

A Multi-scale Approach to the Development of High-rate-based Microstructure-aware Constitutive Models for Magnesium Alloys



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This thesis is dedicated to
my father Robin Wason Marbaniang
who had always supported me in all my endeavours.
Rest in peace.

Abstract

Computational tools are at the forefront of modern day engineering as they offer low cost, timely, and informed approaches to product design, with finite element analysis packages being particularly favoured in industry for predicting the behaviour of physical systems. When high-rate structural components are designed using such approaches, it is typical to allocate constitutive models that reflect experimentally measured material behaviour to the parts being analysed. A common shortcoming of this approach, especially in industrial applications, is the phenomenological nature of the models, which can only make predictions of bulk-level mechanical behaviour, and do not offer insight into the mechanisms driving material behaviour.

Over the last few decades, numerous methodologies to enable the consideration of the lower length-scale phenomena driving the bulk-level mechanical behaviour of polycrystalline-based metals have been proposed, which can be categorised into two branches, mean-field and full-field. As the mechanisms driving plasticity in such materials are found interior to a grain, but the orientation of a collection of grains are found to dictate anisotropic bulk-level mechanical behaviour, crystal plasticity-considered approaches have become popular in literature. Mean-field crystal plasticity-based models provide insight into the relative activity of available micro- and meso-scale deformation mechanisms, as well as their effect on homogenised bulk-level behaviour. Whereas, full-field approaches enable consideration of the heterogeneity of the stress field manifesting in the polycrystalline structure, and thus the relative activity of the deformation mechanisms in individual grains.

Presented in this thesis is a hierarchical full-field-considered approach to the development of high-rate-based microstructure-aware constitutive models for magnesium alloys. At the heart of the full-field polycrystalline-based simulations is a rate-dependent explicitly-run crystal plasticity-based user-subroutine that describes plasticity through both dislocation glide and homogenised twinning mechanisms. The reason for incorporating the user-subroutine into an explicit framework being that they are better suited for high-rate-based analyses. Two magnesium alloys, WE43-T6 plate and AZ31B-O sheet, were selected as model materials to present the developed capabilities as accurate predictions of their high-rate behaviour are difficult to make owing to the low symmetry possessed by the material system's unit cell, and the presence of textures. It was shown through an example where armour plates are blast-loaded, that by fully resolving micro- and meso-structural features, the potential to delve into the phenomena underpinning high-rate bulk-level mechanical behaviour becomes possible, thus offering the ability to design them to improve a material system for its component's specific application.

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List of Abbreviations

2-D, 3-D	Two-, three-dimensional
CRSS	Critically resolved shear stress
CP	Crystal plasticity
CPFEM	Crystal plasticity finite element model
DEST	Discrete element simulation tool
DOF	Degree of freedom
EPSC	Elasto-plastic self-consistent
EBSD	Electron backscatter diffraction
FEA	Finite element analysis
FEM	Finite element model
FETI	Finite element tearing and interconnecting
FFT	Fast fourier transform
GND	Geometrically necessary dislocations
GUI	Graphical user-interface
HATI	Heterogeneous asynchronous time integrators
HCP	Hexagonal close packed
HEM	Homogeneous anisotropic effective medium
ISML	Impact and shock mechanics laboratory
MSE	Mean-square-error
ND	Normal direction
ODF	Orientation distribution function
PDF	Probability density function
RD	Rolling direction
RVE	Representative volume element
SSD	Statistically stored dislocations
TD	Transverse direction
VPSC	Visco-plastic self-consistent

1

Introduction

Computational tools are at the forefront of modern day engineering as they offer low cost, timely, and informed approaches to product design [1], with finite element analysis packages being particularly favoured in industry for predicting the behaviour of physical systems. Advances in computing are continually pushing the limits of what is possible, with headway in stochastic-based methods for assessing system performance [2, 3], data-driven approaches to system design [4, 5], and the development of sophisticated FEA modelling architectures [6, 7] being but a few. One route that offers significant potential is the utilisation of lower length-scale models to inform scales above. This is because a wealth of data becomes available that otherwise would not be predicted if the higher level-models were run with just models for that scale. For example, FEA models are commonly used in the design of structural components in industry. In these, constitutive models that reflect experimentally measured material behaviour are typically allocated to the parts being analysed (e.g. rubber parts are allocated hyper-elastic-based constitutive models, metal parts, plasticity-based constitutive models, etc). A shortcoming of this is that these constitutive models tend to be phenomenological, and as such, do not offer insight into the mechanisms driving material behaviour. However, through the use of physically-based lower

length-scale models, not only are these mechanisms identified, but the ability to design them to improve component performance through choice of processing route becomes realisable.

This thesis strove to develop and exploit such capabilities for magnesium alloy-made (polycrystalline-based metal) structural components destined for high-rate applications, with its format adopting that described in the following. Prior to a literature review or any formal description of theory, a high-level study typical of one conducted in industry was completed. Here, the suitability of replacing a hard steel plate with one magnesium alloy-based for blast shielding applications was explored (the reason being presented later) through use of a FEA model ran using commercially available software. The developments required to then subsequently enable the consideration of magnesium alloys treated to other conditions or comprising differing compositions were then discussed. This example then continued to serve as an overarching narrative to present how microstructure-aware constitutive models could be used to design magnesium alloy-based material systems to better them for their component's specific application, with the relevant literature reviews and descriptions of theory to develop such a capability being conducted on-the-fly where required. To note, the microstructure-aware aspect was achieved through the homogenisation of full-field mesoscale models, and as such the additional opportunities offered by these models were then discussed. After this, the thesis then steered its focus to expected future work and publications, and closed with concluding remarks.

Magnesium alloys were identified as the model material system of choice as they are among the lightest of the structural alloys making them attractive for use in the design of structures where mass is a key constraint (e.g. electric cars, next generation aircraft), and because recent advances have led to the development of various magnesium alloy compositions that possess a good combination of manufacturability, thermo-mechanical behaviour, and environmental in-service properties [10–12]. However, there are complexities associated with their use in high-rate scenarios that necessitates the consideration of their micro- and meso-structures. This becomes evident when the flow stresses with strain-rate and orientation for the rolled magnesium alloys with compositions WE43 (contains 3.7-4.3 wt% yttrium, 2.3-3.5 wt% rare earths, in this case neodymium, and 0.2 wt% [minimum] zirconium), and AZ31, (contains 3.0 wt% aluminium, 1.1 wt% zinc, and 0.49 wt% manganese) are compared (see Figures 1.1 and 1.2). The magnesium alloy WE43 underwent direct chill casting, homogenisation treatment, hot-rolling on a reversing mill, and then heat-treatment to a T6 condition [13]. Whereas, the

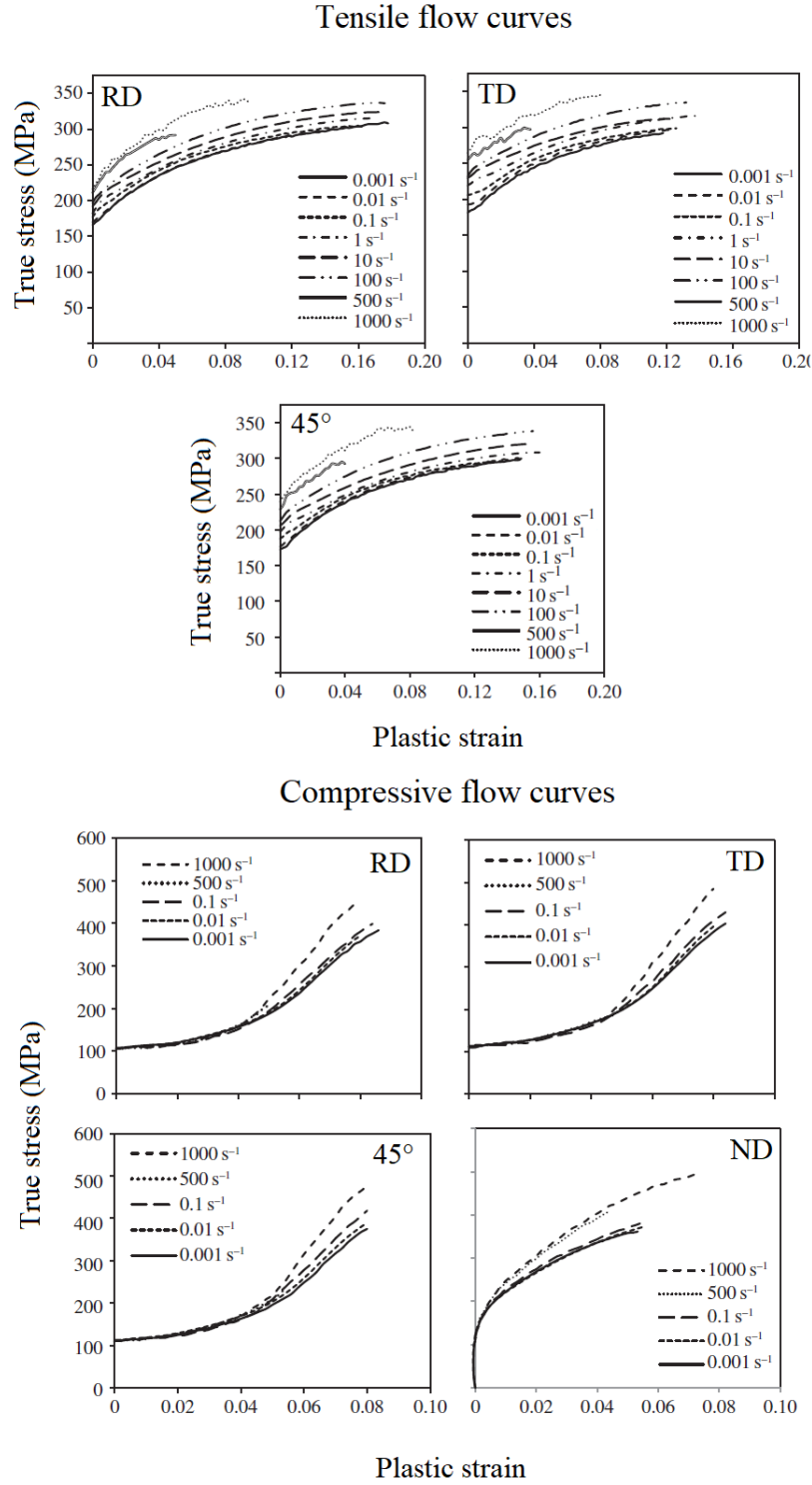


Figure 1.1: Effect of strain-rate and orientation on flow stresses of Mg alloy AZ31B-O sheet [8]. Rate-dependence was observed as an increase in true stress with rate for all loading configurations; minimal orientation dependency was noted for in-plane tensile loading; clear tension-compression asymmetry was exhibited with in-plane loading; and strong orientation dependence was noted between the compressed in-plane and out-of-plane directions (behaviour transitioned from a sigmoid shape to a logarithmic one).

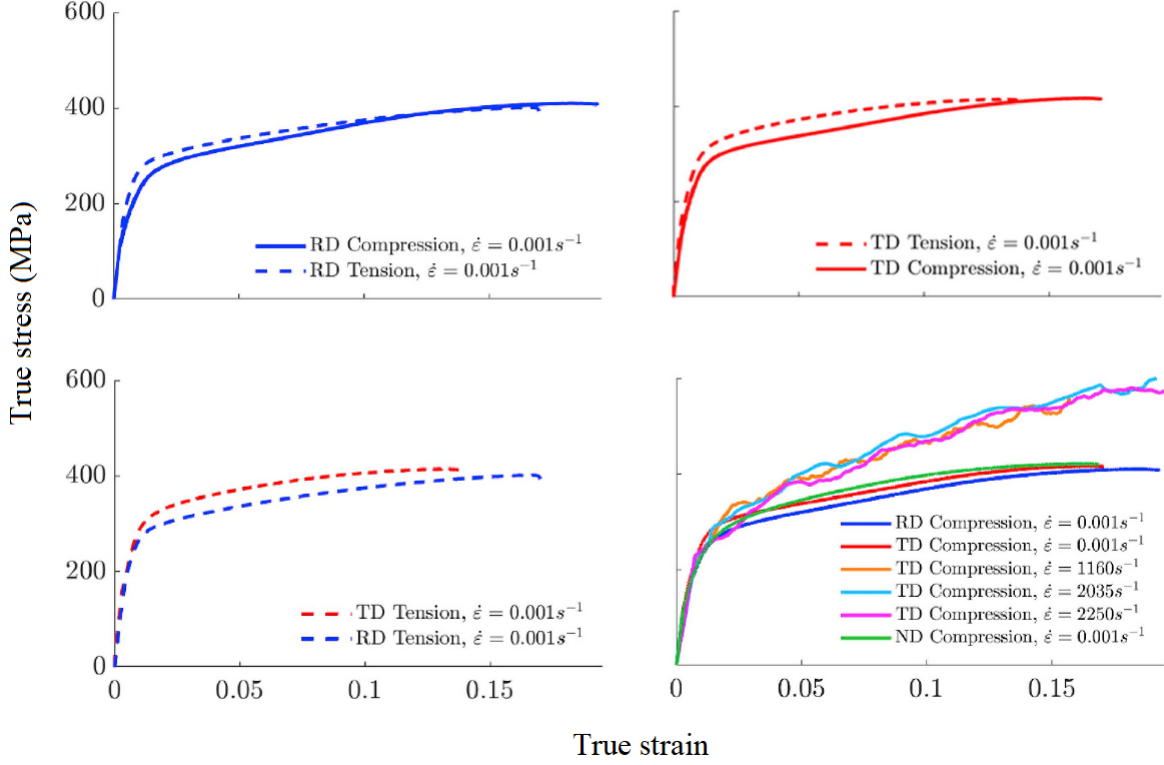


Figure 1.2: Effect of strain-rate and orientation on flow stresses for Mg alloy WE43 plate [9]. When compared to Figure 1.1, this composition’s behaviour seems much more isotropic for both in-plane and out-of-plane loading, and the extent of tension-compression asymmetry is significantly reduced. Similar rate-dependent behaviour was still however observed.

magnesium alloy AZ31 was commercially available in a rolled sheet form supplied in a fully annealed condition (O-temper) [8]. It is clear from these plots that these magnesium alloys exhibit, to various extents, anisotropy, tension-compression asymmetry, and rate dependence, depending on their composition and processing route. The orientation dependency and tension-compression asymmetry is particularly pronounced for AZ31B-O sheet (compare its in-plane and ND compressed, and in-plane compressed and tensioned curves), when compared to the much more isotropically behaving WE43. These variations in flow stresses were specifically believed to arise due to the differences in composition affecting mechanisms found at the micro- and meso-scales. As such, these are discussed next.

The accentuated tension-compression asymmetry and orientation dependency of AZ31B-O sheet, when compared to WE43 plate, can be traced to the low symmetry hexagonal close packed (HCP) unit cells found in magnesium alloys [14, 15]. When magnesium alloys are rolled or extruded, strong textures like that shown in Figure 1.3 develop in the material system through c/a ratio influenced preferential slip [16]. This texture coupled with the low

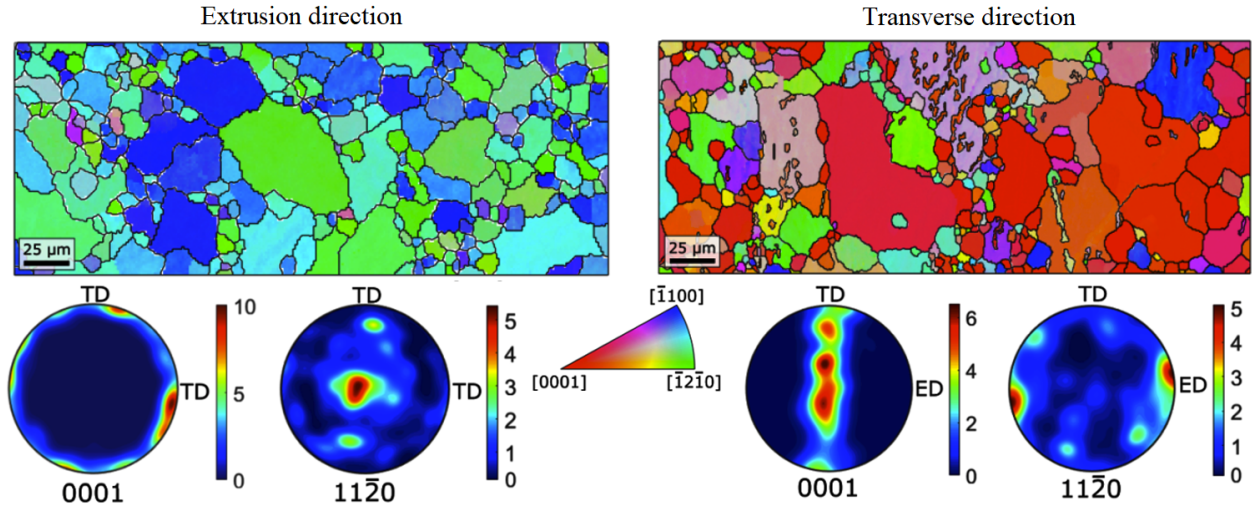


Figure 1.3: Micrograph and texture of extruded AZ31B magnesium alloy as told through inverse pole Figures.

symmetry HCP crystal provides the basis for anisotropic mechanical properties. Examples of intragranular orientation-dependent deformation mechanisms include dislocation glide and twinning (it was twinning that was responsible for the particularly strong tension-compression asymmetry and orientation dependency seen in AZ31B-O sheet [17]). The fact these orientation-dependent mechanisms dictate the bulk mechanical properties so significantly shows that features characterising micro- and meso-structure, such as texture, (that are themselves telling of the material's processing route) need to be considered if the material system is to be designed. Subsequently, if predictions can be made on the performance of a particular magnesium alloy material system based on these features, there exists the possibility to tailor their design through choice of material processing route to better suit them for a component's specific application. It is these types of considerations for magnesium alloy-based material systems destined for high-rate applications that this thesis aims to develop.

A number of research centres have already made significant impact in this area, with PRISMS [18], DAMASK [19], IMDEA [20], and Los Alamos National Laboratory's Visco-plastic self-consistent (VPSC) user-subroutine [21] being but a few. A common link in their strategies to this problem is that they tend to focus on much smaller length-scale problems, they do not concern themselves with making their capabilities available for the design of components, and that information tends to be handled hierarchically (i.e. information is propagated up through length-scales instead of being called concurrently). The exception to the last point is Los Alamos National Laboratory's VPSC user-subroutine that utilises analytical models

based on averaging to predict the plastic deformation of polycrystalline aggregates and as such their constitutive behaviour at the component scale. Here, insight into the relative activity of various crystal plasticity-based mechanisms are made available through use of an anisotropic visco-plastic ellipsoidal inclusion embedded in a homogeneous anisotropic effective medium (HEM) representing the polycrystalline aggregate. However, as the mesostructure is not explicitly modelled, a full-field representation of the stress heterogeneity is not generated, thus inhibiting further investigation of localisation. In contrast, the approaches opted for by PRISMS, DAMASK, and IMDEA do produce full-field stresses. They achieved this by allocating crystal plasticity-based constitutive laws to finite element representations of grains that themselves comprise a polycrystalline structure. These models are frequently referred to as crystal plasticity finite element models (CPFEMs) and have become commonplace when studying full-field stresses or texture evolution of polycrystalline structures. This is because they are better suited for predicting stress and strain heterogeneity for given boundary conditions, especially with the advent of polycrystalline generating algorithms. Implicitly solved CPFEMs [19, 22–25] are favoured in literature with fast spectral solvers [19, 20] also starting to take traction. However, the large time-steps of implicit solvers make them unfavourable for rate-dependent analyses, and the lack of fast spectral-based solvers in commercially available FEA codes was foreseen to hinder the development of spatial multi-scale models that could concurrently run CPFEMs in component-level models (discussed in Section 5.3). Subsequently, it was concluded that a gap in literature existed in the subject areas of upscaling data from high-rate-loaded CPFEMs to the component-level through homogenisation, and high-rate-loaded component-level models that considered mesostructural detail. This thesis aimed to address these gaps using explicit-based solvers which are well suited for high-rate analyses but are not commonly used to solve CPFEMs. However, if they were, they tended to be used to study materials with high symmetry unit cells [26, 27] and as such did not consider twinning. Nonetheless, they were identified as the solver of choice due to their suitability for high-rate analyses and because they are commonly used in component-level analyses, thus offering an easier entry point into developing spatial multi-scale concurrent-based modelling approaches.

The opted for approach for upscaling data involved first building high fidelity full-field models of mesostructure similar to the CPFEMs in Sriram, 2017, Yaghoobi et al., 2019, and Adzima et al., 2017, [27–29], with notable differences being that the crystal plasticity-based user-subroutine

developed in this thesis was implemented into an explicit FEM solver, the formulation considered slip and homogenised-based twinning in a rate-dependent manner, and that the unit cell of the targeted material system had a low order of symmetry. These CPFEMs were then sized into representative volume elements (RVEs), using a high-performance computer cluster, to enable hierarchical parameterisation of component-level constitutive models, thus facilitating scale-bridging. As the CPFEMs enable the study of localised stress field heterogeneities resulting from grain size distributions, texture, etc., and a link between these features and the component-level could be established, the potential to set up optimisations to ascertain characteristics that would yield desirable bulk-level characteristics now existed, thus facilitating a data-driven framework to material design through the active design of micro- and meso-structure.

Further capabilities that full-field homogenisation approaches offer include uncertainty quantification of the effect the aleatoric nature of mesostructure has on bulk mechanical properties. The characterisation of such variation could serve as the basis for stochastic-based models as it could be used to generate a population of parameters for the constitutive models run at the component-level to sample from (e.g. the Johnson-Cook plasticity or VPSC models). However, a problem with this hierarchical parameterisation of longer length-scale models is that a J2-plasticity model with hardening behaviour that reflects the correct functional form needs identifying. This becomes problematic when a material exhibits anisotropic mechanical properties like that of AZ31B-O sheet shown in Figure 1.1. Here, the stress-strain behaviour transitioned from a sigmoid (for in-plane uni-axial loading) to a logarithmic (for out-of-plane uni-axial loading) shape; this problem is discussed in great detail throughout. Moreover, other further capabilities include the potential to introduce additional mechanisms dependent on stress localisation, such as inter- and intra-granular cracking. Having given an account of the bottom-up capabilities offered by such a framework, the top-down opportunities are now discussed.

As the proposed upscaling framework translated crystal plasticity information to component-level models, the potential to add mesostructure detail to discrete areas now exists. This could be achieved in several ways, for example, a component-level model could be set-up with a gradient in mesh resolution to enable mapping of mesostructure resolution. Such a model would be run with a sub-cycling algorithm to facilitate efficient running [30], and could be used to investigate the effect of badly orientated grains in stress-sensitive areas, or to capture the incipient stages of crack initiation; Zhang et al., 2022, [31] utilised such an approach to

reduce the runtime of a FEM that predicted the dynamic response of a nuclear power plant subjected to an impact and the resulting shock induced in the nearby underlying soil/rock. However, if the areas to add mesostructure detail are not known *a priori*, then adaptive mesh refinement could be conducted on-the-fly in areas exhibiting high strain gradients, and mesoscale resolution added when the element size fell below a threshold value [32]. Having now discussed top-down implementations of mesoscale features into high-rate component-level models, the magnesium alloy compositions used as model materials are now detailed.

The developed capabilities were showcased using magnesium alloys WE43 and AZ31. WE43 was chosen because of its superior properties compared to Al-Mg alloy 5083 and conventional Mg alloy AZ31 [33], the fact it remained so isotropic, and to build on the extensive research already conducted on this material through the UK Engineering and Physical Sciences Research Council (EPSRC) grant (EP/R513295/1) that is also funding this work. AZ31 was also chosen as it exhibits strong and unique tension-compression asymmetry (as shown in Figure 1.1) that stems from twinning, thus making it a prime magnesium alloy composition to showcase the meso- to bulk-level upscaling predictive capabilities of the developed framework. Let it be noted that the versatility of the developed capabilities meant that they are not just limited to magnesium alloys but that they could be extended to consider other HCP-based systems, or indeed other crystal systems altogether. Having provided an introduction to the work completed in this thesis, and having given an account of the materials used to showcase the capabilities developed, the questions this thesis ultimately strove to answer are now posed,

- Can constitutive models that correctly predict the flow stresses of WE43-T6 plate and AZ31B-O sheet be developed to enable their consideration in the design of components (such models are currently not available in commercial code)?
- Is it possible to generate approximations of the full-field stress heterogeneity that develops at the mesoscale from bulk mechanical characterisations of a material using CPFEMs?
- Could a hierarchical link between these CPFEMs and component-level constitutive models be established where the effect of altering micro- and meso-scale features (such as solutes and precipitates, texture, grain size distribution, etc.) influences the scale above?
- Subsequently, would it be possible to design these micro- and meso-scale features to improve the performance of a component for its specific application?

- Finally, could the datasets generated through the homogenisation and characterisation of CPFEMs be leveraged to facilitate novel, data-rich modelling strategies?

These questions were addressed by first working through an example that investigated the performance of the magnesium alloy WE43-T6 and AZ31B-O material systems when used as blast resisting armour plating. It was through this example that the need to develop appropriate component-level constitutive models was identified, thus making obvious why the first question was posed. This example was then used as a conduit to discuss the benefits of considering micro- and meso-scale features in the design of a material system, making relevant the second through to fourth question. Finally, the opportunities offered by fully realising mesostructural features were then presented, addressing the last question.

