic grains) and 33.9% (tessellation) for the polycrystalline array. Furthermore, the statistical variation of dislocation junction obstacle density in Figure 26 indicates minor differences across the two grain realisations, supporting the findings in Figure 25. The polycrystalline averages of axial stress for each grain between the tessellation geometry and SCM modelling results again show a low mean difference of 4.7%, which is of the order of the result obtained for the cubic grain geometry. However, a larger variation in axial stress is predicted for the tessellation geometry with $\overline{SD(\sigma_{yy})}^* = 0.538$ which is as a result of the higher geometrical constraint in the realistic geometry. The variation of the hydrostatic stress across the two geometries after creep at 250 MPa is compared in Figure 28. Larger variation of the hydrostatic stress is found for the tessellation geometry with $\overline{SD(\sigma_H)}^* = 1.63$, which is linked to the larger variation of axial stress for the same realisation and is consistent with findings from Section 3.3. A major origin of the discrepancy is the effect of grain shape. The results suggest that there is more local constraint on the deformation of the individual grains arising from the more irregular structure, leading to larger variations in the axial stress. This observation further supports the hypothesis behind the increased variation of stress within the grains during creep as a result of the stress redistribution process. It is worth noting that the values of $\overline{SD(\sigma_e)}^*$ and $\overline{SD(N_d)}^*$ for the tessellation geometry are similar to those obtained for the cubic grain geometry, taking values of 0.1167 and 0.0648, respectively. Although both polycrystalline aggregates are RVEs of the material, which is confirmed by their predicted macroscopic response, local stress or material state may evolve differently. Based on the findings in the present article, it is suggested that the local effects are less likely to affect the global deformation response, but could have more significant effects in damage development (e.g. the nucleation and growth of cavities and cracks) where the detailed distribution of the axial and hydrostatic stresses can play a significant role. The significance of using realistic grain geometries with regard to local evolution of the material's state is further discussed in Section 4. The importance of local stress fields in the development of dislocation obstacle density during creep conditions has also been acknowledged in Section 3.3.

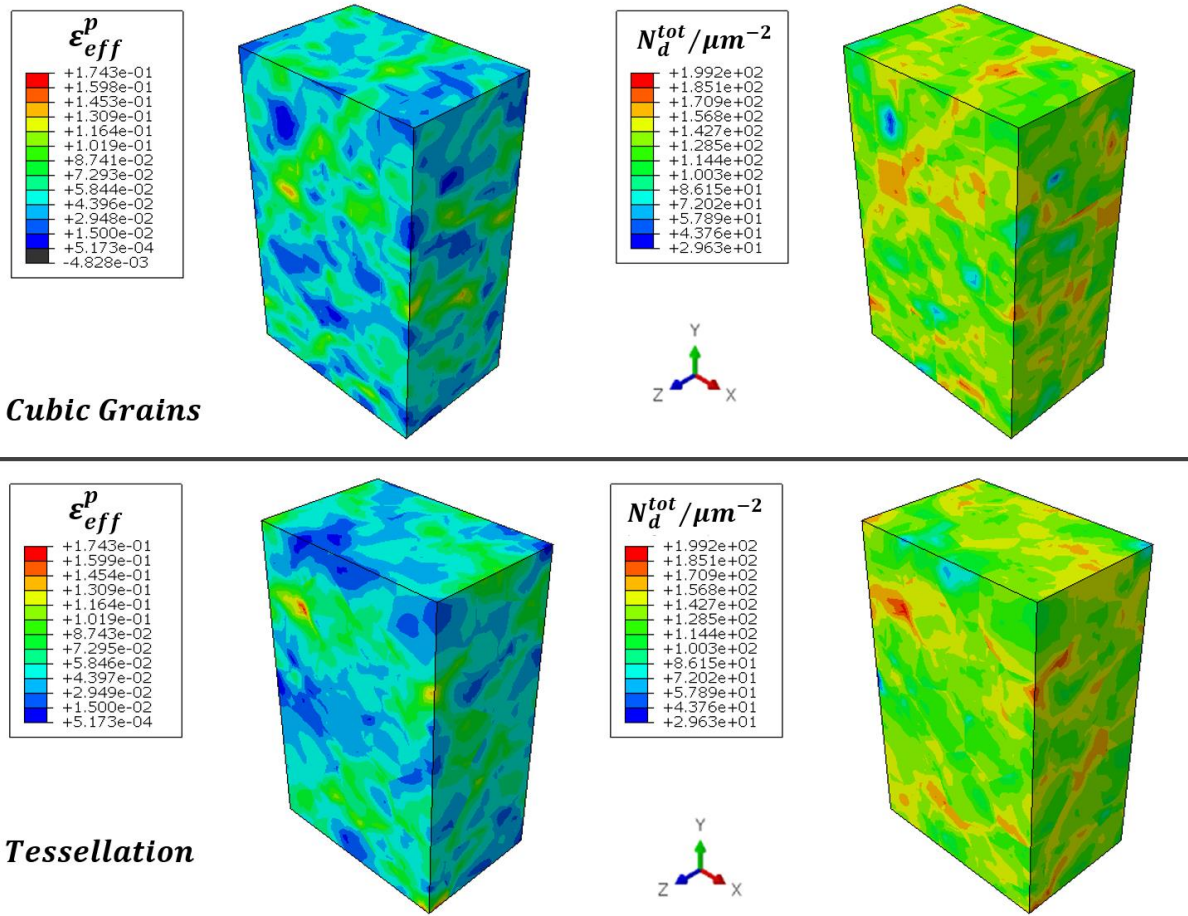


Figure 25. Contour plots of accumulated effective plastic strain and dislocation junction obstacle density in $1/\mu\text{m}^2$, N_d^{tot} , and after creep at 550°C and 250 MPa, 555 h. Top: Cubic grain geometry. Bottom: Tessellation geometry. Peaks in accumulated forest junction density appear similar in both geometries.