2

Blast-loaded plate example

2.1 Chapter Overview

Armour plates are conventionally manufactured from hardened steel, however magnesium alloys such as WE43 are being researched as possible alternatives due to the fact thicker sections can be utilised for the same mass penalty, potentially offering improved protection. This section starts by discussing the complexities associated with designing structural components with magnesium alloys and then moves on to presenting analyses where hardened steel and WE43-T6 armour plates were subjected to blast-loads using boundary conditions and constitutive models available in the widely used FEA package LS-Dyna; this example serves as an overarching narrative throughout the rest of the thesis to present why microstructure-aware constitutive models are beneficial, with literature reviews being conducted on-the-fly where required. The lack of suitable constitutive models to predict the required anisotropy or the sigmoid-shaped flow stresses of sheet AZ31B-O with in-plane compression was subsequently highlighted and the need to develop them identified. The chapter then concludes with the question of whether the bulk mechanical properties of a component could be linked to micro- and meso-scale phenomena, and if these could be designed to improve component performance.

2.2 Study of blast-loaded plates

Designing structures with magnesium alloys presents a multitude of challenges owing to complex microstructure and the inherent transversely isotropic properties of their HCP unit cell. Such challenges include anisotropy, directional-dependent strain-rate sensitivity, and tension-compression asymmetry, all of which stem from the low symmetry of the unit cell and limited number of slip systems available [13, 33–36]. Notably, the difficulty of accommodating $\langle c \rangle$ axis deformation through slip leads to twinning as twinning modes (extension or compression) are more readily activated at room temperature than the relevant $\langle c+a \rangle$ slip systems. As a result, twins are seen to nucleate, propagate, and grow for these load types [37, 38]. Slip systems are re-orientated within these twinned domains and as such could become favourably oriented for activation, thus contributing to the evolving directional-dependent characteristics seen at the bulk-level [39]. Bhattacharyya et al., 2016, Platts, 2019, and Hidalgo-Manrique et al., 2017, [13, 36, 40] also showed that, for magnesium alloy WE43, precipitates have significant bearing on both the critically resolved shear stresses required to drive thermally activated dislocation glide on particular slip systems, and the resulting strain-hardening characteristics, thus further contributing to anisotropy. It is interactions like these that propagate anisotropic and directional-dependent properties from the mesoscale to the material's bulk.

Typically, phenomenological models that use empirical relationships consistent with the aforementioned fundamental theory but not derived from it are the standard constitutive models of choice in industry to model deformation in metals because of their simplicity [27]. The Johnson-Cook model [41], for example, is particularly favoured as it requires a minimum of five material constants to be defined for an isotropic material meaning minimal experimental calibration is necessary. However, their use alone is not sufficient to give insight into the complex mechanisms shown to underpin the high-rate related behaviour of magnesium alloy sheets and plates. Physically-based models such as the Oxford titanium constitutive model [42] developed its theory from micro-mechanic considerations, meaning that its prediction of flow behaviour is physically-based. However, a consequence of this is that its calibration requires the use of large datasets that may be difficult to obtain. Another approach, that is the focus of this work, is to shift aspects of this dependence on in-depth experimental datasets to lower length-scale models, thus enabling exploration of the effects micro- and meso-scale features have on bulk stress-strain behaviour.

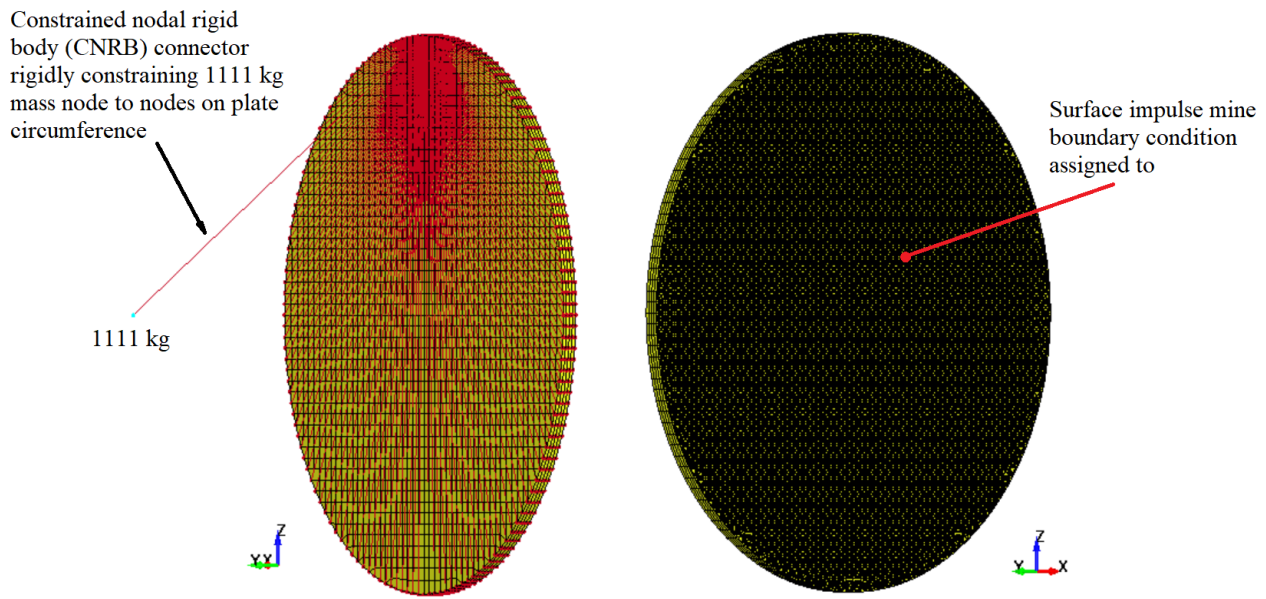


Figure 2.1: Finite element model of disc shaped armour plate from various angles. Constrained nodal rigid body connectors were used to attach a 1111 kg nodal mass to the nodes on the circumference of the disc. The nodes on the circumference were only permitted (0, 1, 0) translational DOF. The impulse mine keyword was assigned to the other side of the plate.

The advantages of using magnesium alloy WE43-T6 armour plating in place of conventional hard steel armour plating, as well as the limitations of the constitutive models currently available to industry, are now demonstrated through a example conducted using the commercially available explicit FEA package LS-Dyna; an explicit solver was used as they are best suited for high-rate analyses due to their small time-steps. The first analysis that was set up investigated the blast response of the hard steel armour plate. A pictorial representation of the FEM is presented in Figure 2.1, with details of the plate, mesh, and called upon boundary conditions and constitutive models being reported in Table 2.1. The impulse mine keyword [44] is a boundary condition that applies initial velocities to selected nodes to emulate the impulse imparted by the detonation of a buried land mine. While the simplified Johnson-Cook constitutive model is one that is based on Eq. 3.52 discussed later, but only considers strain and strain-rate sensitive plasticity, and was set to delete elements that exceeded 0.2 effective plastic strain. The nodes on the circumference of the disc shaped armour plate were only permitted (0, 1, 0) translational DOF and were rigidly constrained to a node of mass 1111 kg in the manner shown. The sequence of images along the top of Figure 2.2 shows the resulting response of the plate with time from front and rear viewpoints. Fracture was observed to occur at 0.6 ms. The plot beneath these images presents the calculated σ_{11} stress with time for the selected elements shown. This plot

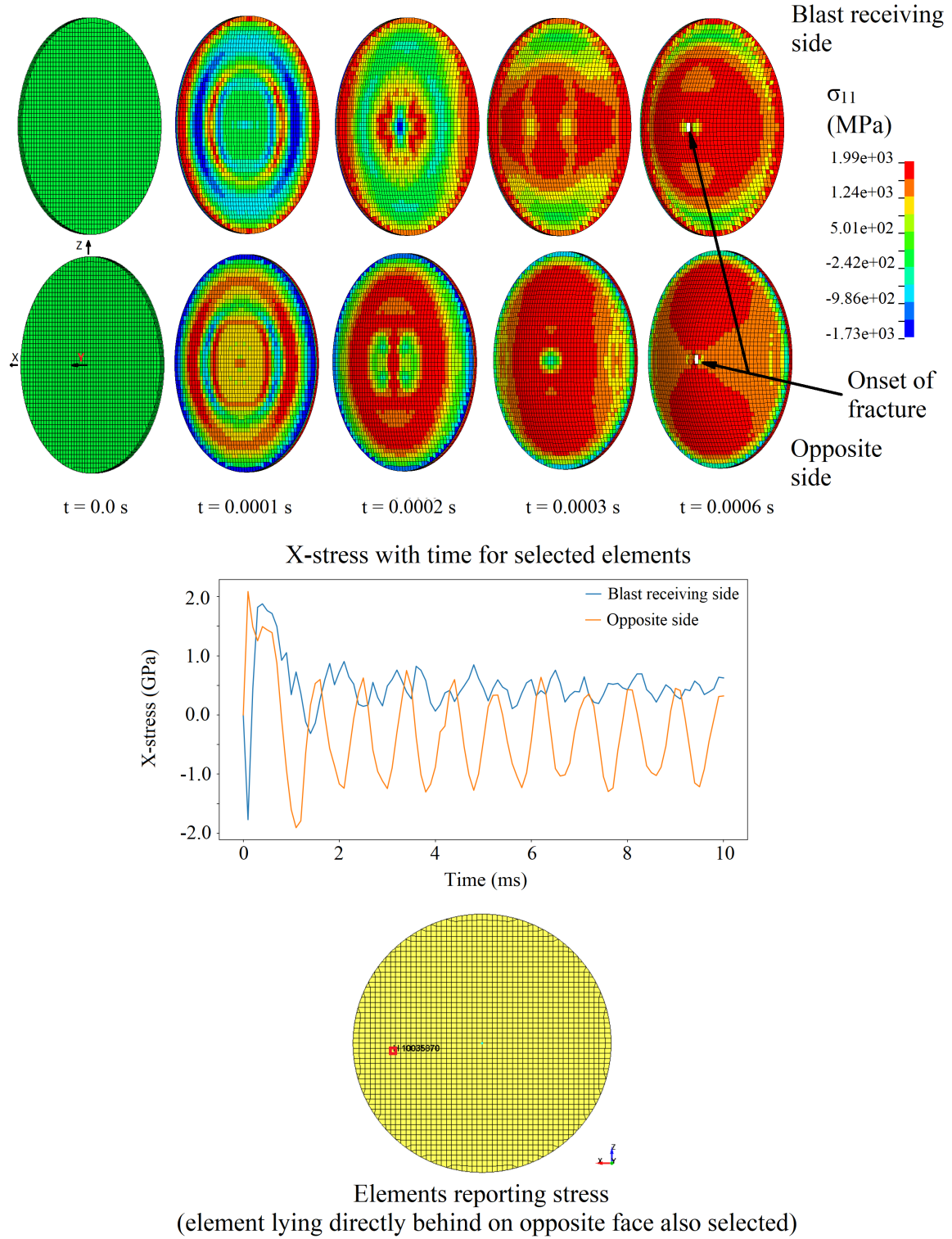


Figure 2.2: (Top) Sequence of images showing the evolving deformation and resulting σ_{11} stress (GPa) of a blast-loaded hard steel plate as viewed from the front and rear. Fracture was observed 6 ms after initial blast. (Bottom) Elements selected from model to report σ_{11} stress. (Middle) Plot showing stress with time for selected elements. Initially, the blast receiving side goes into compression, whereas the opposite side goes into tension. After this, the stress was seen to oscillate in an under-damped manner where the opposite side was seen to oscillate between tension and compression, while the blast receiving face oscillates for the majority in a state of tension.

Parameters	Value	Units
Material	Hard steel [43]	-
Constitutive model	Simplified Johnson-Cook	-
ρ	7.75×10^{-6}	kg/mm ³
E	212.70	GPa
ν	0.30	-
A	1.539	GPa
B	0.477	GPa
n	0.18	-
C	0.012	-
Effective plastic strain at failure	0.20	-
Plate parameters		
Diameter	1000	mm
Thickness	25	mm
Mass	152.17	kg
Impulse mine parameters		
Equivalent mass of TNT	6.0	kg
Density of overburden soil	2.2×10^{-6}	kg mm ⁻³
Depth	140	mm
Mine cross sectional area	4.538×10^4	mm ²
Blast vector	(0, 1, 0)	-
Model settings		
Element size	$19.7 \times 6.25 \times 19.7$	mm $\times$ mm $\times$ mm
No. elements	8160	-

Table 2.1: Parameters used in hard steel plate blast analysis.

identifies that the plate underwent compressive and tensile loading.

The simulation was then repeated with the same settings but the hard steel plate swapped out for a thicker Mg alloy WE43-T6 one of equivalent mass (Table 2.2 summarises this model's parameters). In this instance an anisotropic plasticity model that exhibited tension-compression

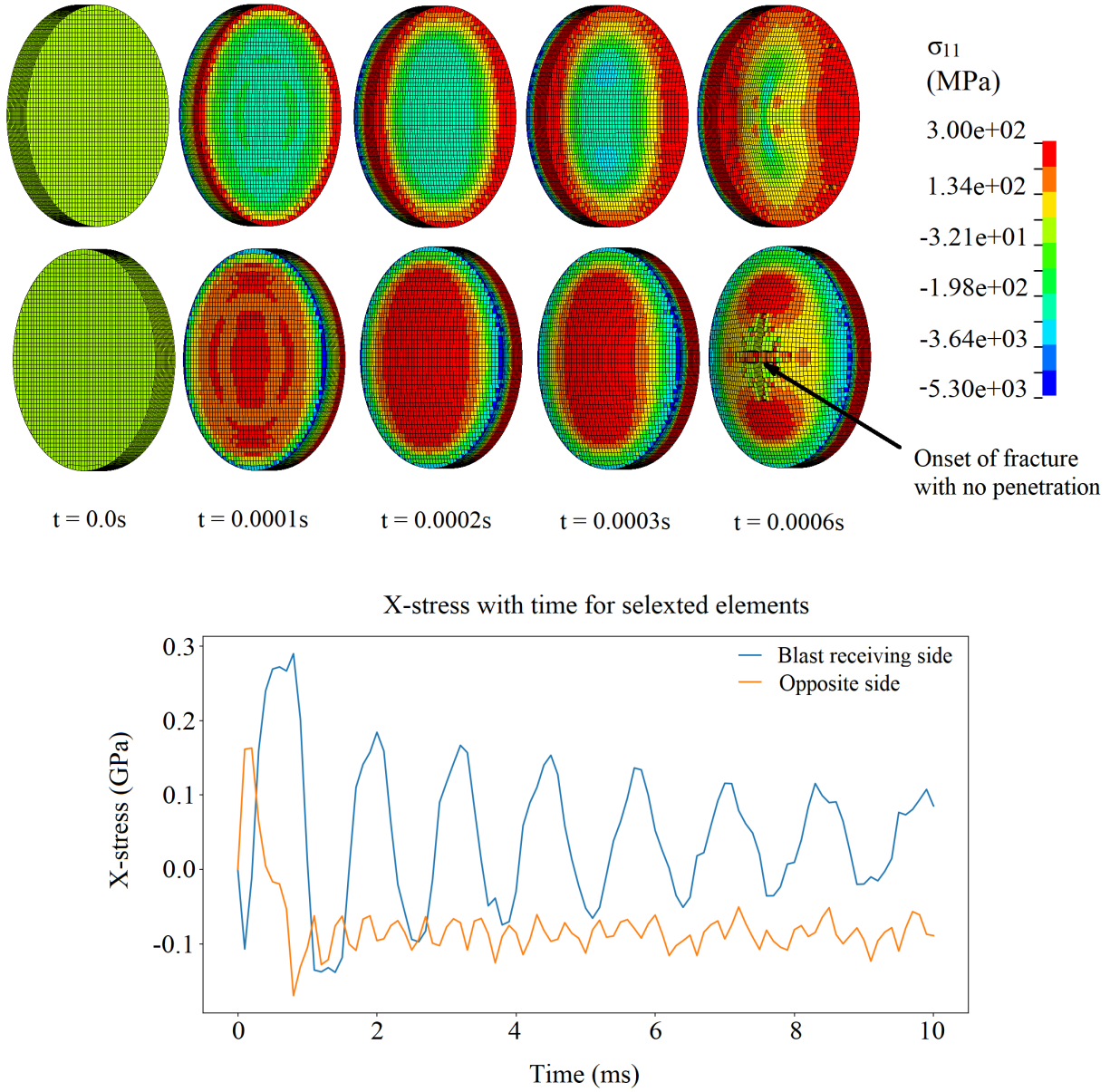


Figure 2.3: (Top) Sequence of images showing the evolving deformation and resulting σ_{11} stress (GPa) of a blast-loaded WE43-T6 plate as viewed from the front and rear. Fracture but no penetration was observed 6 ms after initial blast. (Bottom) Plot showing stress with time for selected elements. Initially, the blast receiving side goes into compression, whereas the opposite side goes into tension. After this, the stress was seen to oscillate in an under-damped manner. The opposite was seen to oscillate in a state of compression, while the blast receiving face oscillates between tension and compression.

Parameters	Value	Units
Material	Magnesium alloy WE43-T6 [13]	-
Constitutive model	Simplified Johnson-Cook	-
Orientation parameters reflect	In-plane (compression)	-
ρ	1.70×10^{-6}	kg/mm ³
E	42.00	GPa
ν	0.27	-
A	0.140	GPa
B	0.340	GPa
n	0.347	-
C	0.0046	-
Effective plastic strain at failure	0.20	-
Plate parameters		
Diameter	1000	mm
Thickness	115	mm
Mass	153.50	kg
Model settings		
No. elements	36721	-

Table 2.2: Parameters used in WE43-T6 plate blast response simulation. The constitutive model parameters reflect in-plane hardening under compression. Parameters not listed re-used the values shown in Table 2.1

asymmetry would have been ideal. However, the tabulated orthotropic Johnson-Cook model in LS-Dyna could not be successfully run without crashing the analysis, and no other anisotropic rate-dependent plasticity models were available. Consequently, the analysis was run using the same simplified Johnson-Cook constitutive model as before but with parameters reflecting the in-plane compression of WE43-T6 plate being used; this decision was made as WE43 was shown to exhibit a relatively small degree of tension-compression asymmetry [9] especially when compared to sheet AZ31B-O. The sequence of images along the top of Figure 2.3 again shows the evolution of the σ_{11} stress with time, and that fracture was observed on the face opposite to the blast, but in this case it was not penetrative at 0.6 ms. The plot beneath clearly

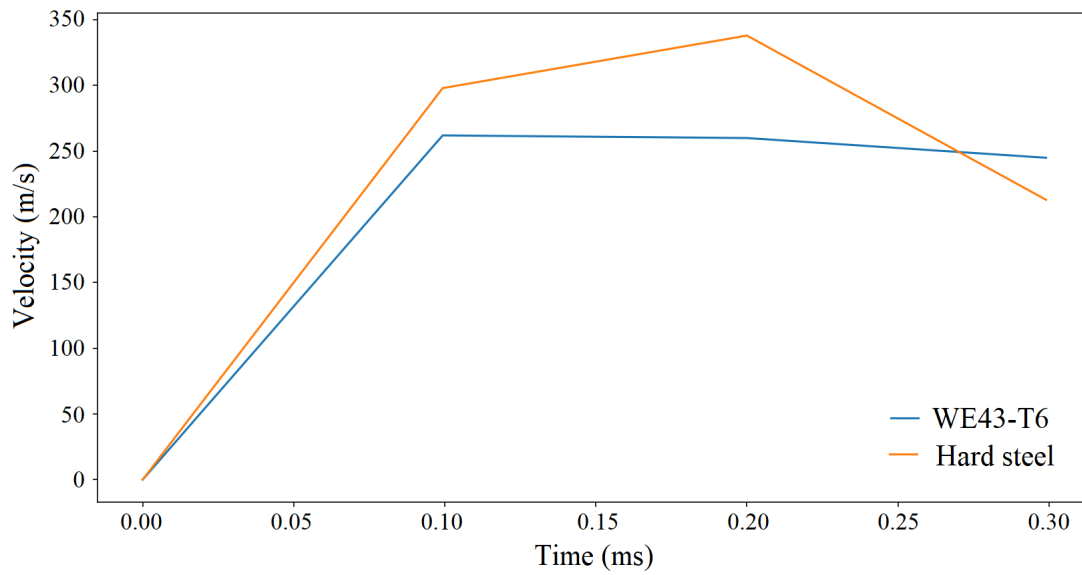


Figure 2.4: Comparison of leading node velocity profiles from both blast simulations.

shows that this plate also experienced compressive and tensile loading. Comparing the velocity profiles of the leading node on the opposite face of the blast of both simulations (see Figure 2.4) quantitatively showed that using a thicker section of armour plate reduced the magnitude of the initial rise of the blast. This coupled with the fact the fracture of the WE43-T6 plate was not penetrative within the same time-period could ultimately mean lives saved if it was used in-place of the hard steel plate without adding extra mass to the system.

The analysis was not run for sheet AZ31B-O as the same justification to run the analysis could not be made due to the fact the its tension-compression asymmetry was so severe. It should also be noted that none of the constitutive models available in LS-Dyna could predict the in-plane compressed sigmoid-shaped flow stresses observed either. As such, these were identified as further shortcomings of the commercially available software package.

Even though a strong argument for using magnesium alloy WE43-T6 armour plating has been presented, it should be noted that the completed simulation may not be as accurate as the hard steel one. This is because an isotropic plasticity model was used to model a material system that was clearly shown to exhibit anisotropy and tension-compression asymmetry (the parameters used in the Johnson-Cook plasticity model in this instance are only reflective of the material under in-plane compression). Therefore, a constitutive model that could predict anisotropy, rate-dependence, and tension-compression asymmetry is required to improve accuracy. Furthermore, plasticity models that could recreate the in-plane compression sigmoid-shaped

flow stresses of sheet AZ31B-O were not available and were also identified as being required if this composition was to be accurately considered. These complexities, as well as general deformation, stem from mechanisms and features found at lower length-scales. Linking them to component performance presents the opportunity for their design to optimise a material system for a component's specific application.

Through the completion of this study, it became clear why some of the questions raised in Chapter 1 were posed. Of these questions, the following were relevant to this body of work (and were answered later in the thesis),

- Can constitutive models that correctly predict the flow stresses of WE43-T6 plate and AZ31B-O sheet be developed to enable their consideration in component-level analyses, as these are not currently available in commercial code?
- Could a link between lower length-scale models and component-level constitutive models be established where the effect of altering micro- and meso-scale features (such as solutes and precipitates, texture, grain size distribution, etc.) influence bulk mechanical properties?
- Would it be possible to design these micro- and meso-scale features to improve the performance of a component for its specific application?

3

Component-level numerical framework

3.1 Chapter Overview

This section strove to answer the questions identified at the end of the last chapter, and starts with a detailed mathematical description of the explicit solver used to run the blast-loaded plate study in Chapter 2. Explicit solvers were favoured over implicit ones due to their small time-steps making them better suited for high-rate analyses. A constitutive model that was able to reproduce the anisotropy of WE43-T6 plate was then identified whose description was provided. This model was however unable to recreate tension-compression asymmetry and so required modifying to do so, with a simplified approach being opted for. This model was subsequently further modified to enable predictions of the sigmoid-shaped flow stresses exhibited by in-plane compressed AZ31B-O sheet. Verification studies were subsequently completed to ensure the desired constitutive behaviour was predicted, and the plate blast analysis from the previous chapter re-run. Having now developed the constitutive models required to predict how the model material systems behave at the component-level (addressing the first question posed), the question was then raised if this behaviour could be related to micro- and meso-scale considered models (addressing the second and third questions).

3.2 Description of Explicit Solver

The blast simulations conducted in the previous chapter were run using the commercially available FEA package LS-Dyna. However, a lot of the early developmental work conducted during this thesis was completed using the in-house developed updated-Lagrangian FEA code DEST, whose formulation is similar to that of LS-Dyna. Within this code, a leap-frog integration scheme is used where increments of deformation are applied to the boundaries of elements, and the material's state variables from the previous time-step are made available, allowing for path-dependent evolution of a system. Equilibrium is enforced through the conservation equations, with the assumption that the stress state is constant over the time-step, allowing for the velocity gradient to be calculated. The description of the explicit solver starts with the requirement that the conservation of mass postulate is satisfied. This is achieved by enforcing,

$$\frac{d}{dt} \int_{\Omega_t} \rho dv = 0, \quad (3.1)$$

where ρ is the instantaneous density, v is the current volume, and Ω_t is the domain that material particles (p) belong to at time t . The equilibrium equations for the system were determined using Hamilton's principle and the Lagrangian (L) that is defined by,

$$L = T - U + W_{nc}, \quad (3.2)$$

where T and U are the total kinetic and potential energies respectively, and W_{nc} is the work done by the non-conservative forces. Hamilton's principle states that the first variation of the integral of Eq. 3.2 (J -integral) with respect to time is zero, thus,

$$\partial J = \int_{t_1}^{t_2} \partial(T - U + W_{nc}) dt = 0. \quad (3.3)$$

For a solid body the components of the Lagrangian are expressed by,

$$T = \frac{1}{2} \int_{\Omega} \rho \dot{\mathbf{u}}^2 dV, \quad (3.4)$$

$$U = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\epsilon} dV, \quad (3.5)$$

$$W_{nc} = \int_{\Omega} \rho \mathbf{b} dV + \int_{\Omega} \nabla \cdot [\boldsymbol{\sigma} \mathbf{u}] dV, \quad (3.6)$$

where $\dot{\mathbf{u}}$ is the velocity vector field, V is the reference volume, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{\epsilon}$ is the strain tensor, $\mathbf{b}$ are body forces, and $\mathbf{u}$ is the displacement vector field. Substituting these into Eq. 3.3 and manipulating yields the momentum balance equation,

$$\rho \mathbf{b} + \nabla \cdot \boldsymbol{\sigma} = \rho \ddot{\mathbf{u}} \quad \forall p \in \Omega. \quad (3.7)$$

Rotational equilibrium is enforced by ensuring symmetry of the Cauchy stress tensor,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T. \quad (3.8)$$

The energy balance equation is derived by first taking the time derivative of the kinetic energy for a body occupying domain Ω ,

$$\dot{T} = \int_{\Omega} \rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} dv. \quad (3.9)$$

The external power acting on the body is then given by,

$$P = \int_{\Omega} \rho \mathbf{b} \dot{\mathbf{u}} dv + \int_{\Gamma_t} \mathbf{t}(\mathbf{n}) \cdot \dot{\mathbf{u}} da, \quad (3.10)$$

where Γ is the domain's boundary. Applying the divergence theorem to the second term in Eq. 3.10 yields,

$$P = \int_{\Omega} [(\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b}) \cdot \dot{\mathbf{u}} + \boldsymbol{\sigma} : \nabla \dot{\mathbf{u}}] dv, \quad (3.11)$$

which for infinitesimal deformations ($\boldsymbol{\sigma} : \nabla \dot{\mathbf{u}} = \boldsymbol{\sigma} : \mathbf{D}$) and applying Eq. 3.7 follows,

$$P = \dot{T} + \int_{\Omega} \boldsymbol{\sigma} : \mathbf{D} dv, \quad (3.12)$$

where $\mathbf{D}$ is the rate of deformation tensor. The heat flow into a body is,

$$Q = \int_{\Omega} \rho r(x) dv - \int_{\Gamma_h} h(\mathbf{x}, \mathbf{n}) da, \quad (3.13)$$

where $r(x)$ is the rate of radiant heat supply density and $h(\mathbf{x}, \mathbf{n})$ is the heat outflow per unit time per unit surface area. The first principle of thermodynamics asserts that there exists a state variable e , called the internal energy density, such that

$$\frac{\partial}{\partial t} \int_{\Omega} \rho e dv = Q + \int_{\Omega} \boldsymbol{\sigma} : \mathbf{D} dv. \quad (3.14)$$

Through the application of a traction vector it can be obtained that,

$$h(\mathbf{x}, \mathbf{n}) = q(\mathbf{x}) \cdot \mathbf{n}, \quad (3.15)$$

where $q(x)$ is the heat flux vector so that for any given domain $H \subset \Omega$,

$$\int_H \rho r dv - \int_{\partial H} \mathbf{q} \cdot \mathbf{n} da = \int_H [\rho r - \nabla \cdot \mathbf{q}] dv, \quad (3.16)$$

which after applying the divergence theorem yields the energy balance equation,

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{D} + \rho r - \nabla \cdot \mathbf{q}. \quad (3.17)$$

To apply the momentum balance equation (Eq. 3.7) to a discretised continuous system, the strong form shown is replaced with a weak form that requires equilibrium be satisfied globally for the entire body. The weak form of this equation describes equilibrium in terms of the virtual work equation through the application of a test function, and integration over the current volume of the body,

$$\partial W = \int_{\Phi_t(\Omega)} (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} - \rho \ddot{\mathbf{u}}) \cdot \delta \mathbf{v} dv = 0. \quad (3.18)$$

Through manipulation this can be expressed as,

$$\partial W = \int_{\Phi_t(\Omega)} \rho \ddot{\mathbf{u}} \cdot \delta \mathbf{v} dv + \int_{\Phi_t(\Omega)} \boldsymbol{\sigma} : \delta \mathbf{D} dv - \int_{\Phi_t(\partial\Omega)} \mathbf{t} \cdot \delta \mathbf{v} da - \int_{\Phi_t(\Omega)} \rho \mathbf{b} \cdot \delta \mathbf{v} dv = 0, \quad (3.19)$$

and rewritten in terms of finite element discretisation,

$$\partial W = \sum_{i=1}^{n=\#\text{nodes}} \delta \mathbf{v}_i \cdot (\mathbf{F}_i^{\text{inert}} + \mathbf{F}_i^{\text{int}} - \mathbf{F}_i^{\text{ext}}), \quad (3.20)$$

where,

$$\mathbf{F}_i^{\text{inert}} = \sum_{e=1}^{m=\#\text{elements}} \int_{\Phi_t(\Omega_e)} \rho \mathbf{N}_i^a \mathbf{N}_i^b \ddot{\mathbf{u}}_i dv, \quad (3.21)$$

$$\mathbf{F}_i^{\text{int}} = \sum_{e=1}^m \int_{\Phi_t(\Omega_e)} \boldsymbol{\sigma} \nabla_x \mathbf{N}_i^a dv, \quad (3.22)$$

$$\mathbf{F}_i^{\text{ext}} = \sum_{e=1}^m \int_{\Phi_t(\partial\Omega_e)} \mathbf{N}_i^a(t) da + \sum_{e=1}^m \int_{\Phi_t(\Omega_e)} \mathbf{N}_i^a \rho \mathbf{b} dv, \quad (3.23)$$

are the inertial, internal, and external force vectors respectively, and N_i represents the element shape function. Since Eq. 3.20 must be satisfied for all cases of the arbitrary virtual velocities, the equation can be rewritten in terms of nodal equilibrium,

$$\mathbf{F}_i^{\text{inert}} + \mathbf{F}_i^{\text{int}} - \mathbf{F}_i^{\text{ext}} = 0. \quad (3.24)$$

If the mass matrix in $\mathbf{F}_i^{\text{inert}}$ is then diagonalised (m_{ii}), the system of differential equations resulting from explicitly integrating Eq. 3.24 through the leap-frog integration method uncouple, meaning they can be solved independently for each degree of freedom through the following,

$$\ddot{u}_{i,N} = m_{ii}^{-1} (f_i^{\text{ext}}(\mathbf{u}_t) - f_i^{\text{int}}(\mathbf{u}_t)), \quad (3.25)$$

$$\dot{u}_{i,t+\Delta t/2} = \dot{u}_{i,t-\Delta/2} + \ddot{u}_{i,t} \Delta t_{t+\Delta t/2}, \quad (3.26)$$

$$u_{i,t+\Delta t} = u_{i,t} + \dot{u}_{i,t+\Delta t/2} \Delta t_{t+\Delta t}, \quad (3.27)$$

where,

$$\Delta t_{t+\Delta t/2} = \frac{\Delta t_t + \Delta t_{t+\Delta t}}{2}. \quad (3.28)$$

Half increments denote variables available during the solve while variables denoted with integers are available at the start and end of the time-steps. The unconditional stability requirement for the explicit leap-frog time-stepping scheme is $\Delta t \leq 2/\omega_{\text{max}}$, where ω_{max} is the element

maximum eigenvalue. A conservative estimate for the stable time increment is,

$$\Delta t \leq \min \frac{L_c}{c_d} \quad \forall \Omega, \quad (3.29)$$

where L_c is the characteristic element length and c_d is the current effective dilatational wave speed of the material. Having presented the formulation of the explicit solver, attention turned to identifying and developing a component-scale plasticity model that exhibited the required anisotropy, tension-compression asymmetry, and sigmoid flow stresses.

3.3 Development of required component-level constitutive model

Constitutive laws are used to evaluate the unknown value of stress in the virtual work equation. As mentioned throughout up to now, plasticity models that exhibit anisotropy, tension-compression asymmetry, rate-dependence, and sigmoid flow stresses are required to accurately predict the behaviour of high-rate loaded structural components made from either WE43-T6 plate or AZ31B-O sheet. The main concepts of plasticity models are the decomposition of the strain-rate, the elastic constitutive law, yielding, plastic flow rules, and hardening laws. Strain-rate at a given stress can be decomposed into two parts, a small recoverable elastic strain and a large irreversible plastic strain for the condition $d\boldsymbol{\sigma}d\boldsymbol{\epsilon}^p \geq 0$; with it only equalling zero if $d\boldsymbol{\epsilon}^p = 0$. The linear elastic strains are related to the applied stress state through,

$$\frac{d\boldsymbol{\epsilon}^e}{dt} = \boldsymbol{S} \frac{d\boldsymbol{\sigma}^e}{dt}, \quad (3.30)$$

where $\boldsymbol{S}$ is the fourth order compliance tensor that can be reduced to a second order 6×6 tensor using Voigt notation.

There are a number of plasticity models available in LS-Dyna that exhibit anisotropy, however each has its own limitation that made them unsuitable for the example presented in Chapter 2. For example, the tabulated Johnson-Cook orthotropic plasticity model [45] was stated to possess a few of the desired traits through use of its J3-dependent yield surface. However, this model was isotropic in the elastic regime, could only predict power-law flow

stresses (making it unsuitable for predicting the required sigmoid shape), and it seemed generally unstable when attempts were made to use it. Another available plasticity model was the Hill-3R-3D model that combines orthotropic elastic behavior with Hills anisotropic plasticity theory [46]. Even though this model offered improvements over isotropic elastic models, it lacked the necessary rate-dependence required to enable accurate predictions of deformation for high-rate loaded structures. Furthermore, it also lacked tension-compression asymmetry, and only allowed the definition of one hardening rule, which again meant it was incapable of predicting both the required logarithmic and sigmoid-shaped flow stresses. Another potentially viable constitutive model available to the author was that developed by Cousins, 2016 [42]. This model is based on the Bammann-Chiesa-Johnson (BCJ) model [47] (dismissed in this work due to its complexity and the need for a high number of input parameters) that was modified to include anisotropy and tension-compression asymmetry. These were incorporated using Hills plasticity theory [46] and the Drucker-Prager criterion [48] (expansion of the von Mises criterion), respectively. Even though this model possessed some desirable traits, the inability to allow for an evolving degree of anisotropy was of concern. Additionally, its formulation inhibited the prediction of sigmoid flow stresses.

Recently, an anisotropic Johnson-Cook plasticity model was developed in the ISML (Impact and Shock Mechanics Laboratory) [49] that was based on a generalised radial-return mapping algorithm for anisotropic von Mises plasticity framed in material eigenspace [50], thus combining anisotropy and rate-dependence. The generalised form of this algorithm meant it could be modified to work with most hardening laws, making it an ideal candidate. What follows is its description and details on how it was modified to deliver on the desired requirements.

3.3.1 Formulation of anisotropic Johnson-Cook plasticity model

For yielding to occur, current plasticity theory states that the stress field vector must lie on the material's yield surface and not exceed it. This is known as a consistency condition. If stress does exceed the yield surface, plastic flow becomes infinite and non-physical. Therefore, the yield surface moves to maintain this condition and consequently transfers energy. Plastic flow rules are used as part of this balance and enable predictions of the components of the plastic strain-rate by requiring the principle of maximum plastic resistance be satisfied. This means that the yield surface must be convex, the plastic strain increment is normal to the yield surface, and the

strain-hardening rate must be ≥ 0 . Hardening laws are then used to describe how the material's state variables (that set the yield surface) evolve with plastic strain; plastic flow potentials that relate the plastic strain-rate to the evolution of the yield surface are known as associative flow rules. The two most common approaches to model the evolution of the yield surface are through isotropic and kinematic hardening laws that are based on J2-plasticity, and see the yield surface scale in size or translate, respectively. Considering this, the most appropriate place to start the description of the ISML anisotropic Johnson-Cook plasticity model was with its yield criteria.

This model uses the the Hill quadratic yield criterion [46] which is a modification of the von Mises criterion that introduced a scaling coefficient (F , G , H , L , M , and N) to each of the six axes defining a hyper-ellipsoid,

$$f_{Hill} = F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2(L\sigma_{23}^2 + M\sigma_{31}^2 + N\sigma_{12}^2) \leq 1, \quad (3.31)$$

that prescribed its anisotropic yield surface. Eq. 3.31 can be written in tensor notation as,

$$\mathbf{s}^\top \mathbf{A} \mathbf{s} \leq 1, \quad (3.32)$$

where $\mathbf{s}$ is a deviatoric stress and $\mathbf{A}$ is a fourth order tensor defining anisotropy. $\mathbf{A}$ can then be reduced to the second order tensor (if symmetry is exploited and Voigt notation used),

$$\mathbf{A} = \begin{bmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{bmatrix}. \quad (3.33)$$

This matrix was derived by first setting $\mathbf{s} = \mathbf{P}_{dev} \boldsymbol{\sigma}$ where $\mathbf{P}_{dev}$ is the deviatoric stress projection

matrix, that in Voigt notation takes,

$$\mathbf{P}_{dev} = \frac{1}{3} \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}. \quad (3.34)$$

Substituting this into Eq. 3.32 gives,

$$(\mathbf{P}_{dev} \boldsymbol{\sigma})^\top \mathbf{A} (\mathbf{P}_{dev} \boldsymbol{\sigma}) = \boldsymbol{\sigma}^\top (\mathbf{P}_{dev})^\top \mathbf{A} (\mathbf{P}_{dev}) \boldsymbol{\sigma} = \boldsymbol{\sigma}^\top (\mathbf{P}_{dev}) \mathbf{A} (\mathbf{P}_{dev}) \boldsymbol{\sigma} = \boldsymbol{\sigma}^\top \mathbf{A} \boldsymbol{\sigma}. \quad (3.35)$$

Working through the above reveals,

$$\begin{bmatrix} a_{11} \\ a_{22} \\ a_{33} \\ 2a_{23} \\ 2a_{31} \\ 2a_{12} \\ a_{44} \\ a_{55} \\ a_{66} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{11}^2 \\ \sigma_{22}^2 \\ \sigma_{33}^2 \\ \sigma_{22}\sigma_{33} \\ \sigma_{33}\sigma_{11} \\ \sigma_{11}\sigma_{22} \\ \sigma_{23}^2 \\ \sigma_{31}^2 \\ \sigma_{12}^2 \end{bmatrix} = 1, \quad (3.36)$$

that when expanding out Eq. 3.31 and relating common terms presents,

$$\begin{bmatrix} a_{11} \\ a_{22} \\ a_{33} \\ 2a_{23} \\ 2a_{31} \\ 2a_{12} \\ a_{44} \\ a_{55} \\ a_{66} \end{bmatrix} = \begin{bmatrix} G + H \\ F + H \\ F + G \\ -F \\ -G \\ -H \\ 2L \\ 2M \\ 2N \end{bmatrix} \equiv \mathbf{A} = \begin{bmatrix} G + H & -H & -G & 0 & 0 & 0 \\ -H & F + H & -F & 0 & 0 & 0 \\ -G & -F & F + G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{bmatrix}. \quad (3.37)$$

From this, expressions for the six coefficients (F , G , H , L , M , and N) can then be deduced by setting up a series of uni-axial loading scenarios where the yield point is unknown (assuming that the principal material axes align with the principal stress axis). Working through the loading scenario,

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (3.38)$$

it was shown that,

$$(\sigma_{11})^2 = \frac{1}{G + H}, \quad (3.39)$$

which following through for the other two principal axes yielded,

$$(\sigma_{22})^2 = \frac{1}{F + H} \quad (3.40)$$

$$(\sigma_{33})^2 = \frac{1}{F + G}. \quad (3.41)$$

These were then rearranged to give expressions for F , G , and H ,

$$F = \frac{1}{2} [(\sigma_{22})^{-2} + (\sigma_{33})^{-2} - (\sigma_{11})^{-2}] \quad (3.42)$$

$$G = \frac{1}{2} [(\sigma_{33})^{-2} + (\sigma_{11})^{-2} - (\sigma_{22})^{-2}] \quad (3.43)$$

$$H = \frac{1}{2} [(\sigma_{11})^{-2} + (\sigma_{22})^{-2} - (\sigma_{33})^{-2}]. \quad (3.44)$$

To determine expressions for the parameters located in the shear components of $\mathbf{A}$, scenarios where uni-axial loads orientated 45° in-between the three principal axes were set-up, thus resulting in three additional load scenarios denoted $'$, $''$, and $'''$, with orientations as shown in Figure 3.1. Coordinate systems were then superimposed on top of these scenarios so that the uni-axial load aligned with a basis vector. For example, $'$ would have a coordinate system that had its 22 principal axis aligned with the uni-axial load. This is equivalent to rotating a coordinate system that is aligned with the principal axes 45° in the anti-clockwise direction around the 11 principal axis. Consequently, loads in this coordinate system were mapped onto the principal axes through,

$$\boldsymbol{\sigma} = (\mathbf{Q}_\theta) \boldsymbol{\sigma}' (\mathbf{Q}_\theta)^\top, \quad (3.45)$$

where $\mathbf{Q}_\theta$ is a rotation matrix. Worked through, this gave,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0.5 & 0.5 \\ 0 & 0.5 & 0.5 \end{bmatrix}, \quad (3.46)$$

that when substituted into $\boldsymbol{\sigma}^\top (\mathbf{P}_{dev}) \mathbf{A} (\mathbf{P}_{dev}) \boldsymbol{\sigma}$ yields,

$$\left(\frac{\sigma'}{6} \right)^2 \begin{bmatrix} -2 \\ 1 \\ 1 \\ 3 \\ 0 \\ 0 \end{bmatrix}^\top \begin{bmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{bmatrix} \begin{bmatrix} -2 \\ 1 \\ 1 \\ 3 \\ 0 \\ 0 \end{bmatrix}. \quad (3.47)$$

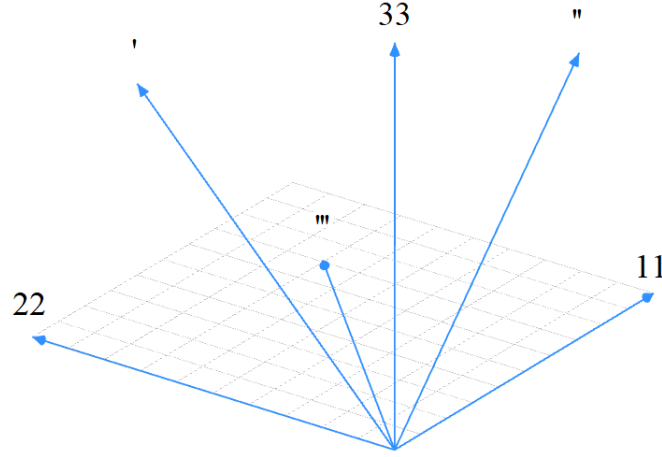


Figure 3.1: Orientation of ' ', ' ', and ' ' uni-axial loads (relative to principal axes) used to determine expressions for parameters in shear components of $\mathbf{A}$.

The following can then be set if the above is expanded out and the assumption is made that the stress field vector lies on the yield surface,

$$1 = 9(G + H + 2L) \left(\frac{\sigma'}{6} \right)^2. \quad (3.48)$$

This was then combined with Eq. 3.39 to give,

$$L = \left(\frac{2}{\sigma'} \right)^2 - \frac{1}{2} (\sigma_{11})^{-2}. \quad (3.49)$$

M and N were then also determined in a similar way,

$$M = \left(\frac{2}{\sigma''} \right)^2 - \frac{1}{2} (\sigma_{22})^{-2} \quad (3.50)$$

$$N = \left(\frac{2}{\sigma'''} \right)^2 - \frac{1}{2} (\sigma_{33})^{-2}. \quad (3.51)$$

Subsequently, the coefficients of the tensor that describe the anisotropic yield surface can now be expressed as functions of the effective flow stress along six different directions.

The yield surface is defined at the start of every time-step by prescribing a Johnson-Cook model to each of the six directions and using tensor $\mathbf{A}$. The Johnson-Cook model takes the form,

$$\sigma^Y = (A + B (\epsilon_{\text{eff}}^p)^n) (1 + C \ln(\epsilon^*)) (1 - (T^*)^m), \quad (3.52)$$

where the first term describes the increase in resistance to plastic flow as a result of plastic straining, the second the effect of strain-rate, and the third the effect of temperature. A , B , n , C , and m are non-physical material parameters, ϵ^* is a normalised effective strain-rate, and T^* is a homologous temperature. Parameters ϵ^* and T^* are defined respectively as,

$$\epsilon^* = \begin{cases} \frac{\dot{\epsilon}_{\text{eff}}^p}{\dot{\epsilon}_0^p} & \dot{\epsilon}_{\text{eff}}^p > \dot{\epsilon}_0^p \\ 1 & \dot{\epsilon}_{\text{eff}}^p \leq \dot{\epsilon}_0^p \end{cases} \quad (3.53)$$

$$T^* = \frac{T - T_r}{T_m - T_r}, \quad (3.54)$$

where $\dot{\epsilon}_0^p$ is a reference plastic strain-rate commonly chosen as 1 s^{-1} , and T_m and T_r are the material melting and reference temperatures, respectively.

Now that a description for an anisotropic yield surface has been established, the formulation of the plastic potential is discussed; this is complex as it depends on the contributions from each of the six Johnson-Cook models. In order to calculate it for a multi-axial load case, the parameter sets for the Johnson-Cook models were mapped to five independent (one per parameter) 6-D hyper-ellipsoids. As the effective parameter set at the beginning of the time-step (t_n) is dependent on the direction of the stress field vector on the yield surface, a scaling back is required. This scaling took the following form,

$$(x_i^{\text{eff}})_n = \frac{(\mathbf{s}_n)^\top (\mathbf{A}_{x_i}) \mathbf{s}_n}{\frac{3}{2} s_{ij} s_{ij}}, \quad (3.55)$$

thus giving values for the effective parameters for a given stress state. Here $(x_i^{\text{eff}})_n$ represent any one of the effective Johnson-Cook parameters (A , B , n , C , and m), and $\mathbf{s}_n$ is the deviatoric stress associated with the stress field vector, σ_n . The anisotropy tensor $\mathbf{A}_{x_i}$ is similar to

that defined earlier and took the form,

$$\mathbf{A}_{x_i} = \begin{bmatrix} G_{x_i} + H_{x_i} & -H_{x_i} & -G_{x_i} & 0 & 0 & 0 \\ -H_{x_i} & F_{x_i} + H_{x_i} & -F_{x_i} & 0 & 0 & 0 \\ -G_{x_i} & -F_{x_i} & F_{x_i} + G_{x_i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L_{x_i} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M_{x_i} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N_{x_i} \end{bmatrix}, \quad (3.56)$$

with the coefficients being determined using a similar methodology,

$$F_{x_i} = \frac{1}{2} [x_{i,22} + x_{i,33} - x_{i,11}] \quad (3.57)$$

$$G_{x_i} = \frac{1}{2} [x_{i,33} + x_{i,11} - x_{i,22}] \quad (3.58)$$

$$H_{x_i} = \frac{1}{2} [x_{i,11} + x_{i,22} - x_{i,33}] \quad (3.59)$$

$$L_{x_i} = 2x'_i - \frac{x_{i,11}}{2} \quad (3.60)$$

$$M_{x_i} = 2x''_i - \frac{x_{i,22}}{2} \quad (3.61)$$

$$N_{x_i} = 2x'''_i - \frac{x_{i,33}}{2}. \quad (3.62)$$

As the flow rule was assumed associative, the plastic strain increment is normal to the yield surface and parallel to the stress field vector. This meant the derived expressions will allow the determination of an effective plastic potential for a given time-step.