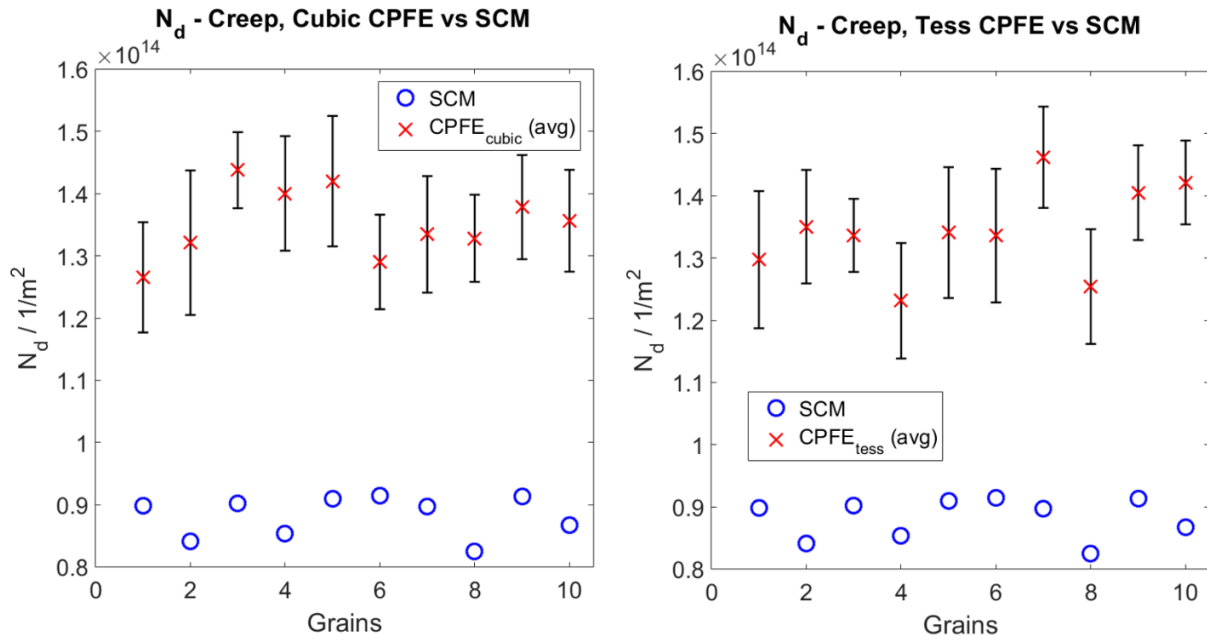


Figure 26. The average values and variation within 10 selected grains, represented via the standard deviation of quantities within a given grain, of $N_{d,tot}$ within the CPFE model for $W_c = 19$ with cubic grains (left) and realistic grains (right), compared to the SCM results after creep for 555 hours at 250 MPa, showing the overall comparable dislocation obstacle density between the two geometries.