Through use of an associative flow rule, where the plastic deformation has proportionality to a plastic multiplier $\Delta\gamma$ (during yielding), as given by,

$$d\epsilon^p = d\gamma \frac{df}{ds}, \quad (3.63)$$

the rate of change of the plastic multiplier can be related to the equivalent plastic strain through the consistency condition and the principle of work equivalency to give,

$$d\epsilon_{\text{eff}}^p = -d\gamma \frac{\partial f_{Hill}}{\partial s_y}. \quad (3.64)$$

Coupling the discussed theory with that from Versino and Bennet, 2018 [50], yielded a framework that enabled a prediction of the plastic multiplier, $\Delta\gamma$, and consequently the effective plastic strain, $\Delta\epsilon_{\text{eff}}^p$, from a trial stress, σ_{tr} . Its formulation begins with taking the total strain increment, $\Delta\epsilon$, decomposing it into elastic, $\Delta\epsilon^e$, and plastic parts, $\Delta\epsilon^p$,

$$\Delta\epsilon = \Delta\epsilon^e + \Delta\epsilon^p = \Delta\epsilon^e + \Delta\gamma\mathbf{A}(\sigma_n + \mathbf{C}\Delta\epsilon^e), \quad (3.65)$$

multiplying both sides by $\mathbf{C}$, and rearranging to give,

$$\Delta\sigma_{tr} = \mathbf{C}\Delta\epsilon = \mathbf{C}\Delta\epsilon^e + \Delta\gamma\mathbf{C}\mathbf{A}(\sigma_n + \mathbf{C}\Delta\epsilon^e). \quad (3.66)$$

$\mathbf{C}$ was then eigendecomposed into $\mathbf{Q}_\mathbf{C}$ and $\mathbf{\Gamma}_\mathbf{C}$ such that $\mathbf{C} = \mathbf{Q}_\mathbf{C}\mathbf{\Gamma}_\mathbf{C}(\mathbf{Q}_\mathbf{C})^\top$. $\mathbf{Q}_\mathbf{C}$ is a matrix of horizontally catenated columnar eigenvectors and $\mathbf{\Gamma}_\mathbf{C}$ is a diagonal matrix of eigenvalues ordered such that each columns on-diagonal element sits in the same columnar position as its corresponding eigenvector does within $\mathbf{Q}_\mathbf{C}$. Substituting these into Eq. 3.66 meant it could be rewritten as,

$$\Delta\sigma_{tr} - \Delta\gamma\mathbf{C}\mathbf{A}\sigma_n = \mathbf{Q}_\mathbf{C}(\mathbf{\Gamma}_\mathbf{C} + \Delta\gamma\mathbf{\Gamma}_\mathbf{C}(\mathbf{Q}_\mathbf{C})^\top\mathbf{A}\mathbf{Q}_\mathbf{C}\mathbf{\Gamma}_\mathbf{C})(\mathbf{Q}_\mathbf{C})^\top\Delta\epsilon^e. \quad (3.67)$$

Two new variables $\mathbf{Q}'_\mathbf{C} = \mathbf{Q}_\mathbf{C}\sqrt{\mathbf{\Gamma}_\mathbf{C}}$ and $\mathbf{B} = (\mathbf{Q}'_\mathbf{C})^\top\mathbf{A}\mathbf{Q}'_\mathbf{C}$ that essentially represent a transformation of basis were then defined. Substituting these into the above yielded,

$$\Delta\sigma_{tr} - \Delta\gamma\mathbf{C}\mathbf{A}\sigma_n = \mathbf{Q}'_\mathbf{C}(\mathbf{I} + \Delta\gamma\mathbf{B})(\mathbf{Q}'_\mathbf{C})^\top\Delta\epsilon^e. \quad (3.68)$$

Given $\mathbf{B}$ is symmetric, another eigendecomposition was performed giving $\mathbf{B} = \mathbf{Q}_\mathbf{B}\mathbf{\Gamma}_\mathbf{B}(\mathbf{Q}_\mathbf{B})^\top$ that was substituted into Eq. 3.68 which was rearranged to,

$$\Delta\epsilon^e = (\mathbf{Q}'_\mathbf{C})^{-\top}\mathbf{Q}_\mathbf{B}[\mathbf{I} + \Delta\gamma\mathbf{\Gamma}_\mathbf{B}]^{-1}(\mathbf{Q}_\mathbf{B})^\top(\mathbf{Q}'_\mathbf{C})^{-1}[\Delta\sigma_{tr} - \Delta\gamma\mathbf{C}\mathbf{A}\sigma_n]. \quad (3.69)$$

$\Delta\epsilon^e$ was then multiplied by $\mathbf{C}$ ($= \mathbf{Q}_\mathbf{C}\mathbf{\Gamma}_\mathbf{C}(\mathbf{Q}_\mathbf{C})^\top = \mathbf{Q}'_\mathbf{C}(\mathbf{Q}'_\mathbf{C})^\top$) to give,

$$\begin{aligned} \Delta\sigma = \mathbf{Q}'_\mathbf{C}\mathbf{Q}_\mathbf{B}[\mathbf{I} + \Delta\gamma\mathbf{\Gamma}_\mathbf{B}]^{-1}(\mathbf{Q}_\mathbf{B})^\top(\mathbf{Q}'_\mathbf{C})^{-1}\Delta\sigma_{tr} - \\ \mathbf{Q}'_\mathbf{C}\mathbf{Q}_\mathbf{B}[\mathbf{I} + \Delta\gamma\mathbf{\Gamma}_\mathbf{B}]^{-1}(\mathbf{Q}_\mathbf{B})^\top(\mathbf{Q}'_\mathbf{C})^\top\mathbf{A}\Delta\gamma\sigma_n. \end{aligned} \quad (3.70)$$

Through substitution of $(\mathbf{Q}'_{\mathbf{C}})^{\top} \mathbf{A} = \mathbf{B} (\mathbf{Q}'_{\mathbf{C}})^{-1}$, and defining $\mathbf{\Lambda} = \mathbf{Q}'_{\mathbf{C}} \mathbf{Q}_{\mathbf{B}}$ and $\tilde{\boldsymbol{\sigma}} = \mathbf{\Lambda}^{-1} \boldsymbol{\sigma}$ (essentially creating a second shift in coordinate system), an expression for $\tilde{\boldsymbol{\sigma}}_n + \Delta \tilde{\boldsymbol{\sigma}}_{tr}$ was arrived at,

$$\tilde{\boldsymbol{\sigma}}_n + \Delta \tilde{\boldsymbol{\sigma}}_{tr} = [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}] (\tilde{\boldsymbol{\sigma}}_n + \Delta \tilde{\boldsymbol{\sigma}}). \quad (3.71)$$

Considering $\tilde{\boldsymbol{\sigma}}_{n+1} = \tilde{\boldsymbol{\sigma}}_n + \Delta \tilde{\boldsymbol{\sigma}}$ and $\tilde{\boldsymbol{\sigma}}_{tr} = \tilde{\boldsymbol{\sigma}}_n + \Delta \tilde{\boldsymbol{\sigma}}_{tr}$ resulted in,

$$\boldsymbol{\sigma}_{n+1} = \mathbf{\Lambda} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \mathbf{\Lambda}^{-1} \boldsymbol{\sigma}_{tr}. \quad (3.72)$$

Given the yield function has the form,

$$f \equiv \frac{1}{2} (\mathbf{s}^{\top} \mathbf{A} \mathbf{s}) = \frac{1}{2} (\boldsymbol{\sigma}^{\top} \mathbf{A} \boldsymbol{\sigma}) \leq 1, \quad (3.73)$$

Yielding at t_{n+1} can then be determined by evaluating,

$$f = \frac{1}{2} (\tilde{\boldsymbol{\sigma}}_{tr})^{\top} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \mathbf{\Lambda}^T \mathbf{A} \mathbf{\Lambda} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \tilde{\boldsymbol{\sigma}}_{tr}. \quad (3.74)$$

As it can be shown that $\mathbf{\Lambda}^T \mathbf{A} \mathbf{\Lambda} = \mathbf{\Gamma}_{\mathbf{B}}$, this resulted in,

$$f = \frac{1}{2} (\tilde{\boldsymbol{\sigma}}_{tr})^{\top} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \mathbf{\Gamma}_{\mathbf{B}} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \tilde{\boldsymbol{\sigma}}_{tr}. \quad (3.75)$$

Defining $\boldsymbol{\kappa} = [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1} \mathbf{\Gamma}_{\mathbf{B}} [\mathbf{I} + \Delta \gamma \mathbf{\Gamma}_{\mathbf{B}}]^{-1}$ then produced,

$$f \equiv \frac{1}{2} (\mathbf{s}^{\top} \mathbf{A} \mathbf{s}) = \frac{1}{2} (\tilde{\boldsymbol{\sigma}}_{tr})^{\top} \boldsymbol{\kappa} \tilde{\boldsymbol{\sigma}}_{tr}. \quad (3.76)$$

Here $\boldsymbol{\kappa}$ is diagonal with its terms given by,

$$\kappa_{ii} = \frac{(\Gamma_B)_{ii}}{(1 + \Delta \gamma (\Gamma_B)_{ii})^2}, \quad (3.77)$$

where $(\Gamma_B)_{ii}$ is the i^{th} diagonal term of $\mathbf{\Gamma}_{\mathbf{B}}$. The criteria for yielding can then be checked and if found to occur, a suitable value for $\Delta \gamma$ can be iteratively converged upon using the consistency condition to ultimately determine the equivalent plastic strain.

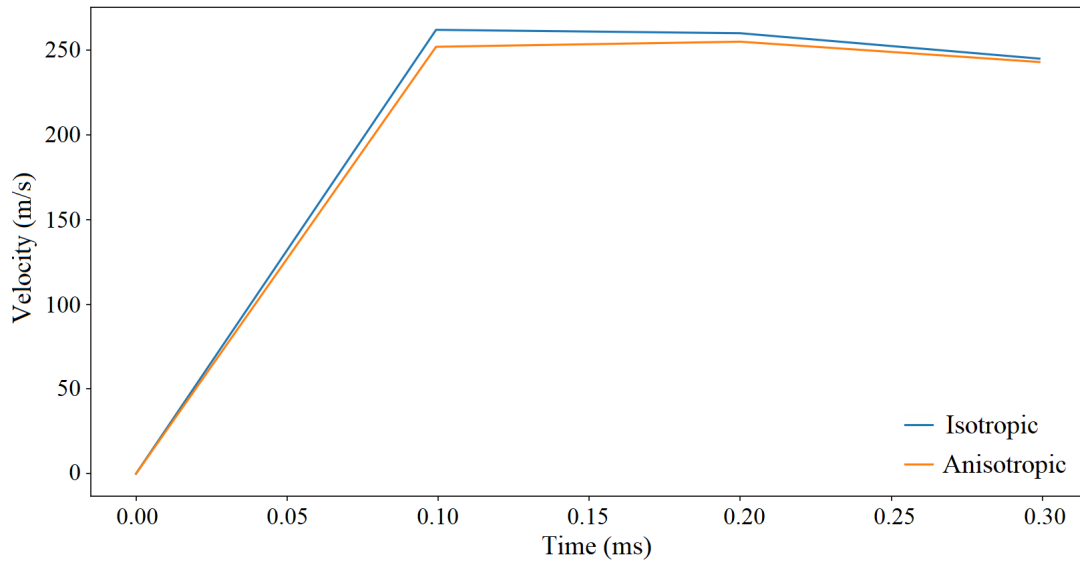


Figure 3.2: Comparison of leading node velocity profiles from blast-loaded WE43-T6 plate simulations that called upon isotropic and anisotropic-based constitutive models. The anisotropic model was observed to predict a reduction of ~ 10 m/s ($\sim 4\%$) in the peak velocity.

3.3.2 Application to blast-loaded WE43-T6 plate analysis

Using the anisotropic plasticity model described thus far, the blast-loaded WE43-T6 plate analysis conducted in Chapter 2 was re-run but with the added consideration of the plate's transversely isotropic mechanical properties. To do so, only the constitutive model of the FEA model needed substituting. All parameters were kept the same except for those required to predict the material's out-of-plane strain-hardening. Here, the values shown in Table 3.1 were used. Where data was not available (i.e. two of the primed vectors in Figure 3.1 if the plate was assumed to exhibit transversely isotropic characteristics), a linear interpolation was assumed ($\mathbf{X}' = \frac{\mathbf{X}_{22} + \mathbf{X}_{33}}{2}$). As no data that characterised the material under tension was available, it was assumed that the material had the same constitutive behaviour in tension as compression even though slight variations were seen at quasi-static strain-rates for other WE43 tempers [9, 36]. Despite this, it was still believed that the accuracy of the model's prediction would be improved as a result of the additional consideration of anisotropy.

Figure 3.2 compares the peak velocity of the leading node from blast simulations that called upon the isotropic and anisotropic-based constitutive models. The anisotropic-based constitutive model predicted a small reduction in velocity throughout, with a ~ 10 m/s ($\sim 4\%$) drop in peak velocity being observed. This was not unexpected as strength was added in the normal direction.

Parameters	In-plane	Out-of-plane	Units
A	0.140	0.189	GPa
B	0.340	0.244	GPa
n	0.347	0.264	-
C	0.0046	0.0043	-

Table 3.1: Anisotropic Johnson-Cook Parameters [13] used in Eq. 3.52 for blast-loaded magnesium alloy WE43-T6 plate analysis.

3.3.3 Modification to include tension-compression asymmetry

The theory described in the previous section is sufficient to describe anisotropy, however it was unable to predict the tension-compression asymmetry of sheet AZ31B-O (this included the observed sigmoid flow stresses with in-plane compression). As such, the ISML model was further modified to incorporate it. Being able to predict the sigmoid flow stress was of particular interest as it stemmed directly from twinning (a microscale phenomenon), making it ideal for showcasing the meso- to macro-scale-bridging capability presented in the following chapter.

Tension-compression asymmetry was implemented using a simplified approach (due to time constraints) that evaluated volumetric strain, more rigorous implementations would be grounded in more sophisticated J3-plasticity theory. To establish if a material point is under compression or tension the volumetric strain for the current time-step was determined using,

$$d\epsilon_V^n = d\epsilon_1^n + d\epsilon_2^n + d\epsilon_3^n. \quad (3.78)$$

Comparing this to the volumetric strain of the previous time-step facilitates the following categorisation of load type,

$$\text{load type} = \begin{cases} \text{tension,} & \text{if } \epsilon_V^n > 0, \\ \text{compression,} & \text{if } \epsilon_V^n < 0. \end{cases} \quad (3.79)$$

Through this characterisation, different hardening laws could be invoked as required for tensile or compressive loading. For example, if an element is classified as being under tension for an arbitrary time-step, then the Johnson-Cook hardening law (Eq. 3.52) could be called upon. Whereas, if the element is under compression, the following hardening rule (as proposed

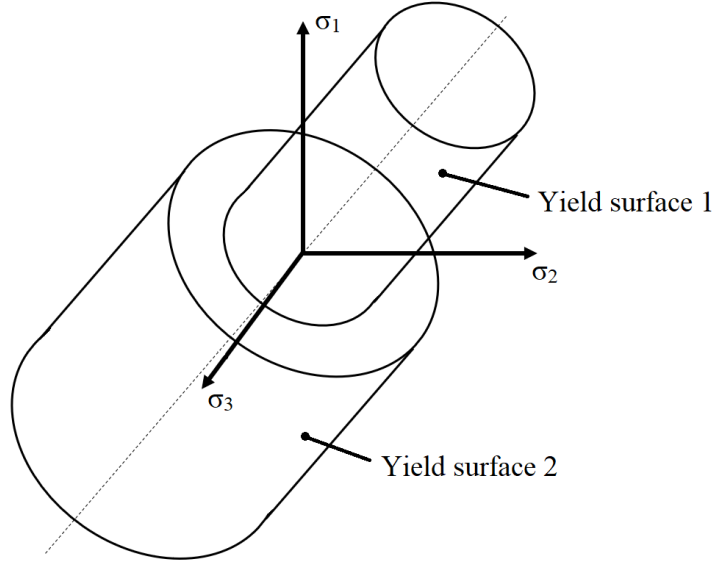


Figure 3.3: Conceptual representation of yield surface for an arbitrary plastic strain (ϵ_{eff}^p) for the developed two hardening law-based constitutive model. The yield surface shown reflects isotropic hardening, whereas anisotropic has been implemented. This would see the circular yield surface replaced by one of irregular shape.

by Kurukuri et al., 2014, [8]) could be used to give the desired sigmoid-shaped flow stress with in-plane compression,

$$\sigma^Y = \frac{K_1 K_2 - \frac{K_3 (\epsilon_{\text{eff}}^p)^{K_4}}{1 - K_5 \dot{\epsilon} - K_6}}{K_2 + (\epsilon_{\text{eff}}^p)^{K_4}}. \quad (3.80)$$

Here, K_1 is the initial yield strength, K_2 controls the extent of the plateau associated with twinning, K_3 is a scaling parameter that controls the slip-dominated region, K_4 controls the point of inflection, and parameters K_5 and K_6 set strain-rate dependencies.

Tension-compression asymmetry implemented in this manner may not be representative of the material system on a whole as both hardening laws are dependent on the effective plastic strain (ϵ_{eff}^p) and the strain-rate ($\dot{\epsilon}$). So, for example, if the plate was initially loaded in tension, it would harden with plastic strain following the Johnson-Cook law. However, as the measure of plastic strain increased, the yield surface associated with compression, as defined by Eq. 3.80, would still evolve, even though the criteria to activate the mechanisms that lead to the observed sigmoid flow stress were not met. This results in the formation of a two part yield surface like that presented in Figure 3.3. This was not deemed problematic for the presented example as the blast resistance of the plate is primarily driven by the initial rise (i.e. not associated with reverse

loading) which is where the majority of plastic strain occurred. Therefore, this implementation comes with the caveat that it may not provide accurate predictions for analyses involving more substantial reverse loading. Another issue that became apparent on inspection of Figure 3.3 is the discontinuity on the deviatoric plane associated with pure shear loading. Further work would be required if this load type was to be considered. Nevertheless, no pure shear loads were encountered in the example, so it was not believed a cause for concern. Regardless of these shortcomings, the developed model was still believed to better predict the blast-load response of AZ31B-O plate compared to FEMs utilising just the isotropic Johnson-Cook model.

A more complete physically-based constitutive model would see the strain-hardening due to dislocation interactions being separated from the hardening due to twinning; this thesis proposed exactly this through the use of physically-based lower length-scale CPFEMs and data-driven approaches (detailed in Chapters 4 and 5). Adopting lower length-scale models also presented the opportunity to address the issue that not all compressed orientations yielded sigmoid flow stresses. Figure 1.1 shows that ND compressed specimens exhibited power-law hardening (consistent with the non-activation of extension twinning), which the currently developed model would not be able to predict (attempts to address it are presented in Chapter 5). Nevertheless, as most of the plate's blast resisting characteristics comes from its in-plane strength, the fact this orientation dependence with compression was not captured was deemed not too problematic.

Considering the description in Section 3.3.1, an effective yield function $f_{\text{eff}}((\epsilon_{\text{eff}}^p)_n, \Delta\epsilon_{\text{eff}}^p, \Delta t, T)$ needed to be formulated for the hardening law, Eq. 3.80, for a given set of K_i^{eff} parameters to compute $\frac{\partial f_{\text{eff}}}{\partial(\Delta\epsilon_{\text{eff}}^p)}$. This expression was arrived at by differentiating Eq. 3.80 with respect to ϵ_{eff}^p ,

$$\alpha = K_1 K_2, \beta = K_2 + (\epsilon_{\text{eff}}^p)^{K_4}, \beta' = K_4 (\epsilon_{\text{eff}}^p)^{K_4-1}, \gamma = \frac{K_3 (\epsilon_{\text{eff}}^p)^{K_4}}{1 - K_5 (\dot{\epsilon}_{\text{eff}}^p)^{-K_6}} \quad (3.81)$$

$$\gamma' = \frac{K_3 \beta'}{1 - K_5 (\dot{\epsilon}_{\text{eff}}^p)^{-K_6}} - \frac{K_3 (\beta - K_2)}{(1 - K_5 (\dot{\epsilon}_{\text{eff}}^p)^{-K_6})^2} (K_5 K_6 (\dot{\epsilon}_{\text{eff}}^p)' (\dot{\epsilon}_{\text{eff}}^p)^{-K_6-1}) \quad (3.82)$$

$$\text{where } (\dot{\epsilon}_{\text{eff}}^p)' = 0 \text{ gives } \gamma' = \frac{K_3 \beta'}{1 - K_5 (\dot{\epsilon}_{\text{eff}}^p)^{-K_6}}. \quad (3.83)$$

$$\text{Finally } \sigma^Y = \frac{\alpha - \gamma}{\beta}, \text{ yields } (\sigma^Y)' = -\frac{\beta' \alpha}{\beta^2} - \frac{\gamma'}{\beta} + \frac{\gamma \beta'}{\beta^2}. \quad (3.84)$$

The implementation of this hardening law into the tension-compression considered generalised eigenspace radial-return mapping algorithm was verified by comparing the predictions of a FEM allocated this constitutive model against those of an analytical model.

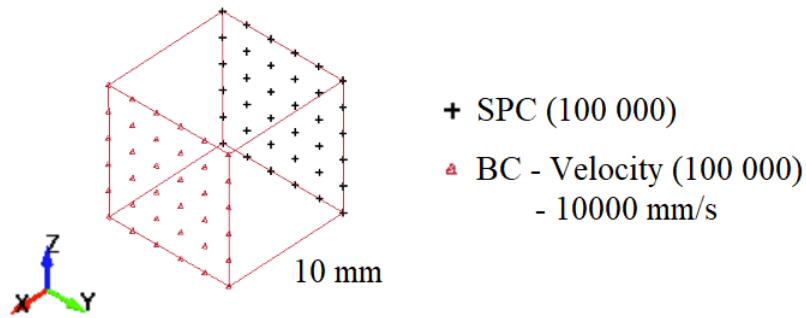


Figure 3.4: Schematic showing mesh and boundary conditions of FEM used to verify sigmoid hardening law implementation.

The models were allocated the parameters presented in Table 3.2, with the FEM being prescribed the boundary conditions shown in Figure 3.4. Figure 3.5 shows good agreement between the two models' predictions of the yield stress with plastic strain. The oscillations at the onset of plasticity were believed to be due to the the shock-wave interfering with itself within the body, and the slight deviation observed due to the distribution of the velocity field throughout the mesh that resulted from how the boundary condition was applied (the analytical model was ideal as it considers the stress to be uniform in the volume). Figure 3.6 supports these claims as it shows the smooth application of velocity to node 1428 on the outer face, and the resulting oscillating velocity profile of the unconstrained interior node 1426. The interior node was also observed to converge to a lower velocity compared to that of the constrained exterior node, showing a distribution in velocity exists throughout.

Parameter	Value	Unit
K1	114.2	MPa
K2	5.3×10^{-5}	-
K3	12.1	-
K4	3.8	-
K5	1.02	-
K6	3.5×10^{-4}	-
$\dot{\epsilon}_{\text{eff}}^p$	1000.0	s^{-1}

Table 3.2: Parameters [8] allocated to analytical and FEMs for verification study.

To assess the implementation of tension-compression asymmetry, the above FEM was adapted to consist of two uni-axial tests as shown in Figure 3.7 (one to investigate tension, the other

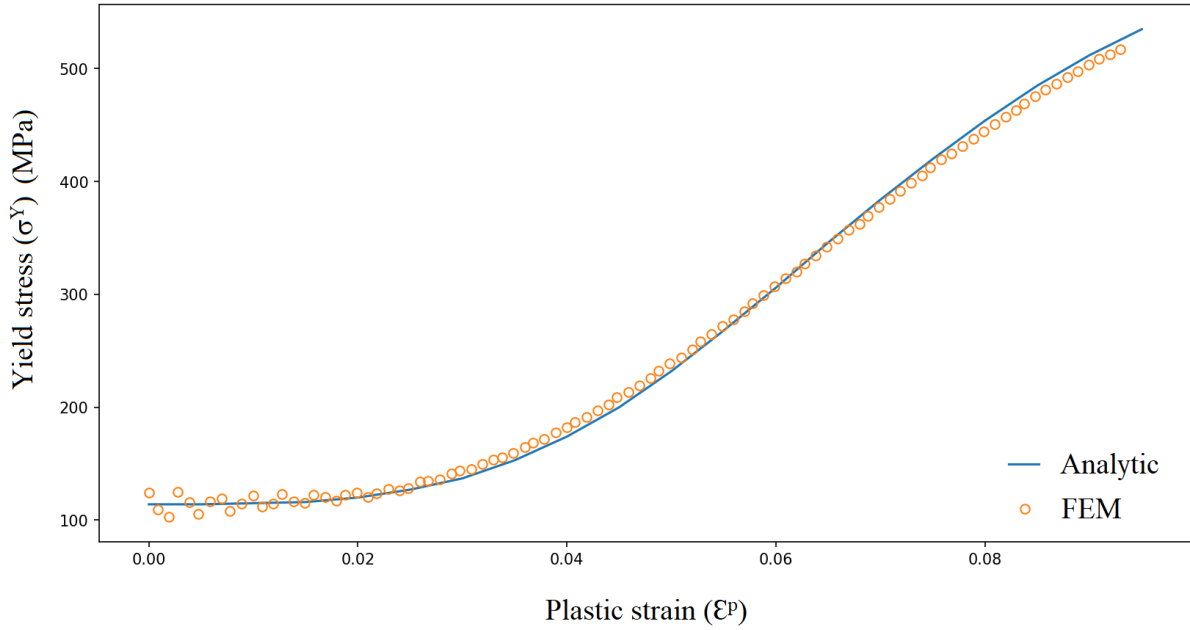


Figure 3.5: Comparison of FEM predicted yield stress with plastic strain to that of the sigmoid hardening law analytical model. Close agreement verifies implementation. Oscillations during the onset of plasticity are believed to be due to the shock-wave interfering with itself. Slight deviation observed is believed to be due to distribution of velocity field throughout mesh due to application of boundary condition.

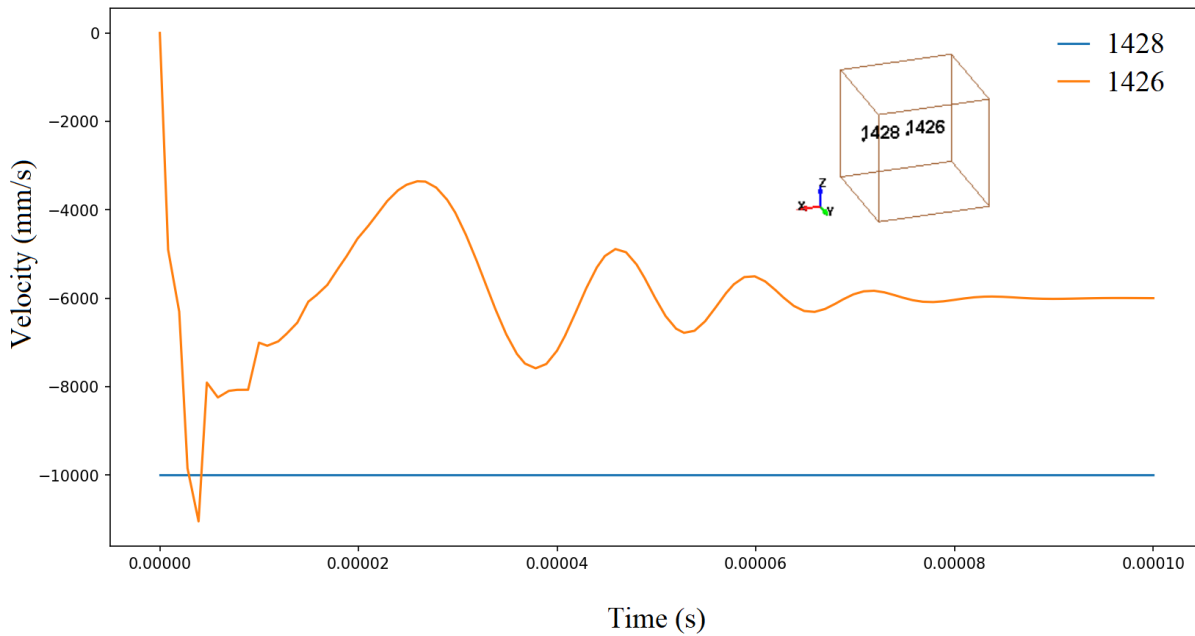


Figure 3.6: Velocity profiles for the shown selected nodes. The unconstrained node was observed to have an oscillating velocity profile, and to converge to a lower velocity. This shows a distribution in velocity existed throughout the mesh.