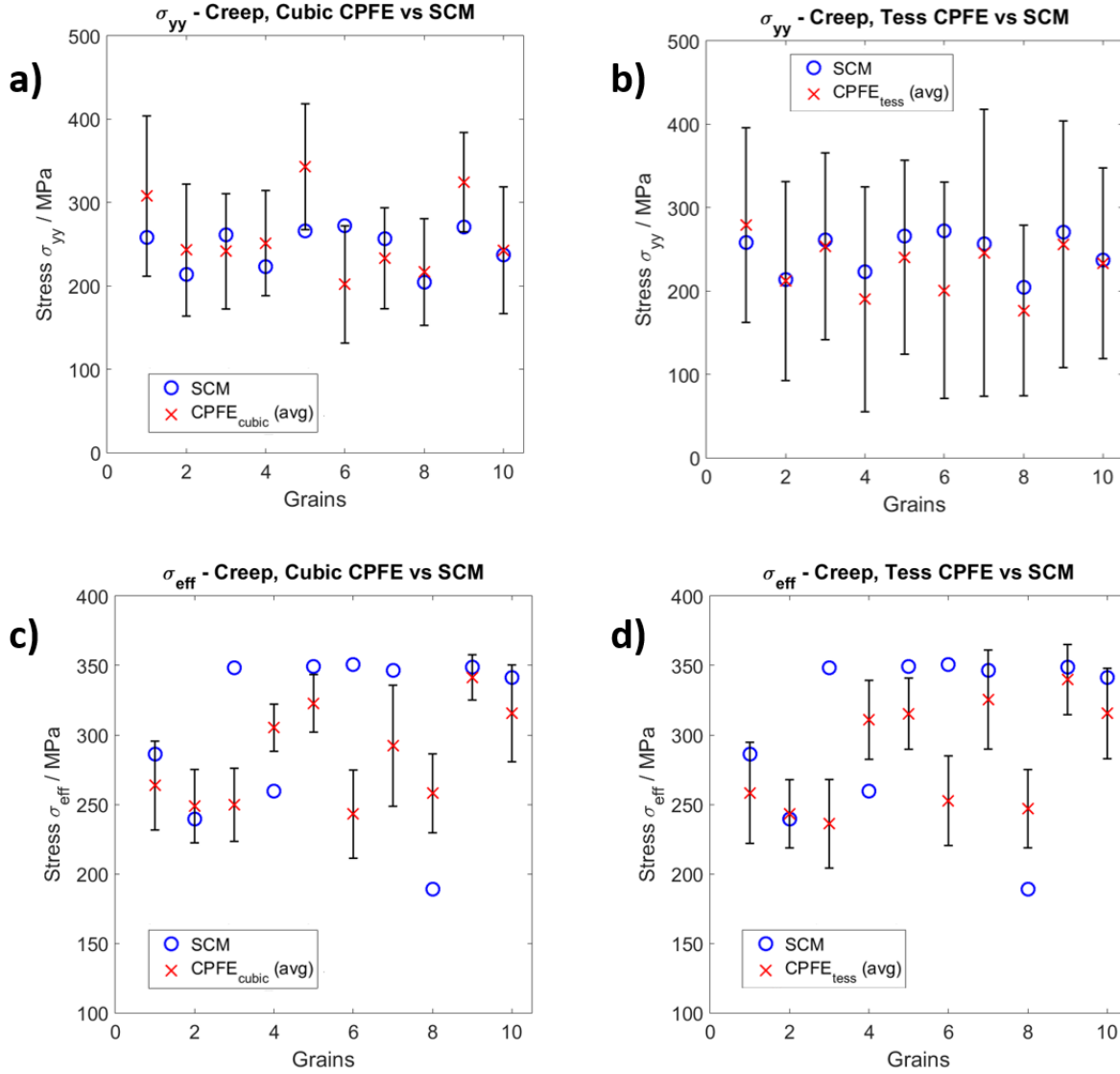


Figure 27. The average values and variation within 10 selected grains, represented via the standard deviation of quantities within a given grain, of σ_{yy} within the CPFE model for $W_c = 19$ with cubic grains (a) and realistic grains (b), compared to the SCM results after creep for 555 hours at 250 MPa. The averaged grain stresses between the aggregates show little difference, but more significant variation of axial stress is found in the tessellation geometry. The variation of σ_{eff} within the CPFE model with cubic (c) and realistic grains (d) is also shown.

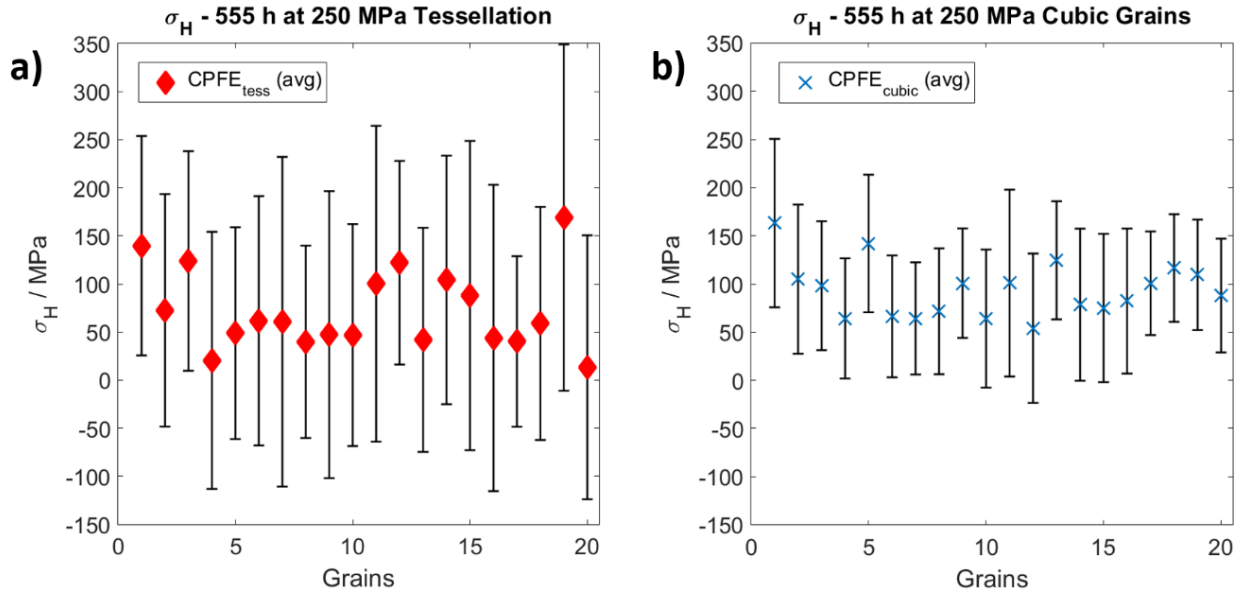


Figure 28. The average values and variation within 20 selected grains predicted via the CPFE model, represented via the standard deviation of quantities within a given grain, of the hydrostatic stress σ_H is shown after 555 hours of creep at 250 MPa for the a) tessellation geometry and b) cubic grain geometry. The averages of the hydrostatic stress for the two geometries are not greatly affected, however, the variation of σ_H within grains is greater in a) because of the increase in the variation in axial stress in the tessellation geometry (see Fig. 27) as a result of the stress redistribution process and the arrangement of stress concentration features, e.g. triple grain junctions.

4. DISCUSSION

4.1 COMPARING CRYSTAL PLASTICITY APPROACHES

In this paper, we have examined the predictive capabilities as well as the advantages and disadvantages of different crystal plasticity approaches for modelling the deformation of polycrystalline aggregates, with an emphasis on the behaviour of ex-service 316H stainless steel. The same physically-based micromechanical model describing the interaction between gliding dislocations and obstacles to their motion at the slip system level, as well as the evolution of material internal state, have been adopted in each model. The degree of model complexity, computational cost and also diversity of results increases from the SCM to CPFE models. The different level of internal constraint between the different models, and even between the different idealisations employed in the CPFE models, gives rise to differences in the predicted response for a given set of material parameters. Ultimately, the objective is to provide an

adequate description of the material response, which is calibrated and validated against material data. A consequence of this is that the models together with the adopted idealisation need to be calibrated independently against a given set of experimental data, although we would not expect a significant variation in the values of these parameters from one approach to another. Parameters determined by fitting the time-independent elastic-plastic response using the SCM, however, also lead to a good description of the material behaviour when employed within the CPFE framework. There is a much greater sensitivity of the response to the precise value of W_c employed within the creep recovery model of Eq. (5), even within different polycrystal idealisations employed using the CPFE approach. Determining how this parameter should be changed when moving between idealisations should be the focus when transitioning from one modelling framework to another. For the simulations presented here W_c needs to be reduced by a factor of 4 from the value employed in the SCM simulations to provide a good fit to the creep data from the CPFE model. The general rule here appears to be the greater the constraint the larger the value of W_c that should be employed.

Each framework is able to capture the trends in deformation behaviour and the redistribution of stress and changes in the material state. They have demonstrated the importance of the evolution of residual stress fields, resulting from grain-to-grain interactions, in predicting the macroscopic deformation response of polycrystalline materials, particularly when the stress state is changed. Examples include the Bauschinger effect (Section 3.2) and the changes in stress state between pre-loading and the primary creep regime in a stress-hold dwell loading history (Section 3.3 and 3.4.3). Other examples include the effects of cyclic loading on long-term stress relaxation under creep conditions, as shown by Petkov et al. [4], which confirm the observations from the present study.

Compared with the SCM, CPFE provides richer features but is at the expense of computational cost (e.g. 1 loading cycle for studies on the Bauschinger effect ~ 24 hrs on a dual processor workstation). However, the discrepancy in the predictions of monotonic short-term plasticity and creep responses between the frameworks and between different geometries used in CPFE highlights the significance of capturing the localization in the deformation behaviour, which can be captured by the sophisticated CPFE method but not by the averaging SCM scheme. The localization consists of two aspects, both of which could affect the global response. Firstly, the local stress concentrations near grain boundaries, particularly at triple grain junctions, can result in accumulation of higher dislocation obstacle density locally, which can affect the static recovery process and localized evolution of residual stress fields. The effect on the global response include the smoother transition in the room temperature tensile reloading curve during the simulation of the Bauschinger effect (Section 3.2), which agrees better with

the experimental data, with the agreement further improved through the adoption of more realistic grain topologies in the CPFE models. Secondly, as the CPFE theory is not limited to small strains, the localized deformation may result in lattice rotations and re-orientation of slip systems in the grains with respect to a reference co-ordinate system. Such lattice rotation may lead to the evolution of texture, particularly when the accumulated strain is large. Therefore, the long-term creep response of the material examined in the present study is more likely to be influenced by the effect of lattice rotation than the short-term elastic-plastic response, where macroscopic strains were of the order 5%. Another loading history in which the deformation response will be significantly affected by the evolution of texture is cyclic stress-controlled loading, or ratcheting, where large strains can accumulate macroscopically [80].

The average and standard deviation of the axial stress, effective stress and dislocation obstacle density within the CPFE multi-grain models are analysed as part of this study. The statistical analyses revealed that small variations in the effective stress and the dislocation obstacle density can influence the deformation rate of the material during creep, with both stress and material state evolving towards a more uniform state. An important finding is the larger variation of hydrostatic stress within grains after creep at a given stress as compared to the variation of the hydrostatic stress after short-term monotonic load-up to the same stress level, due to the relative increase in variation of the axial stress within the material. Although the cubic grain and tessellation geometries yield comparable macroscopic monotonic and creep deformation responses, the statistical analyses of local quantities also revealed significant differences in the variation of local axial and hydrostatic stress fields between the two polycrystalline realisations, with the variation of those quantities within grains being more significant in the tessellation geometry. In addition, it was found that the standard deviation of the effective stress within the CPFE multi-grain framework is lower than values found in the literature (see Section 3.1) which supports the use of the first-order SCM approach (instead of a second-order approach) employed here.

Important consideration should be made concerning the choice of the element type employed in tessellated geometries for which tetrahedral elements are generally used to capture intrinsic grain shapes accurately. The present study suggests that the quadratic C3D10 elements should be used, the disadvantage of which is longer computational times, compared to linear C3D4 tetrahedral elements, since the latter element type usually results in an overly-stiff response due to volumetric locking effects. Although not shown in this article, the authors indeed observed a stiffer response predicted by a converged linear tetrahedral mesh (C3D4) as compared to an equivalent converged quadratic (C3D10)

tetrahedral mesh for the same tessellated geometry; e.g. the difference in predicted macroscopic response via the two meshes was of the order of 20%. Moreover, the authors found that usage of the hybrid formulation of the linear tetrahedral element (C3D4H) in a converged mesh yields identical results to the converged mesh employing quadratic C3D10 elements; the results are not shown here for brevity.