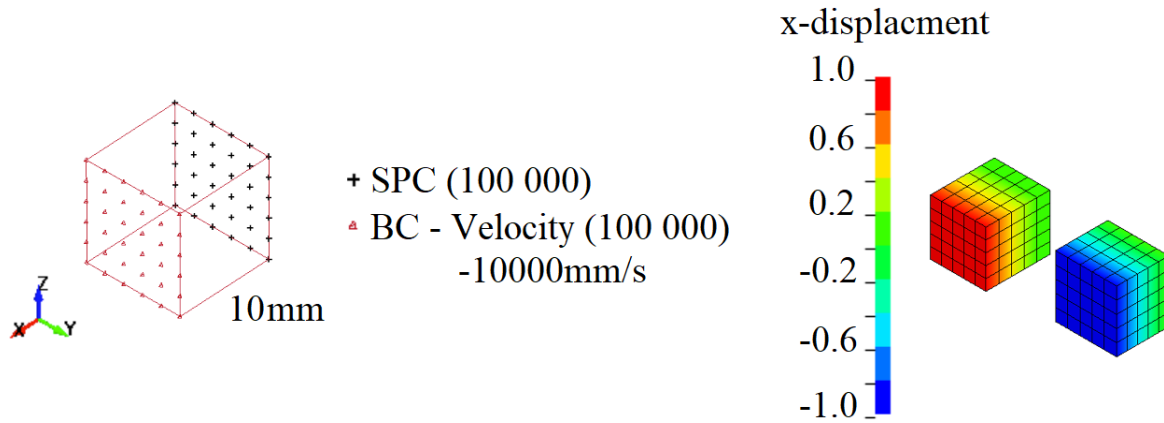


Figure 3.7: FEMs, boundary conditions, and displacements used to investigate implementation of tension-compression asymmetry.

Parameters	Value	Units
A	0.150	GPa
B	0.300	GPa
n	0.4	-
C	0.1	-
Plastic strain failure	0.2	-

Table 3.3: Johnson-Cook parameters used in tension-compression asymmetry implementation verification study. These were determined by fitting Eq. 3.52 to the curves presented in Figure 1.1.

compression). The constitutive model was allocated the parameters detailed in Tables 3.2 and 3.3. The resulting filtered true stress-strain curves (presented in Figure 3.8) show good agreement with the analytically predicted yield stress with plastic strain, therefore verifying its implementation.

Finally, the rate-dependence of the sigmoid hardening law-based constitutive model was verified by comparing the stress-strain response of FEMs allocated it against analytical predictions of the yield stress with plastic strain. The same two bodies as the last verification study were used, but this time they were compressed at 10 s^{-1} and 1000 s^{-1} , respectively. Both sets of models again had their predictions compared (as shown in Figure 3.9). Good agreement was observed, with yield stress increasing with strain-rate and slight deviations being noted (believed to be due to the same reasons as already discussed). Now that the model has been verified to predict the required tension-compression asymmetry, its utilisation in the blast-loaded AZ31B-O plate analysis was presented next.

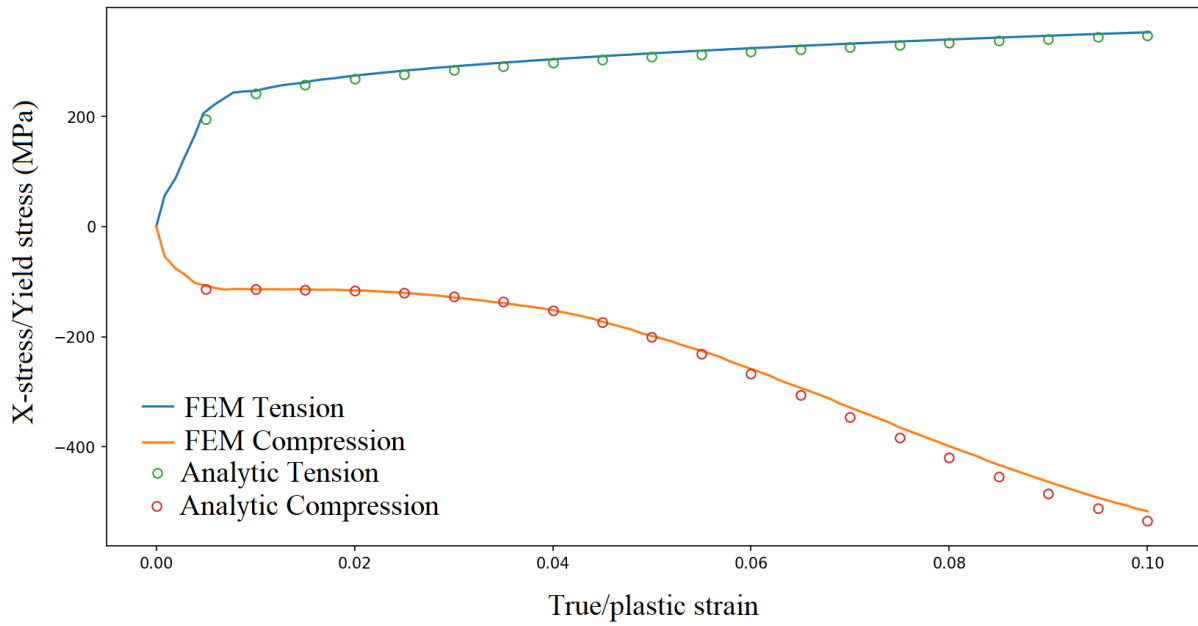


Figure 3.8: True stress-strain curves predicted by FEM compared against analytically predicted yield stress. The good agreement verifies the implementation of tension-compression asymmetry. A moving average filter was applied to smooth out the oscillations at the onset of plasticity.

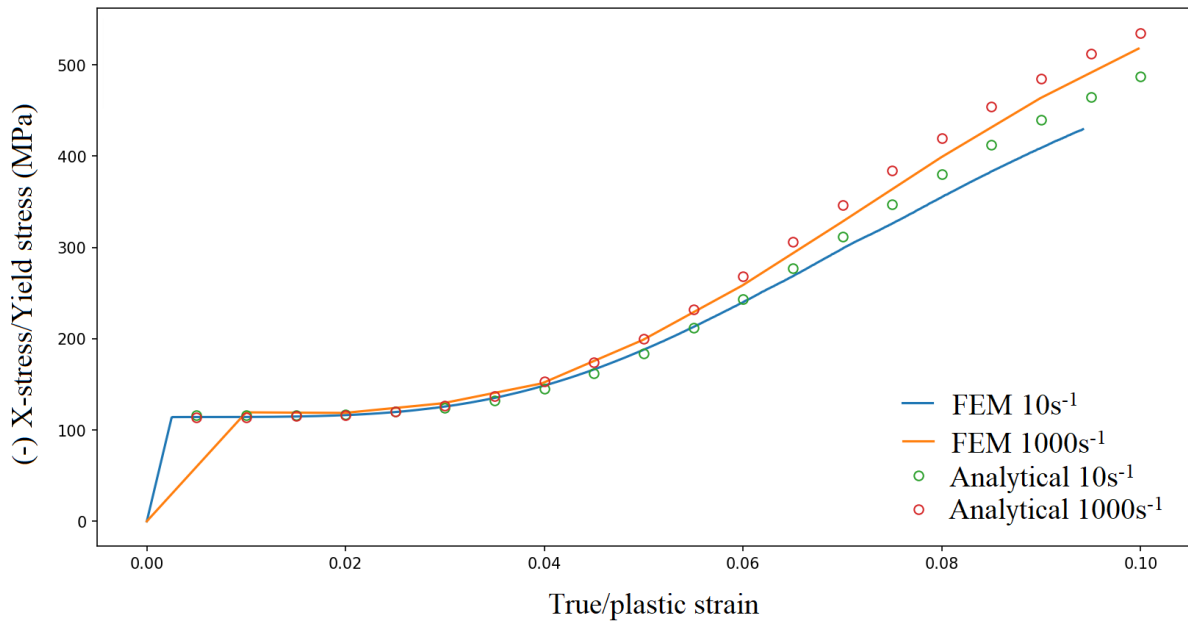


Figure 3.9: True stress-strain curves from FEM compared against analytically predicted yield stress for the shown strain-rates. The good agreement verifies the implementation of rate-dependence. The slight deviation is believed to be due to the non-ideal conditions of the FEMs.

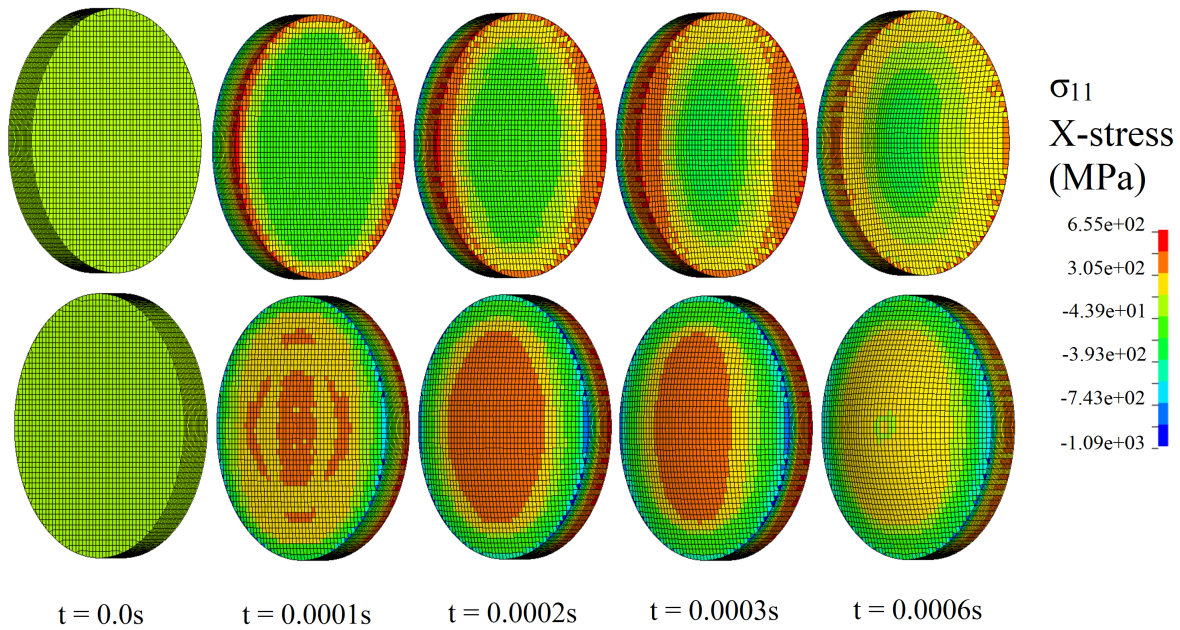


Figure 3.10: Sequence of images showing the evolving deformation and resulting X-stress (MPa) of blast-loaded AZ31B-O plate.

3.3.4 Utilisation of modified ISML anisotropic Johnson-Cook plasticity model in blast-loaded AZ31B-O plate study

Now that the ISML anisotropic Johnson-Cook plasticity model has been modified to exhibit the tension-compression asymmetry seen in AZ31B-O sheet, the blast-loaded plate analysis was run with it. The parameters used were those shown in Tables 3.2 and 3.3, with the evolution of X-stress with deformation, and the leading node velocity profile compared against that from the anisotropic WE43-T6 plate analysis being shown in Figures 3.10 and 3.11, respectively. The shock severity was shown to be ~ 10 m/s ($\sim 4\%$) higher for the AZ31B-O plate. However, no fracture was observed within the same evaluated time-period (occurred at $80\mu\text{s}$), and when it did occur its features were different, as shown in Figure 3.12. This brings into question the methodology used to predict fracture, however, as the main focus of this thesis was to develop microstructure-aware constitutive models, fracture will be discussed only once this capability has been presented. Therefore, if this *delayed* fracture in AZ31B-O plate was assumed accurate, the trade-off for increased shock severity could even be considered desirable. However, putting this digression aside, as the mechanisms driving the strength of the plate are primarily found at the micro- and meso-scales, the performance of the plate could be improved through their identification and design. As such, it is exactly this that the next chapter strove to facilitate.

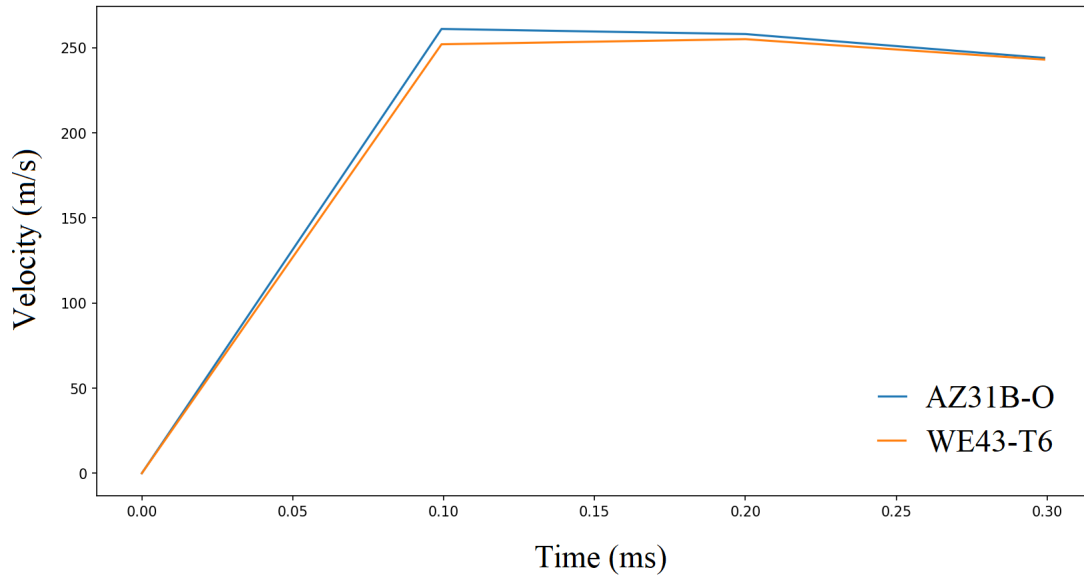


Figure 3.11: Comparison of leading node velocity profiles from blast-loaded AZ31B-O and WE43-T6 plate analyses. WE43-T6 plate was observed to have a peak velocity of ~ 10 m/s ($\sim 4\%$) lower than that of AZ31B-O plate.

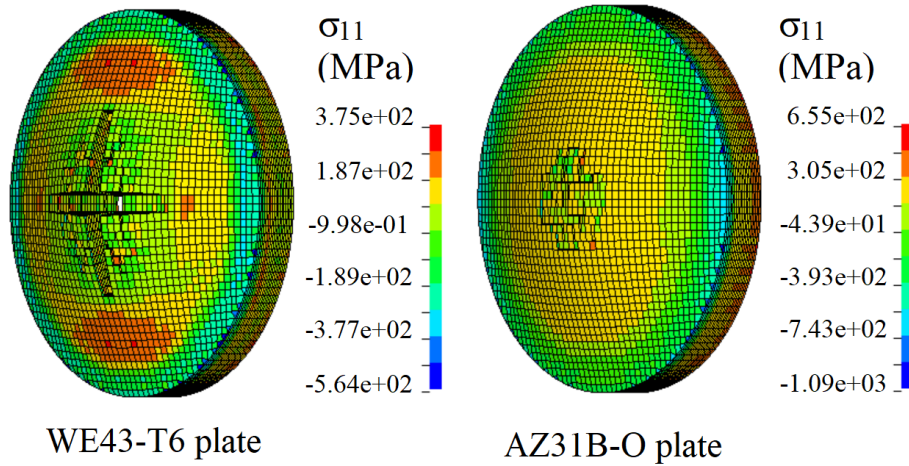


Figure 3.12: Comparison of fracture characteristics observed in plate WE43-T6 and AZ31B-O blast analyses.

3.4 Chapter conclusion

This chapter initially set out to answer the questions listed below,

- Can constitutive models that predict the flow stresses of WE43-T6 plate and AZ31B-O sheet be developed to enable component-level analyses as these are not currently available in commercial code?
- Could a link between lower length-scale models and component-level constitutive models be

established where the effect of altering micro- and meso-scale features (such as solutes and precipitates, texture, grain size distribution, etc.) influence bulk mechanical properties?

- Would it be possible to design these micro- and meso-scale features to improve the performance of a component for its specific application?

In doing so, a constitutive model was identified that could capture the anisotropy of WE43-T6 plate. This model was subsequently modified to enable prediction of the tension-compression asymmetry and sigmoid flow stresses with in-plane compression exhibited by AZ31B-O sheet. These models were then showcased by re-running the blast-loaded plate analyses from the previous chapter, thereby addressing the first question. The second and third questions were not answered in this chapter, however, arguments were made throughout supporting the need for them to be. Furthermore, the following question from those initially posed in Chapter 1 was also identified as becoming relevant,

- Is it possible to generate approximations of the full-field stress heterogeneity that develops at the mesoscale from bulk mechanical characterisations of a material using CPFEMs?

It is hoped that by first focusing on this question, models will become available to aid with the identifying and subsequent designing of mesoscale mechanisms to achieve bulk-level mechanical properties that improves a component's performance for its specific application (hence providing answers to the second and third questions). The proceeding chapter solely focuses on developing and homogenising CPFEMs, and starts with a chapter overview that is thereafter followed by a review of the state of research in this area, and a description of the methodology developed.

4

Toward micro- and meso-scale considered modelling approaches

4.1 Chapter overview

The last chapter saw the development of plasticity models required to reproduce the experimentally measured bulk-level mechanical behaviour of WE43-T6 and AZ31B-O plates. These models, however, could only be used in component-level analyses, and did not offer insight into the mechanisms underpinning bulk mechanical properties. In this chapter, explicitly-run full-field CPFEMs, based on the main deformation mechanisms observed in magnesium alloy crystals (i.e. dislocation glide and twinning), are formulated and homogenised to facilitate the hierarchical scale-bridging parameterisation of the aforementioned plasticity model, thus addressing the questions posed at the end of the last chapter. In order to facilitate this, an in-house polycrystalline generating algorithm was used to produce statistically equivalent models of the microstructure, and a novel explicitly-run crystal plasticity-based user-subroutine was developed, that homogenised twinning via a rate of mixtures rule and considered its contribution

to hardening through a Hall-Petch-based hardening law. As each CPFEM was seeded from a unique polycrystalline realisation that was statistically equivalent to that experimentally measured, the opportunity to quantify the uncertainty arising from the aleatoric nature of mesostructure presented itself. This was achieved through the creation of a distribution via the characterisation of an ensemble of CPFEMs. The characterisation saw flow stresses fitted to the appropriate hardening laws of the component-level plasticity models, with the population being deemed a distribution once measures in second order statistics converged. Having a distribution of parameters to subsequently seed the component-level plasticity models with presented the opportunity for stochastic-based modelling approaches. These are however beyond the scope of this chapter and are discussed in more detail in the following one. What ensues is a review of the current state of research in crystal plasticity modelling, the establishing of the necessary theory for creating CPFEMs, and the uncertainty quantification resulting from their homogenisation and characterisation.

4.2 State of research

Modelling approaches that develop bulk-level constitutive laws from mesoscale features have been extensively developed for magnesium alloys [9, 13, 36, 51]. For example, Bhattacharyya et al., 2016, [36] completed a study to determine the role intergranular deformation modes, such as slip and twinning, play to render WE43-T5 plate more isotropic despite its strong texture. This in-depth analysis was completed using the polycrystal rate-independent elasto-plastic self-consistent (EPSC) model [52] that makes use of the Eshelby inclusion problem [53]. This problem defines a grain by its orientation and considers it an anisotropic elasto-plastic ellipsoidal inclusion embedded in a homogeneous anisotropic effective medium representing the polycrystalline aggregate. Such models are derived from the theory of relating the activation of slip and twin systems to granular flow stresses [54] and thus capture crystalline heterogeneity.

The EPSC model as well as other Taylor-type models (based on similar theory as the EPSC model) are commonly used in multi-scale frameworks [9, 51, 55–57] to predict bulk material properties from mesostructure features. For example, Ardeljan et al., 2016, [51] made use of a two-level homogenisation scheme where the first level used a Taylor-type model to relate the contribution from single crystals to the polycrystal mesoscale, and the second level used an implicit finite element approach to relate the mesoscale to the material bulk; effectively, slip

and twinning in single crystals are captured in the Taylor-type polycrystal homogenisation whose constitutive laws are then embedded into the integration points of the macroscale finite element model. Taylor-type model approaches, however, do not take the heterogeneity of the plastic strain field in a polycrystal into account as they apply a constant deformation gradient to the domain and consequently overpredict plastic flow stresses [58]. Bhattacharyya et al., 2016, [36] however stated that the second level of homogenisation relaxes this iso-strain constraint. Further limitations of these approaches include the predicted intensities of the orientation distribution functions (ODF) being quite poor when compared to experimentally derived textures [59] meaning they should not be relied upon for the prediction of the evolution of texture with strain [58]. Also, the fact that grain boundaries are not discretely considered is another limitation as it is there that localised hardening and fracture often occur [60, 61]. These reasons highlight short-comings associated with using mean-field approaches (i.e. EPSC, VPSC, and Taylor-type models) to predict polycrystalline stress-strain behaviour and texture evolution. As such, full-field approaches are discussed next.

Peirce et al., 1982, [62] formulated crystal plasticity theory into the finite element method therefore allowing the heterogeneous stress fields in a polycrystal to be predicted in a weak form through the principle of virtual work. Consequently, crystal-plasticity finite element models (CPFEM) that use constitutive laws to describe single crystal deformation, have become commonplace when studying full-field stresses or texture evolution of polycrystals [19, 22–26, 62, 63] as they are better suited for predicting stress and strain heterogeneity for given boundary conditions, especially with the advent of polycrystalline generating algorithms (e.g. DREAM3D [64], Neper [65], VorTeX [66]). However, predictions of a material’s bulk properties using these models require careful sizing of the polycrystalline structures into representative volume elements (RVEs), and constraining simulations as boundary value problems (effectively homogenising localised heterogeneity). This is not necessary for the mean-field approaches discussed earlier as their analytical nature automatically satisfies the Hill-Mandel condition [67] required for transitioning from a meso-heterogeneous to a macro-homogenised medium.

Full-field homogenisation (through RVE sizing) or mean-field approaches are essential when investigating the effects of mesostructure on components as wholesale consideration of a large component’s mesostructure in a FEM is not feasible due to the large number of degrees of

freedom which require solving. Approaches that perform homogenization using lower length-scale FEMs to then pass information to larger length-scale ones are considered hierarchical. Alternatively, full-field CPFEMs can be used to inform constitutive behaviour at the integration points in an FEM. Such an approach is coined FE^2 [7] and is categorised as concurrent [68]. Another concurrent-based approach could see spatial refinements, that add finer resolution details to specific portions of a component model that require an increased level of detail (based on *ad-hoc* defined conditions) [69], conducted on-the-fly as the simulation progresses.

Implicit, explicit, and fast Fourier transform (FFT)-based spectral solvers have been used in literature to solve mesostructural-based full-field boundary value problems [19, 20, 23, 26], with each offering particular benefits with their use. Implicitly solved CPFEMs [22, 24, 25] are favoured in literature. Although, their large time-steps make them unfavourable for rate-dependent analyses, and, as such, ill-suited for what's required in this thesis. FFT-based spectral solvers are attractive as they are mesh-free, meaning that the difficulties associated with meshing, and the large number of degrees of freedom to be solved by the full-field calculation are avoided [19]. However, as the intention of this work was to ultimately support the development of an explicit-explicit time-integrated spatial concurrent multi-scale FEA architecture that facilitates microstructure consideration in components subjected to high-rate large deformation loading, efforts were first made to develop the full-field homogenisation capability using an explicit solver. Using this type of solver also presented the opportunity to incorporate intergranular cracking as proposed by Falco et al., 2024, [70] potentially leading to exciting new facets of research.

Benefits of both mean-field and full-field approaches have been discussed, with the ability to utilise VPSC models in component-level FEMs, and being able to model full stress field heterogeneities, being the most forthcoming, respectively. As mean-field approaches have been extensively studied, and a gap in literature seems to exist on the subject of considering mesoscale stress field heterogeneities in component-level analyses, emphasis was placed on developing the latter. Consequently, a hierarchical architecture that utilised explicitly-run CPFEMs and polycrystalline structures sized into RVEs is proposed that in turn was used to parameterise the plasticity models detailed in Section 3 (see the Chapter 5). As each CPFEM realisation has its own unique heterogeneous stress field arising from the variability of polycrystalline structures, the opportunity to quantify uncertainty also presented itself and is discussed later in

this chapter. What follows is a description of the work that went into generating the statistically representative numerical models of mesostructure.

4.3 Generation of statistically representative numerical models of polycrystalline structures

To produce representative numerical models of polycrystalline structures, measurements first need to be made. Experimental techniques that enable this can be classified into two categories, *non-destructive* or *destructive*. An example of a *non-destructive* technique is X-ray diffraction microscopy that generates 3D characterisations of polycrystalline-based materials [71]. An example of a *destructive* technique is focused-ion-beam scanning-electron microscopy (FIB-SEM) that involves serially sectioning a material at given intervals and then producing 2D SEM images to infer 3D metrics [72]. These characterisations in-turn can be used to seed the generation of representative numerical models of mesostructure through *deterministic* or *statistical* approaches. Approaches categorised under *deterministic* aim to build *digital twins* of polycrystalline topologies, whereas approaches categorised under *statistical* aim to reproduce metrics characterising them.