The observations made in this study suggest that from a practical point of view with regard to prediction of macroscopic deformation behaviour under complex loading histories (e.g. HT tension-compression pre-loading with RT re-loading in this study, cyclic loading with relaxation dwells in [4]) the SCM captures the major physical processes. It is also more computationally efficient and can be used to evaluate the evolution of material response over a large number of different types of thermo-mechanical loading histories. Current procedures for assessing the performance of high temperature power generating plant are based on models for the global inelastic response. Design codes place global and local limits on accumulated inelastic strain of the order of 1% and 5%, respectively. The SCM is an ideal candidate for use alongside existing procedures to provide physically based approaches for the determination of the macroscopic response for loading histories for which experimental data is not available. Modelling results obtained using the SCM provide a sufficient level of detail for both the global response and the development of internal residual stress fields to provide meaningful information for use in current assessment procedures. However, when a more detailed understanding of the materials behaviour is required, such as in situations where a more in-depth understanding of damage development leading to failure is required, the CPFE approach offers significant advantages, as described in the following section.

4.2 CONSIDERATIONS ON LOCAL FIELDS AND DAMAGE MODELLING

The processes of stress redistribution, strain localization within confined regions and their effects on the global response as captured by the CPFE models employed in this study provide important insight into the development of high local stresses and how they might lead to the initiation and growth of damage. Since damage development in localised regions of a material is an important pre-cursor to failure [81,82], the CPFE approach is the most appropriate framework out of those examined in this article to study the evolution of creep damage, despite its computational complexity.

The SCM models described here provide information about the grain-average behaviour. It is ideally suited to validation using the neutron diffraction (ND) technique [83], which also provides the average stress state following deformation averaged over different grain families with the same crystallographic

orientation with respect to the global loading axes, see e.g. Hu et al. [2,84]. These techniques can also be used to provide an initial validation of CPFE models, but predictions of local strain and stress fields require other advanced measuring techniques, such as digital image correlation (DIC) [85], to fully validate the more detailed stress and strain fields predicted by the CPFE models.

5. CONCLUSIONS

The major conclusions from this study are:

- 1) Mechanistic deformation models are applied at the slip system level within different crystal plasticity frameworks, allowing the effects of microscopic physical deformation processes related to the evolution of the dislocation network and any obstacles associated with dislocation motion, on the global response to be assessed. The present study validates the previously developed mechanistic model developed by the authors, as applied to austenitic 316H stainless steel, in terms of parameter magnitudes and predictions based on comparison of previous results to full-field solution predictions via CPFE framework considering lattice rotations, texture evolution and realistic grain shapes.
- 2) Comparison of the SCM approach with detailed CPFE simulations, serves to further validate the SCM procedures developed by Hu et al. [2,14], while at the same time highlighting the limitations of the approach. The main limitation of the employed SCM is the inability to capture the stress variation throughout the grains which can affect the macroscopic response predicted, agreeing with observations made in [26].
- 3) The variation of stress within the grains obtained from the CPFE simulations is less than that reported for other models in the literature (see e.g. [34]). This supports the use of a first order SCM scheme for the current crystal plasticity constitutive model, as opposed to the adoption of a higher order approach.
- 4) Care should be taken in cases where averaging modelling schemes, such as the SCM, are used in applications where the hydrostatic effects are of importance, e.g. damage development under multiaxial loading, since the SCM framework possesses a limited capability to capture fully large variations in hydrostatic stresses locally.
- 5) The SCM approach is, however, ideally suited to calibration using neutron diffraction studies. It is also efficient computationally and can be used to simulate industrially relevant thermo-

mechanical loading histories and provide information that is directly relevant to current design and assessment procedures employed in the power generating industry.

- 6) The nature of the CPFE framework used here, however, may result in changes to the physical parameters already established via averaging computational schemes, such as the first-order homogenization SCM. Localised processes and variation in grain geometries, which affect the local constraint and stress fields in the polycrystalline aggregate, are significant and drive these changes. Employing realistic grain shapes, compared to models using cubic-like grains, results in a greater variation of axial and hydrostatic stresses within the grains, suggesting that geometries of realistic grain-shapes should be used where local effects become important, e.g. damage development. Minor variations in the predicted global response are found between the first-order self-consistent homogenization scheme and the CPFE model of time-independent monotonic deformation, when the same parameters are used across the two approaches. Significant differences in predictions of the macroscopic response are found between the two modelling approaches for time-dependent creep deformation, stemming from the greater sensitivity of the static recovery model on the local stress and strain fields, which drive a reduction of the controlling parameter for static recovery by a factor of 4 within the full-field solution.

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APPENDIX A. 3D CRYSTAL PLASTICITY FINITE ELEMENT FRAMEWORK

In this section we describe the implementation of the physical crystal plasticity model described in the last section within a three-dimensional finite strain finite element formalism. The CPFE model has been implemented as a user material subroutine (UMAT) within the commercial FE software ABAQUS. Its numerical implementation is detailed in this section. Implementation of the same model as employed in the SCM allows direct comparison of the predictions from the two approaches. The framework of the developed UMAT and the approach employed for implementation of the plasticity model follow closely those originally developed by Dunne et al. [8].