Of the approaches to generate representative numerical models of polycrystalline structures, *statistical*-based approaches appear most appropriate for the requirements of this thesis as they describe the material in a broader sense rather than recreating specific features. This aligns well with the intention to quantify uncertainty arising from the aleatoric nature of polycrystalline structures and to then use this information to stochastically inform component-level analyses. As SEM micrographs can be produced in-house and seem to be more readily available in literature, their use was opted for to garner statistical metrics characterising a material.

Referring to the micrographs shown in Chapter 1, it is apparent that there exists a range of grain shapes and sizes that could lead to stress field heterogeneities within polycrystalline structures. These in turn could trigger local geometric and physical phenomena such as slip, twinning, crack initiation, or grain reorientation. Consequently, it was deemed crucial that sufficient effort was made to generate realistic representations. This therefore negates the use of regular morphologic polycrystalline generating algorithms [73, 74], and puts preference toward Voronoi-based tessellation algorithms that are capable of capturing such irregularities. More complex methods based on grain-growth kinetics have been proposed (e.g. Phase-Field

[75], Surface Evolver [76]) that can capture the irregular morphologies of individual grains that Voronoi-based methods cannot, as they model convex grains with straight edges and planar faces. However, their high computational cost makes them unattractive due to the large number of realisations required in this work.

Among the Voronoi-based tessellation algorithms available, Poisson-Voronoi, Hardcore-Voronoi, and Laguerre-Voronoi formulations are widely accepted to generate tessellations statistically representative of real polycrystalline structures [77]. However, as the Laguerre-Voronoi formulation offers a wider range of granular structures when compared against the other two due to constraints it imposes on the initial state [65], the algorithm, VorTeX [66] (that is based on this formulation), was opted for to generate the polycrystalline structures considered in this thesis. Nevertheless, prior to discussing this particular algorithm, the classic formulation was presented first as to make clear the reason for this choice.

Voronoi tessellations decompose space, $\mathfrak{R}^n$ (where n denotes the number of dimensions), into cells that themselves are seeded from individual nuclei. This means space can be discretised into N finite cells based on N nuclei. What defines a cell R_{P_i} that seeds from nucleus $\mathbf{P}_i$ is that any point, $\mathbf{x}$, in $\mathfrak{R}^n$ is closer to nucleus $\mathbf{P}_i$ than any other nucleus $\mathbf{P}_j$. This can be written as,

$$\begin{aligned} \{R_{P_i}\} = \{x \in \mathfrak{R}^n : ||\mathbf{P}_i - \mathbf{x}|| \leq ||\mathbf{P}_j - \mathbf{x}||\} \\ j = 1, 2, \dots, N : j \neq i. \end{aligned} \quad (4.1)$$

Considering this, it becomes apparent that the size and shape of the cells are dependent on the position of the nuclei $\mathbf{P}_i$ in space $\mathfrak{R}^n$. To overcome this dependence on position, the Hardcore-Voronoi tessellation algorithm [78] proposes a control through a scalar value, ρ (the Hardcore radius), that controls the minimum distance between nuclei during the seeding process, dictating the sphericity of a grain. This control takes the form,

$$\begin{aligned} ||\mathbf{P}_i - \mathbf{P}_j|| = \sqrt{\sum_{k=1}^n (P_{i_k} - P_{j_k})^2} > \rho \\ \forall(i, j) = 1, 2, \dots, N : j \neq i. \end{aligned} \quad (4.2)$$

Even with this additional control, Hardcore-Voronoi-based algorithms are not able to generate the wide range of grain sizes seen in polycrystalline structures. This is where the additional controls of the Laguerre-Voronoi tessellation offer benefits.

The Laguerre-Voronoi tessellation introduces a power-distance rule that allocates weights w_i to individual nuclei and takes the form,

$$\text{pow}(\mathbf{x}, (\mathbf{P}_i, w_i)) = \|\mathbf{P}_i - \mathbf{x}\|^2 - w_i. \quad (4.3)$$

As with Voronoi tessellations, a boundary segment of a cell is defined by two nuclei and is perpendicular to the line connecting them. All points on this plane are described by,

$$\mathbf{x} \in \mathbb{R}^3 : 2\langle \mathbf{x}, \mathbf{P}_i - \mathbf{P}_j \rangle = \|\mathbf{P}_i\|^2 - \|\mathbf{P}_j\|^2 + w_j - w_i. \quad (4.4)$$

If the weights are constrained to being positive, this allows a relationship to the radii of the sphere to be defined. This consequently allows the formulation to be written as,

$$\begin{aligned} \{R_{P_i}\} &= \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{P}_i - \mathbf{x}\| - r_i^2 \leq \|\mathbf{P}_j - \mathbf{x}\| - r_j^2\} \\ &j = 1, 2, \dots, N : j \neq i. \end{aligned} \quad (4.5)$$

With the addition of nuclei weights manifests the non-univocal relation between cells and nuclei that can potentially compromise the resulting tessellation. Such cases include the following *degenerated* conditions,

- Nuclei not guaranteed to generate cells,
- Cells can violate the one-to-one relationship with nuclei,
- Nuclei may not be contained within the cell they generate.

Each of these conditions are identified in Figure 4.1; cell i does not contain its nucleus P_i , cell j contains multiples nuclei, and the nucleus P_k does not generate any cell.

As stated in Falco et al., 2017, [77], from the examples shown and the mathematical description, the occurrence of undesired cells can be avoided by imposing a non-overlapping condition on the spheres that depends on the weights of the nuclei. Therefore, to ensure that every nucleus generates a cell, and lies within it, VorTeX utilises an innovative technique for efficiently generating dense packings of spheres. This technique uses a conditioning method based on a distribution of radii, tangency conditions, and an adaptation of the 3D-clew algorithm

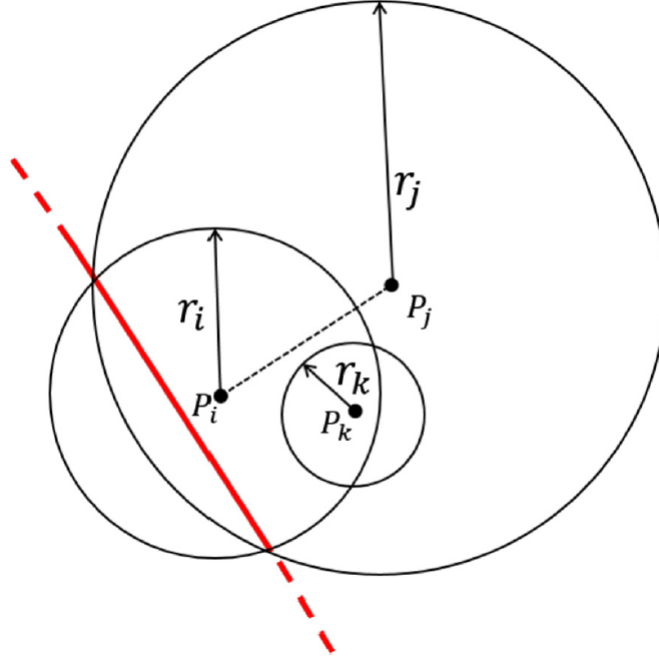


Figure 4.1: Illustration of a grain boundary (red line) between cell i (left) and cell j (right) generated by the nuclei P_i and P_j [77]. Three degenerate conditions are shown; cell i does not contain its nucleus P_i , cell j contains multiples nuclei, and the nucleus P_k does not generate any cell.

[79]. It proceeds by placing and designating the first sphere as the *central*, the second sphere is then placed tangent to it, and the line connecting the centre of these spheres is set as the X-axis. Each sphere after this is then added by imposing a tangency condition to both the *central* and previously placed spheres. This process is repeated till a sphere cannot be placed. In this instance the layer is considered saturated and the *central* sphere is updated. The spheres are prescribed radii equal to the square root of the weight and the resulting structure takes the form of a 3-D spiral. The algorithm implements guards to ensure that no overlapping takes place, and that a layer is adequately saturated before proceeding to the next. Consequently, random packings of non-overlapping spheres with radii seeded from a distribution are generated, that in-turn, as shown in Figure 4.2, serve as the basis for $\mathbf{x}$ and r in the Laguerre-Voronoi tessellation.

4.3.1 Generating statistically representative numerically-based polycrystalline structures of WE43-T6

The process to generate representative numerical models of polycrystalline structures like those seen in magnesium alloys is now presented. First, the distribution in grain radii as per an EBSD micrograph of hot-rolled WE43-T6 plate [13] was measured. This was done by taking

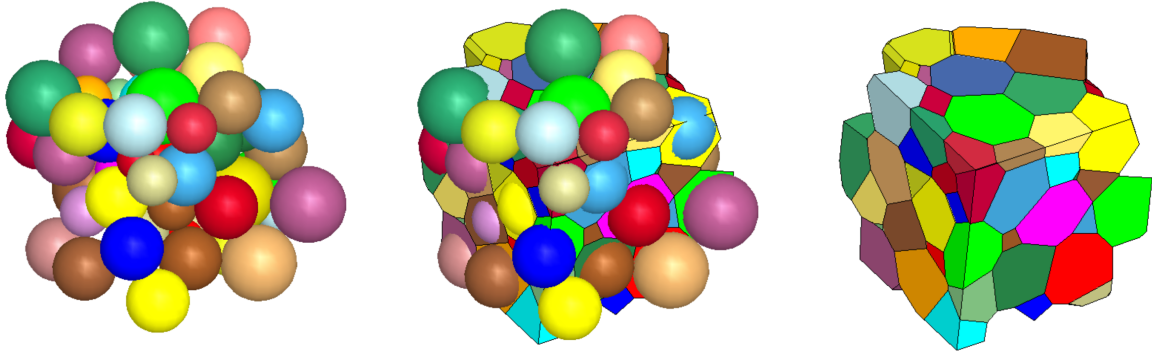


Figure 4.2: (left) Sphere packing resulting from conditioning method, (middle) overlay of packing on tessellation, (right) tessellation.

the areas of whole grains [80], and inferring the equivalent grain size in 2D by mapping these areas onto circles and determining their radii. These equivalent grain sizes were subsequently put into a histogram consisting of unevenly sized bins (to give a tapering with grain size distribution [77]) and passed into VorTeX to seed the generation of a sphere packing, thus facilitating the generation of a cubic domain tessellation (an example of such a 3-D tessellation is shown in Figure 4.3). This domain was then sliced along planes at regular intervals with face normals aligning with the global Z-axis as shown in Figure 4.4. The equivalent grain sizes on each slice were then evaluated and compared against that of the EBSD micrograph to verify that the numerically-based mesostructure was representative of that experimentally measured. The comparisons shown in Figures 4.5 and 4.6 highlight the qualitative likeness achieved. Figure 4.5 shows the γ -probability density functions (γ -PDFs) of the sectioned tessellation using dash-dotted lines, while a solid line was used to identify the one that derived from the micrograph; the higher count of small grains was due to the slicing of the mesostructure having the potential to intersect a grain arbitrarily meaning more grains are not cut at their largest, thus resulting in an increased count of smaller grains.

Having generated a high fidelity numerically-based representation of mesostructure with metrics that match experimental data, attention turned to developing the crystal plasticity-based constitutive model required by the framework. Any subsequent polycrystalline structures discussed from this point onward were generated using this methodology.

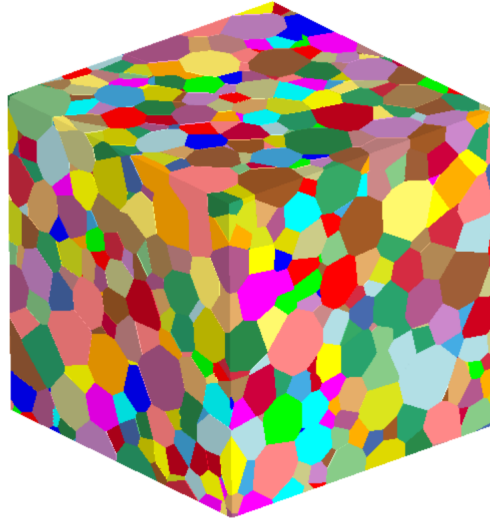


Figure 4.3: 750x750x750 μm Laguerre-Voronoi tessellation representative of WE43-T6.

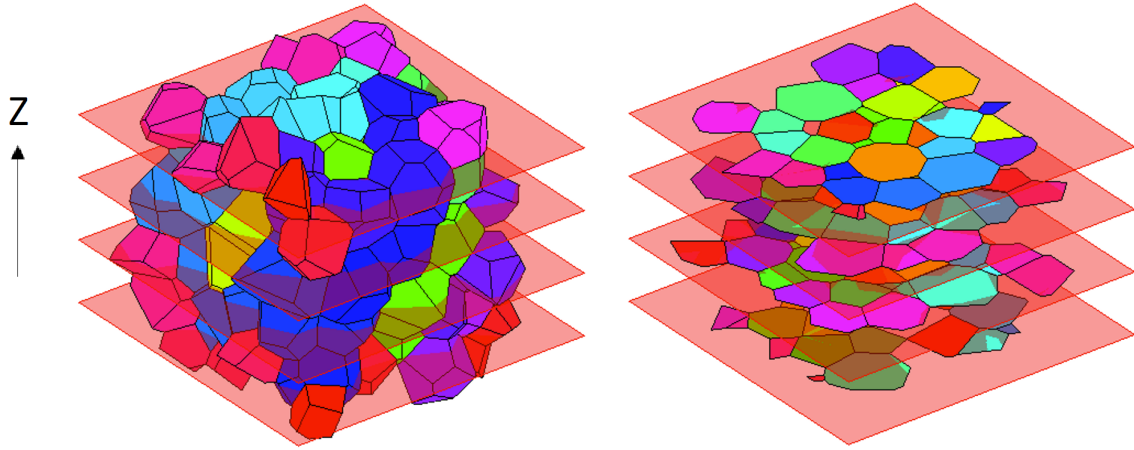


Figure 4.4: Serial sectioning of a 3D structure with planes (left), and relative 2D projections (right).

4.4 Development of a crystal plasticity-based constitutive model

Plasticity in crystalline structures is carried by various mechanisms, with one such mechanism being slip. This mechanism sees dislocations glide on slip planes when shear stresses exceed a critical magnitude. Schmid's law,

$$\tau = \mathbf{s} \cdot \boldsymbol{\sigma} \cdot \mathbf{n}, \quad (4.6)$$

can be used to determine the shear stress on a plane by projecting the stress state onto it. Here, τ is the resolved shear stress, $\mathbf{s}$ is the vector describing the slip direction, and $\mathbf{n}$ is the

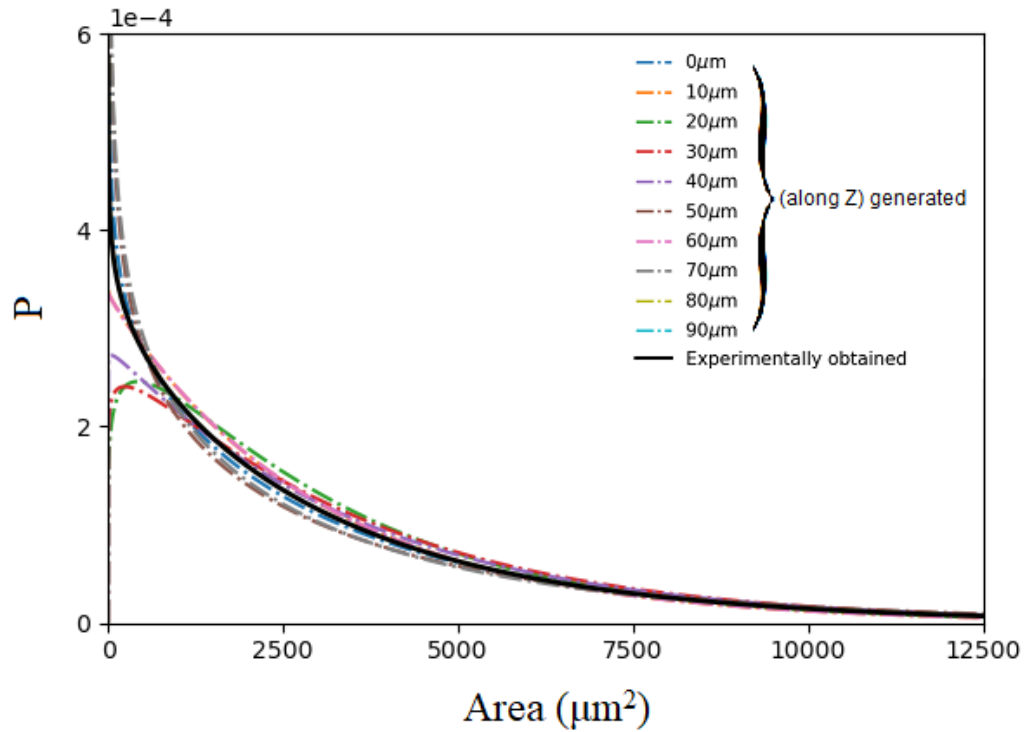


Figure 4.5: Comparison of γ -PDFs generated through (1) the serial slicing of a tessellation by planes at regular 10 μm intervals and the subsequent measuring of relative 2D projections of a grain's area onto them (dash dotted lines), (2) experimental means (solid line).

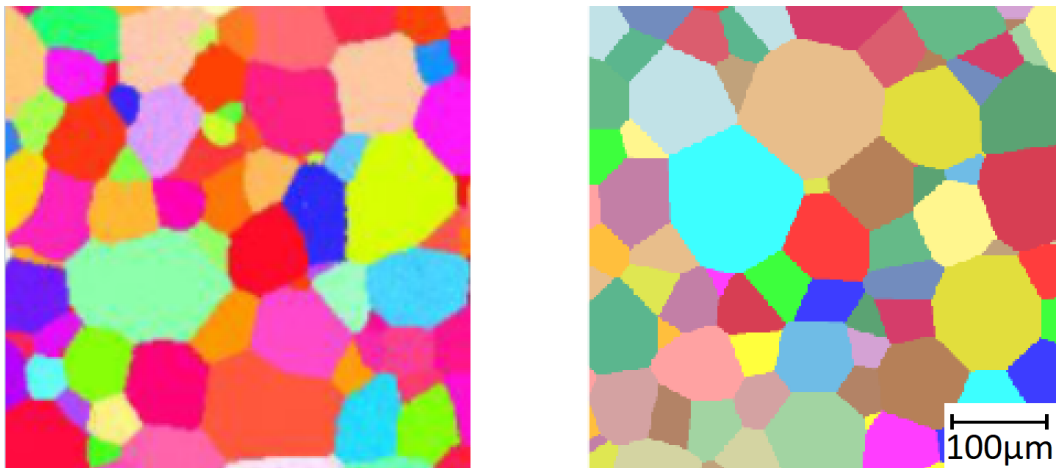


Figure 4.6: Comparison of 500x500 μm areas taken from WE43-T6 EBSD micrograph [13] (left) and Laguerre-Voronoi Tessellation (right).

vector describing the slip plane normal. Another mechanism that carries plasticity is twinning. Twinning is more readily activated in low symmetry metals, under high-rate loading, and in cold conditions, and tends to occur when the stress state is sufficiently localised and cannot be accommodated by slip alone. Twins are observed as mirrored images of the crystal lattice structure and form along specific or sets of planes (known as twin planes) in the crystal [37], with the line this mirror symmetry forms along being referred to as a twin boundary. Twin boundaries are a distinct interface where the crystal lattice of one part is oriented differently from that of the other. Significant effort has gone into implementing such physically-based phenomena into finite element codes and as such are discussed next.

Current crystal plasticity formulations mostly derive from the already discussed works of Pierce, Needleman, and Asaro [62, 81] who made the assumption that deformation modes can activate and contribute to shear simultaneously. This formulation has been adapted to work within the VPSC framework, as well as implicit and explicit finite element codes. As the intention of this thesis was to develop high-rate-based considered CPFEMs that in turn could be used to establish the foundation on which an explicit-explicit time-integrated spatial concurrent multi-scale FEA architecture could be built upon (see earlier discussion and Chapter 5), the following presents the steps taken to develop an explicit run crystal plasticity-based constitutive model that could facilitate this.

Explicit run CPFEMs tend to be used less frequently than implicit ones in literature, and if they are, they tend to be used to describe high symmetry materials [63, 82] like copper [27], and aluminium alloys [26]. Sarsfield [83] attempted to develop an explicitly-run crystal plasticity model for the low symmetry HCP-based material system (Figure 4.7 presents the HCP unit cell with some of its available slip systems), titanium alloy Ti6Al4V, using the work of Anand et al., 1996 [84]. However, this attempt only considered slip and lacked the ability to predict strain hardening behaviour. As such, it was only able to make piecewise bi-linear predictions of constitutive behaviour where the point after yield had a zero gradient.

Clearly, a gap in literature exists on the subject of explicitly-run crystal plasticity-based constitutive models for low symmetry metals that exhibit twinning. Therefore, in order to formulate one that met the requirements of this project, commonalities in theory shared between the previously discussed explicit constitutive models, that do not consider twinning, were first identified.

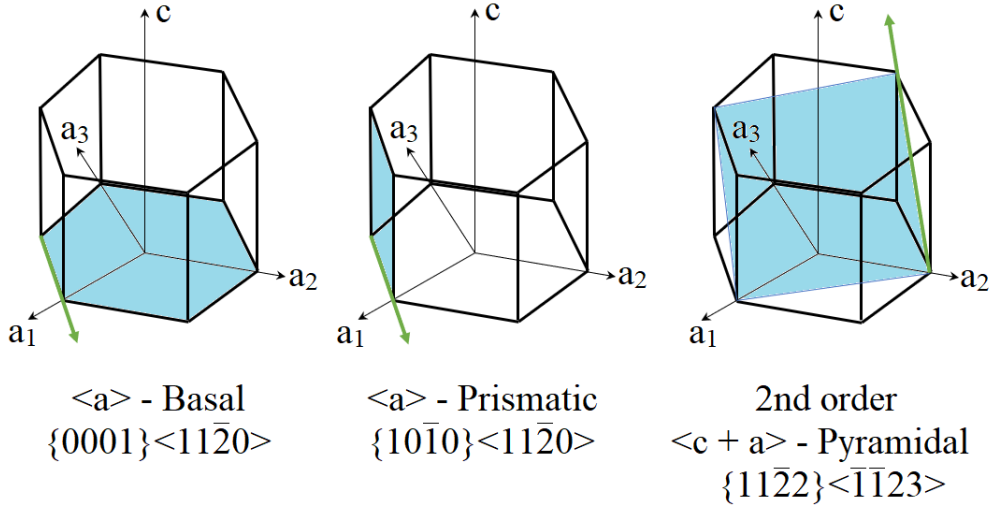


Figure 4.7: Pictorial representations of HCP slip systems.

4.4.1 Formulation of crystal plasticity-based constitutive model

The aforementioned models (as well as the VPSC model) start with the assumption that the velocity gradient is specified and can be additively decomposed into elastic and plastic parts,

$$\mathbf{L} = \mathbf{L}^e + \mathbf{L}^p, \quad (4.7)$$

where $\mathbf{L}^p$ represents plastic deformation through shearing (from various mechanisms) and $\mathbf{L}^e$ captures elastic deformation through the stretching of metallic bonds, as well as rigid crystal lattice rotation. The rate of deformation ($\mathbf{D}$) and spin ($\mathbf{W}$) tensors can then be expressed as their symmetric and skew-symmetric parts respectively through,

$$\mathbf{D} = \frac{1}{2}(\mathbf{L}^T + \mathbf{L}), \quad (4.8)$$

$$\mathbf{W} = \frac{1}{2}(\mathbf{L}^T - \mathbf{L}). \quad (4.9)$$

Expressing the plastic velocity gradient as the sum of the product of the shearing rate, and the dyadic product of the slip plane normal ($\mathbf{n}$) and slip direction ($\mathbf{s}$) for activated slip systems κ ,

$$\mathbf{L}^p = \sum_{\kappa} \dot{\gamma}^{\kappa} \mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa}, \quad (4.10)$$

where $\dot{\gamma}$ is the shearing rate, means the plastic rate of deformation and spin tensors can be expressed as,

$$\mathbf{D}^p = \text{sym} \left(\sum_{\kappa} \dot{\gamma}^{\kappa} \mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa} \right), \quad (4.11)$$

$$\mathbf{W}^p = \text{skew sym} \left(\sum_{\kappa} \dot{\gamma}^{\kappa} \mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa} \right), \quad (4.12)$$

that in-turn can be used to determine increments in stress and lattice rotations, respectively.