Within a crystal plasticity framework, the plastic part of the velocity gradient for an FCC material can be expressed as

$$\mathbf{L}^p = \sum_{\alpha} \dot{\gamma}^{(\alpha)} (\bar{\mathbf{s}}^{(\alpha)} \otimes \bar{\mathbf{n}}^{(\alpha)}) \quad (\text{A.1})$$

where $\dot{\gamma}^{(\alpha)}$ is the shear strain-rate for the α slip system given by either Eqn. (8) or (9), and the summation is over all active slip systems. The slip direction $\bar{\mathbf{s}}^{(\alpha)}$ and normal direction to the slip plane $\bar{\mathbf{n}}^{(\alpha)}$ are rotated incrementally by the elastic component of the continuum spin tensor. Within a UMAT routine the deformation gradients at the beginning and end of the time increment, $\mathbf{F}_t$ and $\mathbf{F}_{t+\Delta t}$ are provided as inputs; the purpose of the UMAT itself is to find the true stress at the end of the increment, provide the material Jacobian ($\partial \Delta \sigma / \partial \Delta \epsilon$) and update all state variables of interest. An implicit scheme, using an elastic predictor and plastic corrector terms similar to the one used by Dunne et al. [8], has been developed to achieve convergence of stress for a given set of deformation gradients through a Newton-Raphson scheme. By expressing the stress at the end of increment as $\sigma_{t+\Delta t}$ through the elastic predictor stress, $\sigma_{trial} = \sigma_t + \mathbf{C}^{rot} \Delta \epsilon$, and increment in plastic strain $\Delta \epsilon^p$, one obtains

$$\sigma_{t+\Delta t} = \mathbf{C}^{rot}(\epsilon_t^e + \Delta \epsilon^e) = \sigma_{trial} - \mathbf{C}^{rot} \Delta \epsilon^p \quad (\text{A.2})$$

The matrix $\mathbf{C}^{rot}$ is the anisotropic stiffness matrix of a crystal with respect to global coordinates obtained by rotating the local stiffness matrix defined in the crystal lattice coordinates, $\mathbf{C}$, using the transformation matrix, $\mathbf{T}_k$:

$$\mathbf{C}^{rot} = \mathbf{T}_k \mathbf{C} \mathbf{T}_k^T \quad (\text{A.3})$$

In Voigt notation, $\mathbf{T}_k$ is the matrix, which rotates the stress vector from the local lattice, coordinates to the global specimen reference frame according to

$$\mathbf{T}_k = \begin{bmatrix} R_{11}^2 & R_{12}^2 & R_{13}^2 & 2R_{11}R_{12} & 2R_{11}R_{13} & 2R_{12}R_{13} \\ R_{21}^2 & R_{22}^2 & R_{23}^2 & 2R_{21}R_{22} & 2R_{21}R_{23} & 2R_{22}R_{23} \\ R_{31}^2 & R_{32}^2 & R_{33}^2 & 2R_{31}R_{32} & 2R_{31}R_{33} & 2R_{32}R_{33} \\ R_{11}R_{21} & R_{12}R_{22} & R_{13}R_{23} & R_{11}R_{22} + R_{21}R_{12} & R_{11}R_{23} + R_{21}R_{13} & R_{12}R_{23} + R_{22}R_{13} \\ R_{11}R_{31} & R_{12}R_{32} & R_{13}R_{33} & R_{11}R_{32} + R_{12}R_{31} & R_{11}R_{33} + R_{13}R_{31} & R_{12}R_{33} + R_{13}R_{32} \\ R_{21}R_{31} & R_{22}R_{32} & R_{23}R_{33} & R_{21}R_{32} + R_{22}R_{31} & R_{21}R_{33} + R_{23}R_{31} & R_{23}R_{32} + R_{22}R_{33} \end{bmatrix} \quad (\text{A.4})$$

The matrix $\mathbf{R}$ is the rotation matrix transforming a vector from lattice coordinates into global coordinates. This is the inverse of the $\mathbf{G}_{ori}$ matrix ($\mathbf{G}_{ori}^{-1} = \mathbf{R}$) defined according to the three Euler orientation angles - ϕ_1 , Φ and ϕ_2 - of each single crystal after Randle and Engler [86] as

$$\mathbf{G}_{ori} = \begin{bmatrix} \cos \phi_2 & \sin \phi_2 & 0 \\ -\sin \phi_2 & \cos \phi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{bmatrix} \begin{bmatrix} \cos \phi_1 & \sin \phi_1 & 0 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (\text{A.5})$$

The total strain increment can be expressed in terms of the velocity gradient as

$$\Delta \varepsilon = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T)\Delta t \quad (\text{A.6})$$

where $\mathbf{L}$ is expressed in terms of the total deformation gradient and its rate as

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} \quad (\text{A.7})$$

The resolved shear stress on each slip system can be expressed as

$$\tau^{(\alpha)} = [\text{sym}(\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)})] : \sigma_t \quad (\text{A.8})$$

where $:$ denotes the outer product. Following Eq. A.6, the plastic strain increment is expressed by the plastic velocity gradient as

$$\Delta \varepsilon^{pl} = \frac{1}{2}(\mathbf{L}^p + \mathbf{L}^{pT})\Delta t = \text{sym}(\mathbf{L}^p)\Delta t \quad (\text{A.9})$$

In order to determine the stress at the end of the increment, Eq. A.2 is rearranged in terms of a residual stress term, Ψ , leading to

$$\Psi = \sigma_{t+\Delta t} - \sigma_{trial} + \mathbf{C}^{rot}\Delta \varepsilon^p \quad (\text{A.10})$$

which in differential form becomes

$$\delta \Psi = \delta \sigma_{t+\Delta t} - \delta \sigma_{trial} + \mathbf{C}^{rot}\delta \Delta \varepsilon^p \quad (\text{A.11})$$

Depending on the constitutive flow rule used in Eq. A.1, $\delta \Delta \varepsilon^p$ will have different forms. In this study, two distinct flow rules – a) simple power-law (Eq. 9) for room temperature plasticity and b) thermally-activated glide (Eq. 8) at high temperature – are employed. The forms of $\delta \Delta \varepsilon^p$ for the two rules are obtained from Eq. A.1 and Eq. A.9 as

$$\delta \Delta \varepsilon^p = \text{sym} \left[\sum_{\alpha} \frac{\dot{\gamma}_0}{(\tau_{cr}^{\alpha})^p} p(\tau^{\alpha} + (\bar{\tau}_m^r))^{p-1} \Delta t (\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)}) \delta \tau^{\alpha} \right] \quad (\text{A.12a})$$

$$\delta \Delta \varepsilon^p = \text{sym} \left[\sum_{\alpha} Z \Delta t (\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)}) \delta \tau^{\alpha} \right] \quad (\text{A.12b})$$

where

$$Z = \dot{\gamma}_0 \exp \left(-\frac{\Delta F_0}{kT} \left(1 - \left(\frac{\tau^{\alpha} + (\bar{\tau}_m^r)}{(1 + F_{sol})\tau_{cr}^{\alpha}} \right)^p \right)^q \right) \left(-q \frac{\Delta F_0}{kT} \left(1 - \left(\frac{\tau^{\alpha} + (\bar{\tau}_m^r)}{(1 + F_{sol})\tau_{cr}^{\alpha}} \right)^p \right)^{q-1} \right) \left(-p \left(\frac{\tau^{\alpha} + (\bar{\tau}_m^r)}{(1 + F_{sol})\tau_{cr}^{\alpha}} \right)^{p-1} \right) \frac{1}{\tau_{cr}^{\alpha}} \quad (\text{A.13})$$

It is important to note that the differentials in Eqs. A.12 and A.13 are positive. Note that F_{sol} is assumed to be zero for the current study. For simplicity we assume that $\delta\tau^{(\alpha)} = [sym(\bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)})] : \delta\sigma_{t+\Delta t}$ and the above differentiated expressions are substituted by $\mathbf{P}$ [8], leading to

$$\delta\Delta\varepsilon^p = \mathbf{P}\delta\sigma_{t+\Delta t} \quad (A.14)$$

where

$$\mathbf{P} = \sum_{\alpha} \frac{\dot{\gamma}_0}{(\tau_{cr}^{(\alpha)})^p} p(\tau^{(\alpha)} + (\bar{\tau}_m^r))^{p-1} \Delta t \mathbf{A}^{\alpha} \otimes \mathbf{A}^{\alpha} \quad (A.15)$$

$$\mathbf{P} = \sum_{\alpha} Z \Delta t \mathbf{A}^{\alpha} \otimes \mathbf{A}^{\alpha} \quad (A.16)$$

with $\mathbf{A}$ written as a [6x1] vector with components defined by

$$\mathbf{A}^{\alpha} = \bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)} \quad (A.17)$$

Substitution of Eq. A.14 into Eq. A.11 yields

$$\delta\boldsymbol{\Psi} = \delta\sigma_{t+\Delta t} - \delta\sigma_{trial} + \mathbf{C}^{rot}\mathbf{P}\delta\sigma_t \quad (A.18)$$

Through a Taylor series expansion, as suggested in [8], and setting the target for the residual stress to $\boldsymbol{\Psi} \rightarrow 0$, one obtains

$$\boldsymbol{\Psi} + \frac{\partial\boldsymbol{\Psi}}{\partial\delta\sigma_{t+\Delta t}}\delta\sigma_{t+\Delta t} = \sigma_{t+\Delta t} - \sigma_{trial} + \mathbf{C}^{rot}\Delta\varepsilon^p + (\mathbf{I} + \mathbf{C}^{rot}\mathbf{P})\delta\sigma_{t+\Delta t} = 0 \quad (A.19)$$

where $\mathbf{I}$ is the identity matrix. Expressions for the increment in stress are obtained from Eq. A.2, which are used iteratively within a Newton-Raphson scheme until the residual stress decreases to a specified tolerance ($\boldsymbol{\Psi} < 1 \times 10^{-10}$ MPa)

$$-(\mathbf{I} + \mathbf{C}^{rot}\mathbf{P})^{-1}[\sigma_{t+\Delta t} - \sigma_{trial} + \mathbf{C}^{rot}\Delta\varepsilon^p] = \delta\sigma_{t+\Delta t} \quad (A.20)$$

Depending on the flow rule used (see Eqs. A.12) their forms are

$$\delta\sigma_{t+\Delta t} = (\mathbf{I} + \mathbf{C}^{rot}\mathbf{P})^{-1} \left[\sigma_{trial} - \sigma_{t+\Delta t} - \mathbf{C}^{rot} sym \left(\sum_{\alpha} \dot{\gamma}_0 \left| \frac{\tau^{(\alpha)} + (\bar{\tau}_m^r)}{\tau_{cr}^{(\alpha)}} \right|^p sgn(\tau^{(\alpha)}) \Delta t \bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)} \right) \right] \quad (A.21)$$

$$\begin{aligned} \delta\sigma_{t+\Delta t} = (\mathbf{I} + \mathbf{C}^{rot}\mathbf{P})^{-1} & \left[\sigma_{trial} - \sigma_{t+\Delta t} \right. \\ & - \mathbf{C}^{rot} \text{sym} \left(\sum_{\alpha} \dot{\gamma}_0 \exp \left(-\frac{\Delta F_0}{kT} \left(1 \right. \right. \right. \\ & \left. \left. \left. - \left| \frac{\tau^{(\alpha)} + (\bar{\tau}_m^r)}{(1 + F_{sol})\tau_{cr}^{(\alpha)}} \right|^p \right)^q \right) \text{sgn}(\tau^{(\alpha)}) \Delta t \bar{s}^{(\alpha)} \otimes \bar{n}^{(\alpha)} \right) \left. \right] \end{aligned} \quad (\text{A.22})$$