Shearing occurs on slip system κ if the resolved shear stress (τ^{κ}) on it exceeds its critically resolved shear stress (τ_c^{κ}). The resolved shear stress on each slip system for a given stress state can be calculated using the Cauchy stress tensor through,

$$\tau^{\kappa} = \boldsymbol{\sigma} : (\mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa}). \quad (4.13)$$

The shearing rate can then be predicted using the rate-dependent power-law formulation,

$$\dot{\gamma}^{\kappa} = \begin{cases} \dot{\gamma}_0 \text{sign}(\tau^{\kappa}) \left| \frac{\tau^{\kappa}}{\tau_c^{\kappa}} \right|^{\frac{1}{m}}, & \text{if } |\tau^{\kappa}| \geq \tau_c^{\kappa} \\ 0, & \text{if } |\tau^{\kappa}| < \tau_c^{\kappa} \end{cases}, \quad (4.14)$$

where $\dot{\gamma}_0$ is the reference shear strain rate, and m is the strain-rate sensitivity coefficient. Now that the accumulated shearing rates can be approximated, the stress increment can be determined. The Lie Derivative ($\overset{\nabla}{\boldsymbol{\sigma}}$) can be written as,

$$\begin{aligned} \overset{\nabla}{\boldsymbol{\sigma}} &= \mathbf{C} : \mathbf{D}^e, \\ &= \mathbf{C} : (\mathbf{D} - \mathbf{D}^p), \end{aligned} \quad (4.15)$$

and the Cauchy stress rate as,

$$\dot{\boldsymbol{\sigma}} = \mathbf{C} : (\mathbf{D} - \mathbf{D}^p) + \mathbf{W}\boldsymbol{\sigma} - \boldsymbol{\sigma}\mathbf{W} - (\mathbf{W}^p\boldsymbol{\sigma} - \boldsymbol{\sigma}\mathbf{W}^p) - \boldsymbol{\sigma} \text{tr}(\mathbf{D}), \quad (4.16)$$

where $\mathbf{C}$ is the fourth order elasticity tensor. If the spins are small and the material is assumed

in-compressible, this can be approximated as,

$$\dot{\boldsymbol{\sigma}} \approx \mathbf{C} : (\mathbf{D} - \mathbf{D}^p), \quad (4.17)$$

This incremental Cauchy stress tensor can then be added to the previous stress state, allowing for predictions on the path-dependent evolution of the stress state.

This approach to determine the stress increment works for the aforementioned explicitly time-integrated formulations as the projected stress state tends to exist near the critically resolved shear stress due to the high symmetry of the metals analysed and the small time-steps associated with their use. However, problems arise when twinning is incorporated into the formulation. This is because modelling the crystal substructure reorientation observed when twin laths nucleate and propagate can locate previously inactive slip systems in such a way that the resolved shear stress projected onto them is many times larger than their critically resolved shear stress. Consequently, if the power-law shown in Eq. 4.14 is invoked to predict the shearing rate, exceedingly large values are computed due to the large exponent term that results from the relatively low-rate sensitivity term seen for magnesium alloys [85]. This means use of the approximation, $\dot{\boldsymbol{\sigma}} = \mathbf{C} : (\mathbf{D}_{t-\Delta t/2} - \mathbf{D}_{t+\Delta t/2}^p)$, (where $t + \Delta t/2$ denotes the current time-step and $t - \Delta t/2$ denotes the previous) that has already been discussed, can yield results that do not satisfy consistency. Therefore, the explicit-based crystal plasticity formulation proposed in this work incorporates the Newton-Raphson-based method put forward in Dunne et al., 2007 [23] to help identify when consistency is violated and thus establish an upper limit on the shearing rate to ensure it does not become unmanageable.

The formulation of the Newton-Raphson-based method follows a similar decomposition of the total velocity gradient into elastic and plastic parts. However, this can now be further expanded to include the shearing from both slip ($\mathbf{L}^{slip}$) and twinning ($\mathbf{L}^{twin}$) mechanisms,

$$\begin{aligned} \mathbf{L}_{t+\Delta t/2} &= \mathbf{L}_{t+\Delta t/2}^p + \mathbf{L}_{t+\Delta t/2}^e, \\ \mathbf{L}_{t+\Delta t/2}^p &= \mathbf{L}_{t+\Delta t/2}^{twin} + \mathbf{L}_{t+\Delta t/2}^{slip}. \end{aligned} \quad (4.18)$$

Slip was modelled following the same formulation already discussed except that the criteria for activation was modified to $\tau^\kappa / \tau_c^\kappa \geq 0.5$. This was to allow slip systems to harden for less

severe stress states and to therefore develop resilience in case they are *twinned* into orientations that result in significantly larger resolved shear stresses.

If the resolved shear stress activates slip, the shearing rate in explicit-based methods (as discussed) is approximated using the stress state of the previous time-step ($\boldsymbol{\sigma}_t$), hence allowing the stress increment to be calculated using Eq. 4.17. In actuality, the magnitude of the shearing rate is unknown and a numerical method like the Newton-Raphson method is required to bring the plastic strain field and the stress field vectors together. To construct one, first an expression incorporating the incremental plastic strain ($\Delta\boldsymbol{\epsilon}^p$), trial stress ($\boldsymbol{\sigma}^{tr}$), Cauchy stress, and a vector stress residual (Ψ) is required [23] and can be formulated as,

$$\Psi = \boldsymbol{\sigma} - \boldsymbol{\sigma}^{tr} + \mathbf{C}\Delta\boldsymbol{\epsilon}^p = 0. \quad (4.19)$$

Applying the differential operator yields,

$$\delta\Psi = \delta\boldsymbol{\sigma} - \delta\boldsymbol{\sigma}^{tr} + \mathbf{C}\delta\Delta\boldsymbol{\epsilon}^p = 0, \quad (4.20)$$

where the differential of the plastic strain tensor increment is,

$$\delta\Delta\boldsymbol{\epsilon}^p = \text{sym} \left(\sum_{\kappa} \dot{\gamma}_0 \left(\frac{1}{m} \right) \Delta t \left| \frac{\tau_t^{\kappa}}{\tau_c^{\kappa}} \right|^{(\frac{1}{m}-1)} \mathbf{s}^{\kappa} \otimes \mathbf{n}^{\kappa} \delta\tau^{\kappa} \right), \quad (4.21)$$

where $\delta\tau^{\kappa} = (\mathbf{n}^{\kappa} \otimes \mathbf{s}^{\kappa}) : \delta\boldsymbol{\sigma}$. Writing all variables in Voigt notation gives,

$$\delta\Delta\boldsymbol{\epsilon}^p = \text{sym} \left(\sum_{\kappa} \dot{\gamma}_0 \left(\frac{1}{m} \right) \Delta t \left| \frac{\tau_t^{\kappa}}{\tau_c^{\kappa}} \right|^{(\frac{1}{m}-1)} \mathbf{A}^{\kappa} \otimes \mathbf{A}^{\kappa} \right) = \mathbf{P}\delta\boldsymbol{\sigma}. \quad (4.22)$$

where $\mathbf{A}^{\kappa}$ is given by,

$$\mathbf{A} = (\mathbf{s} \otimes \mathbf{n})_{\kappa}. \quad (4.23)$$

Substituting Eq. 4.22 into Eq. 4.20 and rearranging yields the following Newton-Raphson formulation,

$$\Psi + \frac{\partial\Psi}{\partial\boldsymbol{\sigma}}\delta\boldsymbol{\sigma} = [\boldsymbol{\sigma} - \boldsymbol{\sigma}^{tr} + \mathbf{C}\Delta\boldsymbol{\epsilon}^p] + [\mathbf{I} + \mathbf{C}\mathbf{P}]\delta\boldsymbol{\sigma} = 0, \quad (4.24)$$

that updates the stress through,

$$\delta\boldsymbol{\sigma} = [\mathbf{I} + \mathbf{C}\mathbf{P}]^{-1}[\boldsymbol{\sigma}^{tr} - \boldsymbol{\sigma} - \mathbf{C}\Delta\boldsymbol{\epsilon}^p], \quad (4.25)$$

until a tolerance is met. This increment in stress is then added to the previous stress state to give the current stress that the explicit solver then uses to determine the nodal forces at $t + \Delta t$.

Twinning can be considered by either *discretely* modelling them or by *homogenising* their effects. Due to their localised nature *discrete*-based approaches would be favourable as this would predict the heterogeneity of the stress field more accurately, however, to do so is computationally expensive. Ardeljan et al., 2015, 2017, Grilli et al., 2020, and Ghosh et al., 2017, [25, 85–87] are examples where twins have been discretely modelled. The work of Grilli et al., and Ardeljan et al. show that to model twin laths, additional subroutines are required, thus, limiting their application to localised areas (comprising of at most tens of grains) within a polycrystalline structure. Ghosh et al., were able to extend their studies to representative volume element sizes, however to do so necessitated the use of an adaptive multi-time-domain subcycling algorithm to optimise the use of computational resources. Initially, attempts were made to develop a similar approach, however, it was realised, due to the workload, that to do so was not attainable and so it was not further pursued. Even so, the use of an adaptive multi-time domain subcycling algorithm is presented later as a means to facilitate component-level analyses that consider mesostructural detail. Alternatively, *homogenised*-based approaches negate the need for additional subroutines through the use of rate of mixture-based considerations, and are therefore an attractive alternative option.

Van Houtte et al., 1978, [88] and Kalidindi et al., 1998, [89] developed what has become to be known as the pseudo-slip model to account for the nucleation and growth of twins. Their approach has earned this name as it adopts a formulation similar to slip where the stress field tensor is projected onto the planes defining the twin systems. Accordingly, the extent of twinning is predicted through,

$$\dot{\gamma}^\alpha = \begin{cases} \dot{\gamma}_0^{\text{twin}} \left| \frac{\tau^\alpha}{\tau_c^\alpha} \right|, & \text{if } \tau^\alpha \geq \tau_c^\alpha \\ 0, & \text{if } \tau^\alpha < \tau_c^\alpha, \end{cases} \quad (4.26)$$

where α identifies a particular twin system. The resulting twin volume fraction evolution of a particular twin system, f^α , was then predicted using, $\dot{f}^\alpha = \frac{\dot{\gamma}^\alpha}{S^\alpha}$, where S^α is the characteristic shear strain that has been stated to be 12.89% for magnesium-based alloys [13]. Kurukuri et al., 2014 [8] stated that twin growth is rate independent hence why Eq. 4.26 took the rate-independent form shown. The shear due to twinning was then accounted for using,

$$\mathbf{L}^{twin} = \sum_{\alpha} \dot{f}^\alpha S^\alpha \mathbf{s}^\alpha \otimes \mathbf{n}^\alpha, \quad (4.27)$$

and remains valid till the volume fraction of twin systems reaches unity, i.e. $\sum_1^n \Delta f^\alpha = 1$ for n strain increments. Having incorporated the shear from slip and twinning in the parent grain, shear due to slip in the twinned domain was considered in the developed model by adopting the philosophy of the predominant twin reorientation scheme [90]. This philosophy involves tracking the volume fraction of each individual twin system, and then designating the first one to exceed a threshold value as the predominant twin system. The twinned domain was then given characteristics reflecting this twin. Subsequently, the contribution of slip from both domains can be rewritten as [38],

$$\mathbf{L}^{slip} = (1 - \sum_{\alpha=1}^{ntwin} f^\alpha) \sum_{\kappa} \dot{\gamma}^\kappa \mathbf{s}^\kappa \otimes \mathbf{n}^\kappa + \sum_{\alpha=1}^{ntwin} f^\alpha \sum_{\kappa} \dot{\tilde{\gamma}}^\kappa \tilde{\mathbf{s}}^\kappa \otimes \tilde{\mathbf{n}}^\kappa, \quad (4.28)$$

where variables denoted $\sim$ are variables associated with the transformed twinned domain.

One consideration that has not been discussed yet is rigid lattice rotation due to shearing. The explicit solver used only handles non-shearing related continuum rotation and so needs to be corrected to reflect lattice rotation. In essence this means that two changes in coordinate system take place as shown in Figure 4.8. First, the solver transforms the global coordinate system to the material's coordinate system (accounts for continuum rotation). Then, the user-subroutine transforms the material's coordinate system into the crystal's one (accounts for rotation due to shearing) by taking the plastic spin tensor of the prior time-step ($t - \Delta t/2$) and using it to calculate the rotation increment,

$$\Delta \mathbf{R}_{t+\Delta t/2} = \mathbf{I} + \mathbf{W}_{t-\Delta t/2}^p \Delta t, \quad (4.29)$$

that updates the rotation matrices orientating the crystal,

$$\mathbf{R}_{t+\Delta t/2} = \Delta \mathbf{R}_{t+\Delta t/2} \mathbf{R}_{t-\Delta t/2}, \quad (4.30)$$

hence predicting incremental rotation. The material point's rate of deformation tensor can then be rotated from the global reference frame (g) into the local reference frame (l),

$$\mathbf{D}_{t+\Delta t/2}^l = \mathbf{R}_{t+\Delta t/2}^T \mathbf{D}_{t+\Delta t/2}^g \mathbf{R}_{t+\Delta t/2}. \quad (4.31)$$

It is this rate of deformation tensor that is used by the crystal plasticity-based user-subroutine to determine the stress increment. Having now established how crystal rotation is tracked, the transformation associated with the twin can now be predicted. This is done using the orthogonal transformation tensor ($\mathbf{R}^\alpha$) [91], which is a function of the the normal of the plane belonging to the predominant twin system ($\mathbf{n}^{\alpha,PTS}$),

$$\mathbf{R}^\alpha = 2\mathbf{n}^{\alpha,PTS} \otimes \mathbf{n}^{\alpha,PTS} - \mathbf{I}. \quad (4.32)$$

This transformation matrix then re-orientates the parent grain's slip systems into the twinned domain (turning $\mathbf{s}$ and $\mathbf{n}$ into $\tilde{\mathbf{s}}$ and $\tilde{\mathbf{n}}$). As twinning was assumed to occur at the speed of sound in the material [38], and because the explicit time integration scheme used bases its forward stepping interval on it, twinning was considered an instantaneous event. Another factor that requires consideration is that the contribution to elastic behaviour will have changed as the grain now comprises of two domains with transversely isotropic properties at differing orientations to each other. This was considered by making the elasticity tensor dependent on the rate of mixtures rule. Consequently, the Cauchy stress rate shown in Eq. 4.17 became,

$$\dot{\boldsymbol{\sigma}}_{t+\Delta t}^l \approx \mathbf{C}' : \mathbf{D} - (1 - \sum_{\alpha=1}^{ntwin} f^\alpha)[\mathbf{C}' : \mathbf{D}^p] - \sum_{\alpha=1}^{ntwin} f^\alpha[\mathbf{C}' : \tilde{\mathbf{D}}^p], \quad (4.33)$$

where $\mathbf{C}'$ is a volume fraction-based fourth order elasticity tensor, and $\tilde{\mathbf{D}}^p$ denotes slip in the twinned domain. Having now established the necessary formulation to determine the shearing rate contribution from all domains, and consequently the resulting stress increment, attention turned to incorporating strain hardening behaviour.

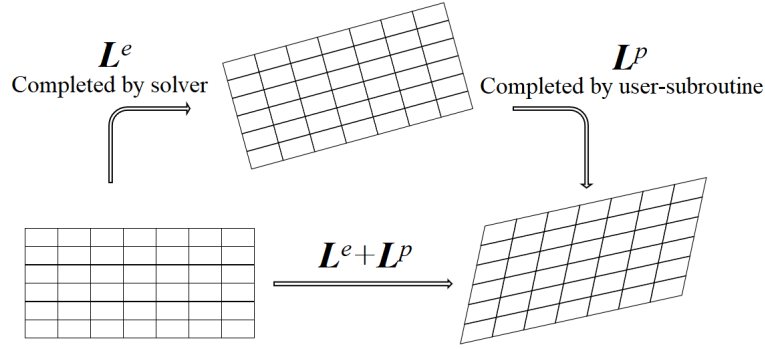


Figure 4.8: Pictorial depiction of velocity gradient ($\mathbf{L}$) decomposition into elastic and plastic components alongside routines responsible for transformations.

It has been well documented that polycrystalline metals undergo strain hardening due to the interaction of dislocations with themselves, solutes, precipitates, and grain-boundaries within their substructures [92–94]. Pierce, Needleman, and Asaro in their series of papers [62, 81] proposed the generic hardening model,

$$\dot{\tau}_\epsilon^\kappa = \mathbf{H}_{\kappa\beta} \dot{\gamma}^\beta, \quad (4.34)$$

to phenomenologically account for this. In this equation the tensor $\mathbf{H}_{\kappa\beta}$ denotes the hardening matrix that governs self and latent hardening between slip systems and takes the form,

$$\mathbf{H}_{\kappa\beta} = [q + (1 - q)\delta_{\kappa\beta}]h(\gamma), \quad (4.35)$$

$$\text{with } h(\gamma) = h_0^\kappa \text{sech}^2\left(\frac{h_0^\kappa \gamma}{\tau^{*,\kappa} - \tau_0^\kappa}\right), \quad (4.36)$$

where $\delta_{\kappa\beta}$ is the Kronecker delta, q is the latent hardening parameter, $\gamma = \int \sum_\kappa \dot{\gamma}^\kappa dt$ is the accumulated glide on all slip systems, h_0^κ is the initial hardening slope, $\tau^{*,\kappa}$ is the saturation stress, and τ_0^κ is the initial critical resolved shear stress for slip system κ . This strain hardening behaviour can be one of many contributing factors that influence the critically resolved shear stress for a slip system. These factors can be additively summed to give the resolved shear stress required to activate slip. For example, the crystal could have an initial critically resolved shear not dependent on strain hardening that can be accounted for through,

$$\tau_c^\kappa = \tau_0^\kappa + \Delta\tau_\epsilon^\kappa. \quad (4.37)$$

Other variations of formulating this strain hardening behaviour have also been developed, with the VPSC adopting the Voce hardening form [21]. The generic hardening model was chosen in this work as it was used in the initial set of papers published by Pierce, Needleman, and Asaro [62, 81]. The intention was to then substitute this hardening model for a dislocation density-based one after initial implementations had been verified. However, due to complications arising elsewhere in the project, it was decided that the generic hardening model would suffice. Nevertheless, this theory is reviewed here as significant effort went into attempting to implement it (Hall-Petch hardening resulting from size effects and twin formation was successfully incorporated and is discussed after). Tomé et al., 2001, Beyerlein et al., 2008, Knezevic et al., 2008, Bhattacharyya et al., 2016, and Feather et al., 2019, [9, 22, 36, 56, 95] each subsequently evolved a dislocation density-based hardening model derived from the work of Mecking and Kocks, 1981 [96]. The attempted model derives from these works, and, as such, the expression for the critical resolved shear stress took the form,

$$\tau_c^\kappa = \tau_0^\kappa + \Delta\tau_{sub}^\kappa + \Delta\tau_{for}^\kappa, \quad (4.38)$$

where $\Delta\tau_{sub}^\kappa$ and $\Delta\tau_{for}^\kappa$ evolve with the substructure and forest dislocation densities, respectively. Such a form was shown to be a sensible approximation for mixtures of weak (solute) and strong obstacles (precipitates and dislocations) [97]. The evolution of each of these terms were subsequently calculated using,

$$\Delta\tau_{sub}^\kappa = k_{sub}\mu b^\kappa \sqrt{\Delta\rho_{sub}} \log\left(\frac{1}{b^\kappa \sqrt{\Delta\rho_{sub}}}\right), \quad (4.39)$$

$$\Delta\tau_{for}^\kappa = b^\kappa \mu \sqrt{\chi^{ss'} \Delta\rho_{for}^\kappa}, \quad (4.40)$$

where k_{sub} is a material-independent constant, μ is the shear modulus and b^κ is the Burger's vector for slip system κ . The substructure and forest dislocation densities are represented by ρ_{sub} and ρ_{for} , respectively, and $\chi^{ss'}$ is a dislocation interaction matrix where the diagonal terms are set to 0.81 and the off diagonal terms, zero (analogous to $\mathbf{H}_{\kappa\beta}$ in the generic hardening model without any latent hardening).

Forest dislocation density evolution is governed by the rate of generation and annihilation

equations,

$$\frac{\partial \rho_{for}^\kappa}{\partial \gamma^\kappa} = \frac{\partial \rho_{gen,for}^\kappa}{\partial \gamma^\kappa} - \frac{\partial \rho_{rem,for}^\kappa}{\partial \gamma^\kappa} = k_1^\kappa \sqrt{\rho_{for}^\kappa} - k_2^\kappa \rho_{for}^\kappa, \quad (4.41)$$

$$\Delta \rho_{for}^\kappa = \frac{\partial \rho_{for}^\kappa}{\partial \gamma^\kappa} |\Delta \gamma^\kappa| \quad (4.42)$$

where k_1^κ and k_2^κ are coefficients for dislocation storage and dynamic recovery, respectively. These are related through,

$$\frac{k_1^\kappa}{k_2^\kappa} = \frac{1}{\sqrt{(\chi^{s's})^{-1} \left(\frac{\tau_{sat}^\kappa}{b^\kappa \mu^\kappa} \right)^2}}, \quad \tau_{sat}^\kappa = \frac{D^\kappa (\beta^\kappa)^3 g^\kappa \mu^\kappa}{(D^\kappa (b^\kappa)^3) - kT \ln(\frac{\dot{\epsilon}}{\dot{\epsilon}_0})}, \quad (4.43)$$

where k , $\dot{\epsilon}_0$, g^κ , and D^κ are the Boltzmann's constant, a reference value of strain rate (10^7 s^{-1}), the activation enthalpy, and the drag stress. Substructure dislocation densities evolve through,

$$\Delta \rho_{sub} = \sum_{\kappa} q^\kappa b^\kappa \sqrt{\rho_{sub}} \frac{\partial \rho_{rem,for}^\kappa}{\partial \gamma^\kappa} |\Delta \gamma^\kappa|, \quad (4.44)$$

where q^κ is a coefficient defining the amount of debris from the recovered dislocation population. Even though dislocation density-based hardening could not be successfully implemented, Hall-Petch (τ_{HP}^κ) hardening due to size effects and twin formation was. This was achieved by including τ_{HP}^κ into Eq. 4.37 to yield,

$$\tau_c^\kappa = \tau_0^\kappa + \Delta \tau_\epsilon^\kappa + \Delta \tau_{HP}^\kappa. \quad (4.45)$$

The formulation of this additional term is discussed next.

Proust et al., 2007 [90] derived this hardening term from geometric considerations of what is known as the composite grain model. To start, they formulated the contribution to the critically resolved shear stress as,

$$\tau_{HP}^\kappa = \frac{h_{HP}^\kappa}{\sqrt{d_{mfp}}}, \quad (4.46)$$

where h_{HP}^κ is a Hall-Petch coefficient, and d_{mfp}^s is the mean-free-path between boundaries (these could be the grain boundaries if no twins were present). They then assume, after twin formation, equally spaced twins of thickness (d^{twin}) form in a grain of size (d^g) that then grow

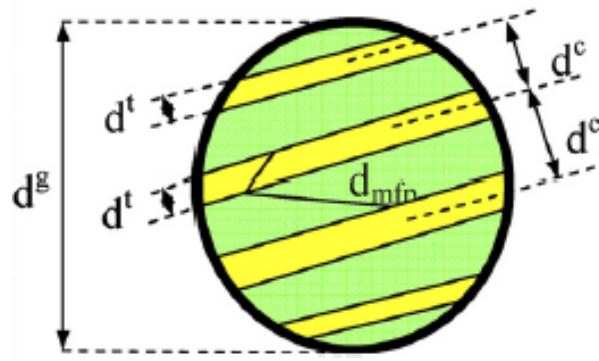


Figure 4.9: Composite grain schematic [90]. The green bands represent the parent grain, and the yellow, twin laths.

under deformation to a maximum thickness (d_{max}^{twin}). The separation of the centre planes of these twins (d^c) is commonly set to $0.2 d^g$ [9]. All the aforementioned terms are identified in Figure 4.9, which also highlights that the mean-free-path reduces for slip systems that intersect a twin boundary. The mean-free-path is introduced for each system through,

$$d_{mfp} = \frac{d^{twin}}{\sin\theta} \text{ in the twin,} \quad (4.47)$$

$$d_{mfp} = \frac{d^{matr}}{\sin\theta} \text{ in the twin,} \quad (4.48)$$

where $d^{twin} = f^{PTS} d^c$ and $d^{matr} = (1 - f^{PTS}) d^c$. Here θ is the angle made by the intersection of the predominant twin plane and a slip plane. Having now detailed what was believed to be all the necessary mechanisms required to appropriately capture slip system hardening, attention turned to incorporating a model that sufficiently described the hardening of twin formation due to nucleation, propagation, and growth.

Wu et al., 2015, [98] developed and implemented into the VPSC model a constitutive law to describe twin nucleation, propagation, and growth in magnesium crystals. Xie et al., 2016, [38] then modified this implementation using a phenomenological description that softened the critical resolved shear stress (τ_c^α) for twinning, through the consideration of the twin volume fraction (f^α), to reproduce the shear localisation that is typical of twin laths. Figure 4.10 shows a side by side comparison of the twinning stage to the CRSS of a twin system. As shown, when the twin volume fraction increases, τ_c^α decreases until the twin volume fraction reaches the threshold, f_g^α ; this stage in the model reflects twin band propagation. After this threshold value, the twin

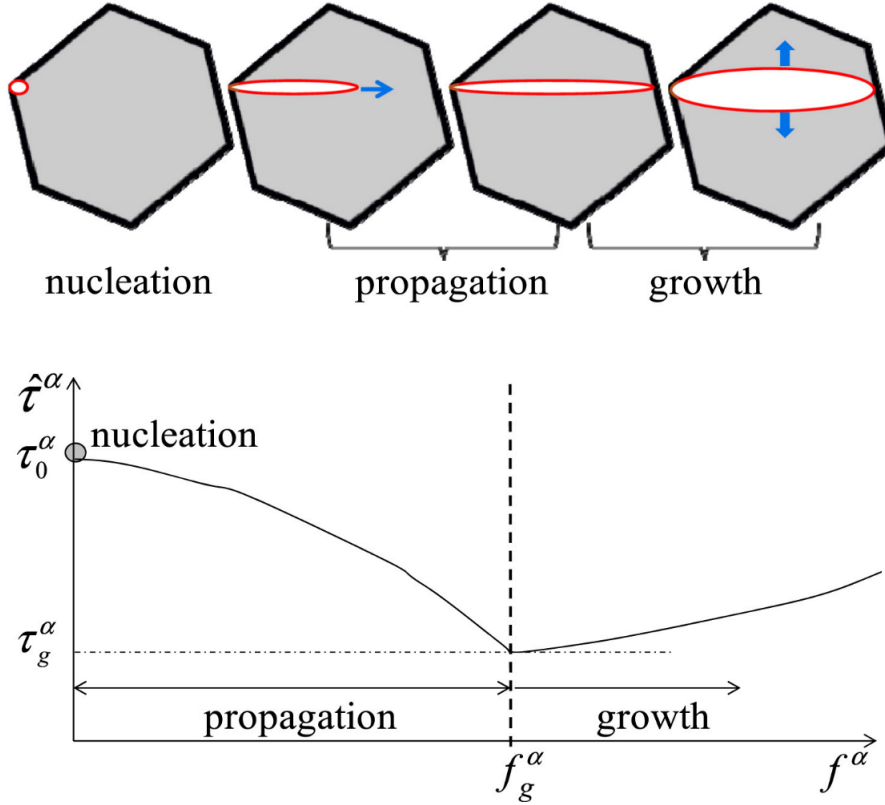


Figure 4.10: (Top) Sequence of images identifying various stages of twinning. (Bottom) Example of the evolution of the critical resolved shear stress for each of these stages [98]. The reduction of the twin systems' CRSSs encourages twin localisation.