Lastly, the Jacobian stiffness matrix $\mathbf{J}$ is calculated following the procedure in [8]; for $\boldsymbol{\Psi} \approx 0$ and $\delta\sigma_{trial} = \mathbf{C}^{rot}\delta\epsilon$, one obtains

$$\mathbf{J} = \frac{\partial\sigma}{\partial\epsilon} = (\mathbf{I} + \mathbf{C}^{rot}\mathbf{P})^{-1}\mathbf{C}^{rot} \quad (\text{A.23})$$

All state variables are updated after the stress and plastic strain at the end of increment are obtained. The predictive capabilities of this 3D CPFE framework will be assessed in the following section for high temperature deformation of ex-service 316H stainless steel and compared with SCM predictions.

APPENDIX B. MESH CONVERGENCE OF TESSELLATION GEOMETRY

The mesh convergence of the tessellation geometries was carried out following a macroscopic response criterion under which convergence was assumed when the difference between the macroscopic creep strain predicted at the end of the creep test was lower than 3% with further mesh refinement. In the case of the 216-grain geometry four meshes, comprising of 33797, 46473, 60081 and 96205 elements (C3D10), were examined. The predicted macroscopic creep curves used to establish mesh convergence are shown in Figure B.1, indicating the suitability of the mesh comprising of 60081 elements.

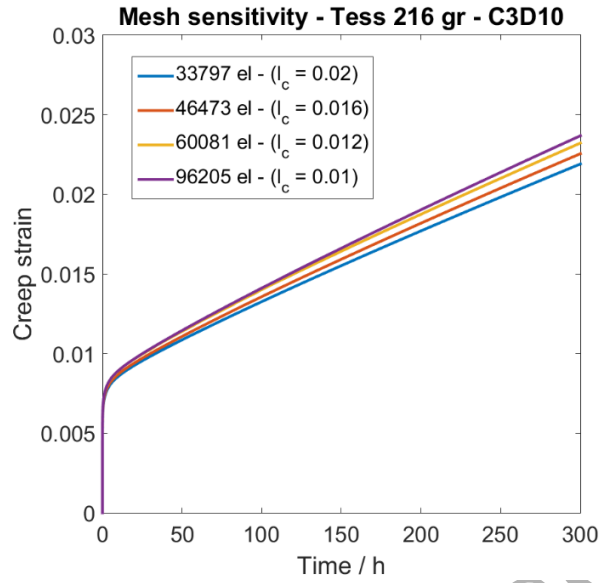


Figure B.1. Macroscopic creep curves at 250 MPa for different meshes of the 216-grain geometry.

The statistical variation of stress and obstacle density within selected grains for the different meshes, examined in Figure B.1, was also investigated to further support the mesh convergence studies. An example is shown in Figure B.2. for the dislocation obstacle density variation within a selected grain from which it is evident that the selected mesh of 60081 elements for the 216-grain geometry provides a sufficient level of detail.

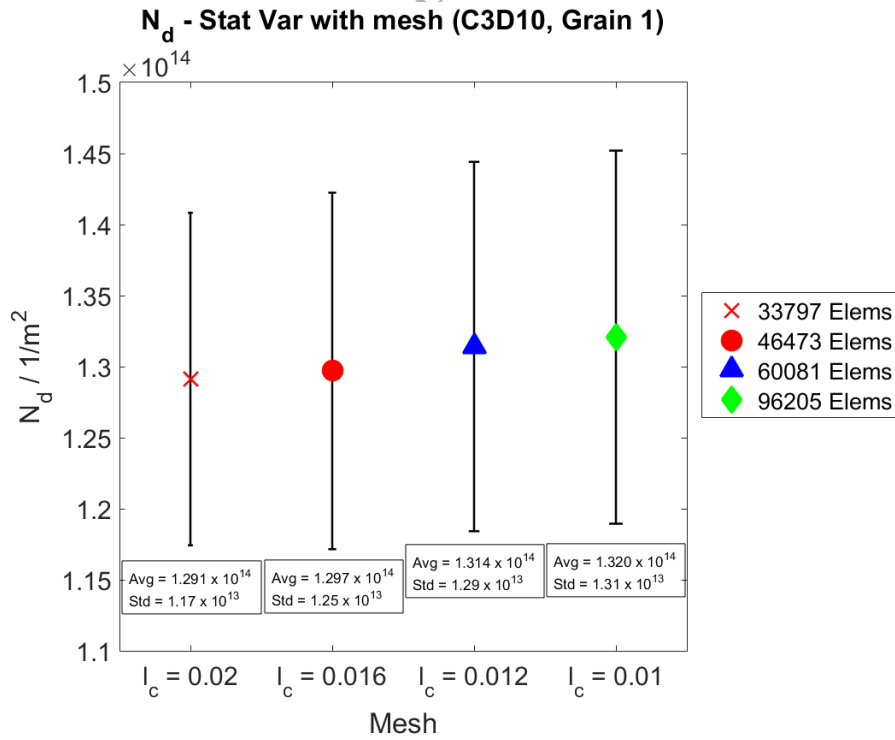


Figure B.2. Mesh convergence study – average dislocation obstacle density and variation within a selected grain with mesh refinement.

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