CRSS grows, thus reflecting twin growth. The expressions used to formulate such behaviour are,

$$\tau_c^\alpha = \begin{cases} \tau_0^\alpha - \frac{\tau_0^\alpha - \tau_g^\alpha}{f_g^\alpha} & \text{if } f^\alpha \leq f_g^\alpha, \\ \tau_g^\alpha \left(\frac{f_{\text{final}}^\alpha - f_g^\alpha}{f_{\text{final}}^\alpha - f^\alpha} \right), & \text{if } f^\alpha > f_g^\alpha \end{cases}, \quad (4.49)$$

where τ_0^α and τ_g^α are the initial and maximum threshold stresses of twinning, respectively, and f_{final}^α is the final volume fraction of twin system α . Having now incorporated all the necessary hardening terms to capture the various stages of twin lath formation, attention turned to considering thermal effects.

Due to the high-rate application of this developed user-subroutine, handles on thermal softening were introduced by adopting the following form that draws similarities to that of the Johnson-Cook constitutive model [26],

$$\tau_c^\kappa = \tau_c^\kappa \left(1 - \frac{T_{t+\Delta t/2} - T_{ref}}{T_{melt} - T_{ref}} \right)^n. \quad (4.50)$$

Here, $T_{t+\Delta t/2}$ is the temperature for the current time-step, T_{ref} is the room temperature, T_{melt} is the melting temperature of the material, and n is a user-set sensitivity parameter. As shown, the extent of thermal softening is dependent on temperature, which was assumed to be increased with plastic work. To calculate the rise in temperature, a fraction (z) of the incremental plastic work (ΔG) for the current time-step, that is the product of the Cauchy stress field vector ($\boldsymbol{\sigma}$) and the incremental plastic strain,

$$\Delta G = \boldsymbol{\sigma}_{t+\Delta t} \Delta \boldsymbol{\epsilon}^p, \quad (4.51)$$

was considered transformed into thermal energy, and was subsequently summed with the last,

$$E_{t+\Delta t/2} = E_{t-\Delta t/2} + z\Delta G. \quad (4.52)$$

The current thermal energy was then used to calculate the current temperature through,

$$T_{t+\Delta t/2} = \frac{E_{t+\Delta t/2}}{\rho C_p}, \quad (4.53)$$

where C_p is the specific heat capacity of the material. Through this procedure, temperature increases associated with work soften the material.

Now that a homogenised twin-considered explicit crystal plasticity-based constitutive model with all the necessary handles to sufficiently predict all expected flow stresses has been formulated, focus shifted to verifying the implementation outlined in Algorithm 1.

4.4.2 Verification of crystal plasticity-based constitutive model

Correct implementation of the crystal plasticity model user-subroutine was verified using FEM-based studies that compared its responses against those of analytical solutions. The studies were conducted using the reduced integration eight node elements available in LS-Dyna. The first study verified whether the anisotropic fourth order elasticity tensor was implemented following Eq. 3.30 by determining if the variation in stiffness with orientation was as expected. To do so, two sets of uni-axially loaded blocks allocated the elastic properties shown in Table 4.1 were stressed in tension along the global Z-axis which relates to the [0001] crystal direction. The underlying material coordinate system was then incrementally rotated around the X and

Algorithm 1 Implementation of explicit crystal plasticity-based user-subroutine into LS-Dyna

```

1: Arguments:  $\Delta\epsilon_{t+\Delta t/2}$ ,  $\sigma_t$ ,  $\Delta t$ ;
2: Compute  $\mathbf{R}_{t+\Delta t/2}$  using  $\mathbf{W}_{t-\Delta t/2}^p$  and Eqs. 4.29 and 4.30;
3: Compute total twin volume fraction,  $\sum_{\alpha=1}^{ntwin} f^\alpha$ ;
4: if Total twin volume fraction  $\geq$  PTS activation criteria then
5:   Set PTS and twinned domain's evolution trackers equal to parent domain's;
6: end if
7: if PTS then
8:   Compute  $\mathbf{R}^\alpha$  using Eq. 4.32;
9:   Compute  $\mathbf{C}'$  via a mixture rule;
10: end if
11: Rotate  $\Delta\epsilon_{t+\Delta t/2}$  and  $\sigma_t$  from material into local coordinate system;
12: Compute  $\sigma^{tr}$  using  $\sigma_t + \mathbf{C}'\Delta\epsilon_{t+\Delta t/2}$ ;
13: Compute  $\tau^\kappa$  using Eq. 4.13, and similarly  $\tau^\alpha$ ;
14: if PTS then
15:   Rotate PTS slip systems by  $\mathbf{R}^\alpha$ ;
16:   Compute  $\tilde{\tau}^\kappa$ ;
17: end if
18: if  $\tau^\kappa/\tau_c^\kappa \geq 0.5$  or  $\tau^\alpha/\tau_c^\alpha \geq 0.5$  or  $\tilde{\tau}^\kappa/\tilde{\tau}_c^\kappa \geq 0.5$  then
19:   while  $|\sigma^{tr} - \sigma - \mathbf{C}'\Delta\epsilon^p| \leq 10^{-8}$  MPa do
20:     Compute  $\Delta\epsilon_{t+\Delta t/2}^p$ ,  $\mathbf{L}_{t+\Delta t/2}^p$ , and  $\delta\sigma$  using Eqs. 4.14, 4.22, 4.25, 4.26, and 4.33;
21:     Update  $\tau^\kappa$  according to new stress state, and similarly  $\tau^\alpha$  and  $\tilde{\tau}^\kappa$  if required;
22:   end while
23:   Compute  $f^\alpha$  using  $\int \frac{\dot{\gamma}^\alpha}{\dot{\gamma}_c^\alpha} dt$ ;
24:   Compute  $\mathbf{D}_{t+\Delta t/2}^p$ ,  $\mathbf{W}_{t+\Delta t/2}^p$ , and  $\epsilon_{eff}^p$ ;
25:   Transform  $\sigma_{t+\Delta t}$  from local to material coordinate system;
26:   Compute  $\gamma = \int \sum_\kappa \dot{\gamma}^\kappa dt$ ;
27:   Strain harden parent domain slip systems using Eq. 4.34;
28:   if PTS then
29:     Evolve CRSS values of twin systems using Eq. 4.49;
30:     Strain harden twinned domain slip systems using Eq. 4.34;
31:     Hall-Petch harden parent and twin domain slip systems using Eq. 4.46;
32:   end if
33:   Thermally soften slip systems by scaling CRSS values following Eq. 4.50;
34: else
35:   Set  $\sigma_{t+\Delta t} = \sigma^{tr}$ ;
36:   Transform  $\sigma_{t+\Delta t}$  from local to material coordinate system;
37: end if
38: Return  $\sigma_{t+\Delta t}$ ;

```

Y-axes ($[11\bar{2}0]$ and $[\bar{1}100]$ crystal directions, respectively), depending on their set. Figure 4.11 shows the variation in stiffness with orientation from these runs against those analytically calculated; no variation was noted for rotations around the $[0001]$ direction (as expected), so this was not shown. Close agreement was observed, with slight variations occurring at the stationary points whose cause was deemed due to the approximated method for generating the rotated fourth order elasticity tensor in the analytical solution.

Parameter	Value	Units
ρ	1.83×10^{-15}	$\text{kg}/\mu\text{m}^3$
E_1	45.45	GPa
E_2	45.45	GPa
E_3	50.74	GPa
G_{12}	16.75	GPa
G_{23}	16.40	GPa
G_{13}	16.40	GPa
ν_{12}	0.36	
ν_{23}	0.25	
ν_{13}	0.23	

Table 4.1: Density and elastic parameters of WE43, [13] where 1, 2, and 3 represent the X, Y, and Z basis vectors respectively.

Correct activation of slip systems for a given stress field was verified by adopting an approach similar to the elastic verification study, except the material's coordinate system was incrementally rotated around the X, Y, and Z-axes (depending on the set), for Z-axis tensile loaded blocks. The CRSS values used for the basal $\langle a \rangle$, prismatic $\langle a \rangle$, and 2^{nd} order pyramidal $\langle c+a \rangle$ slip systems were 35, 75.8, and 116.7 MPa [13], respectively; hardening was deactivated for this study so the yield stress reflected saturated strain hardening. The variation in yield stress with orientation for both the CPFEM and analytical solutions are shown in Figure 4.12 with close agreement being noted.

To ensure correct implementation of the corotational stress rates and that objectivity was maintained, a single element with a local stress vector of $\sigma_{yy} = 25$ MPa was set to rotate around

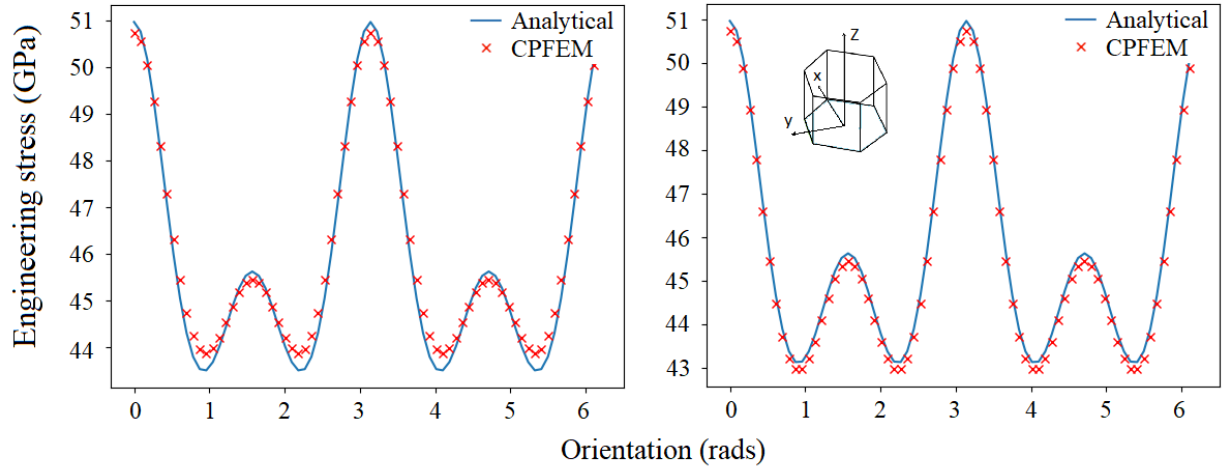


Figure 4.11: Comparison of predicted variation in stiffness with orientation around (left) X-axis ($[11\bar{2}0]$ direction) and (right) Y-axis ($[\bar{1}100]$ direction) for CPFEM and analytical solutions with Z-axis loading. Good agreement verified implementation.

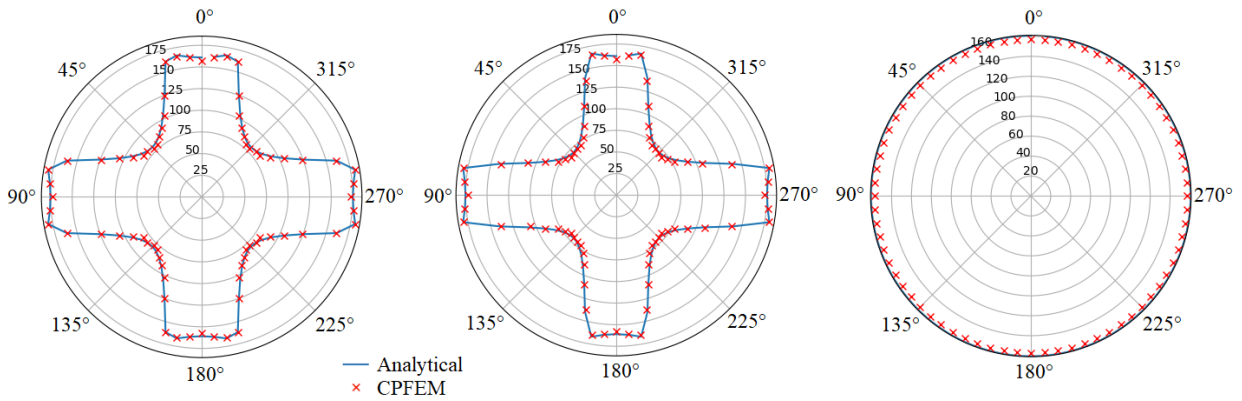


Figure 4.12: Comparison of predicted variation in yield stress with orientation around (left) X, (middle) Y, and (right) Z-axes ($[11\bar{2}0]$, $[\bar{1}100]$, and $[0001]$ directions, respectively) for CPFEM and analytical solution with Z-axis loading. Good agreement verified implementation.

the X-axis ($[11\bar{2}0]$ direction). As shown in Figure 4.13, the expected harmonic response in the global reference frame was predicted (reflecting Mohr's circle).

The implementation of the hardening law detailed in Eq. 4.34 was verified through comparison against experimentally obtained data. As its parameterisation required a representative volume element-sized CPFEM (i.e. sufficiently homogenised stress field), details on how such a model was developed is discussed in the following section.

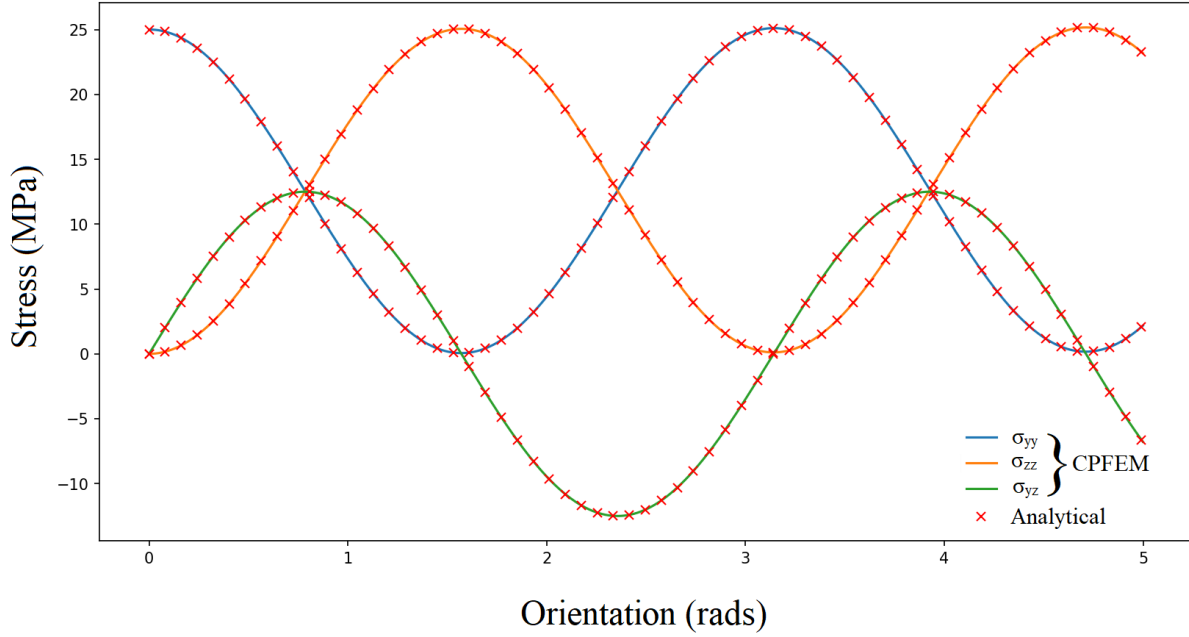


Figure 4.13: Global measured stress state of element first uni-axially loaded to 25 MPa then rotated around X-axis ($[11\bar{2}0]$ direction). The sinusoidal variation shows objectivity. Good agreement between CPFEM and analytical predictions verified implementation.

4.5 Full-field homogenisation scheme

A complexity associated with parameterising the crystal plasticity model is that most experiments characterising a material are conducted using test coupons typically in-between millimetres to centimetres in size. This means the individual hardening response of the various deformation mechanisms of micron-sized magnesium crystals cannot be specifically targeted and characterised. Furthermore, finite element models of large scale components cannot directly consider mesoscale resolutions without adopting some kind of *hierarchical* or *concurrent* multi-scale framework due to the high number of degrees of freedom requiring solved. Therefore, an intermediary step is required to bridge the two. Through use of a *hierarchical* framework and an optimiser it became possible to converge on crystal plasticity-based parameter settings that yielded measured bulk-level mechanical behaviour, and thus provide an approximation of the mesoscale stress field heterogeneity. However, to facilitate this, the limit defining the separation of scales (i.e. a representative volume element) needed determined. It is this activity that is presented in the following.

4.5.1 Sizing polycrystalline structures into RVEs

To define an RVE, and thus satisfy the Hill-Mandel condition [99], the internal energy density stored within the mesoscale should match the energy stored in the material point at the bulk-level. That is, the rate of energy increase or loss across the heterogeneous RVE must match that of the homogeneous reference medium. Therefore, in order to maximise computational efficiency, the homogenisation strategy must seek the minimum volume for which the averaged stress of the heterogeneous mesostructure matches that of the bulk. The average stress over a volume can be represented using the linear momentum balance Eq. 3.7, and noting that tractions are $\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$, through,

$$\frac{1}{v} \int_{\Omega} (\boldsymbol{\sigma}) dv = \frac{1}{v} \left[\int_{\partial\Omega} (\mathbf{t} \otimes \mathbf{x}) da - \int_{\Omega} \rho(\ddot{\mathbf{u}} - \mathbf{b}) \otimes \mathbf{x} dv \right], \quad (4.54)$$

$$\text{with } \sigma_{ij} = \sigma_{ik}\delta_{jk} = \sigma_{ik}x_{j,k}. \quad (4.55)$$

Note, that $\mathbf{t} = 0$ at internal interfaces in equilibrium, therefore internal discontinuities do not need to be considered as stresses are continuous, however, they do need to be considered for strains. Falco et al., 2022, [100] presented a CPFEM RVE sizing strategy based on the convergence of strain energy density with domain size for brittle ceramic-based polycrystalline microstructures. It was this that has been adopted and is presented in the following.

Each time VorTeX was run, unique tessellations statistically equivalent to those described in Section 4.3.1 were generated as the Laguerre-Voronoi algorithm used created unique sphere packings with each execution. These tessellations were then shaped into cubic domains of various sizes that were then spatially discretised into structured raster meshes comprised of uniformly sized hexahedral elements at varying densities (as shown in Figures 4.14 and 4.15) to enable RVE sizing and mesh sensitivity studies. To initiate the process of determining the parameters of the crystal plasticity model, first a model of sufficiently fine mesh resolution, as to maintain likeness of the grain boundaries in the tessellation, and sufficient size, comprised of up to ten grains along each edge, was generated. An algorithm was then set-up to ascertain the crystal plasticity parameters that could reproduce the measured true stress-strain curves of WE43-T6 plate shown in Figure 4.16.

The algorithm used was a metamodel-based optimisation with a sequential domain reduction strategy. A flowchart showing this procedure is shown in Figure 4.17. The optimisation was set

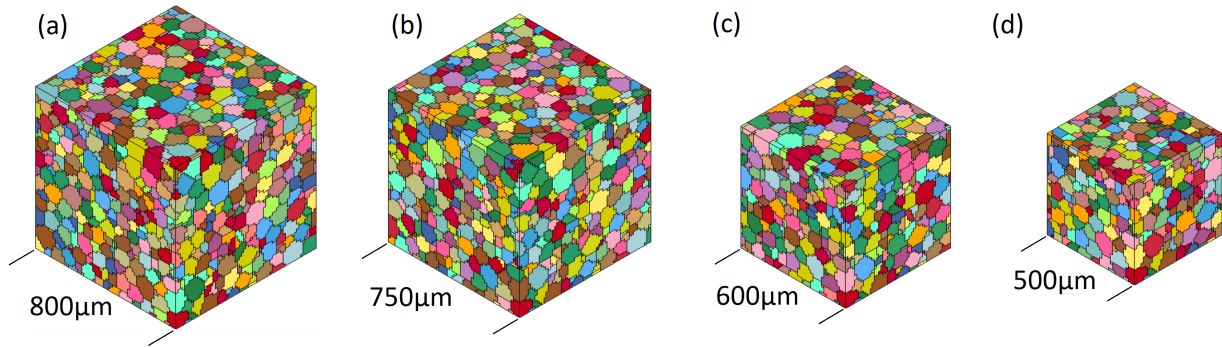


Figure 4.14: Domains of different sizes (Domain edge lengths: (a) 800 μm (b) 750 μm (c) 600 μm (d) 500 μm) from the same tessellation. Element edges have been hidden for clarity.

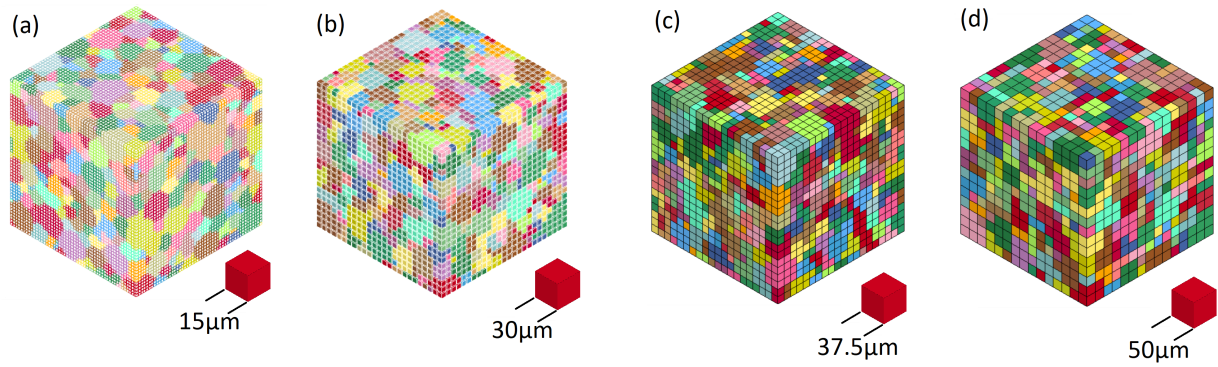


Figure 4.15: Discretisation of equal size domain with elements of varying sizes ((a) 15 μm (b) 30 μm (c) 37.5 μm (d) 50 μm) from a tessellation.

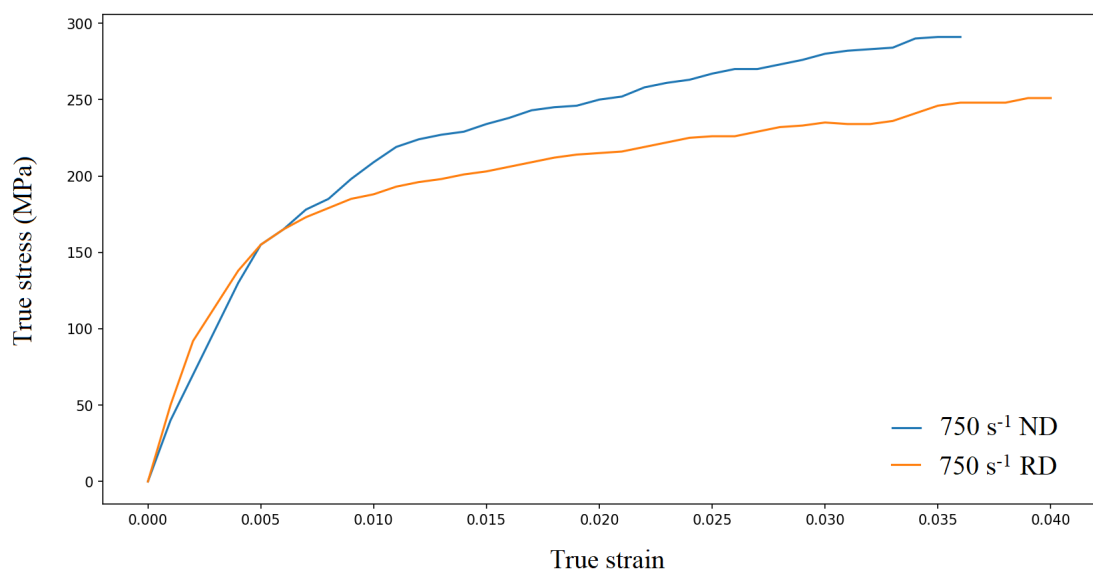


Figure 4.16: Experimentally measured true stress-strain data for WE43-T6 loaded in normal direction (ND) and rolling direction (RD) at 750 s^{-1} [13].

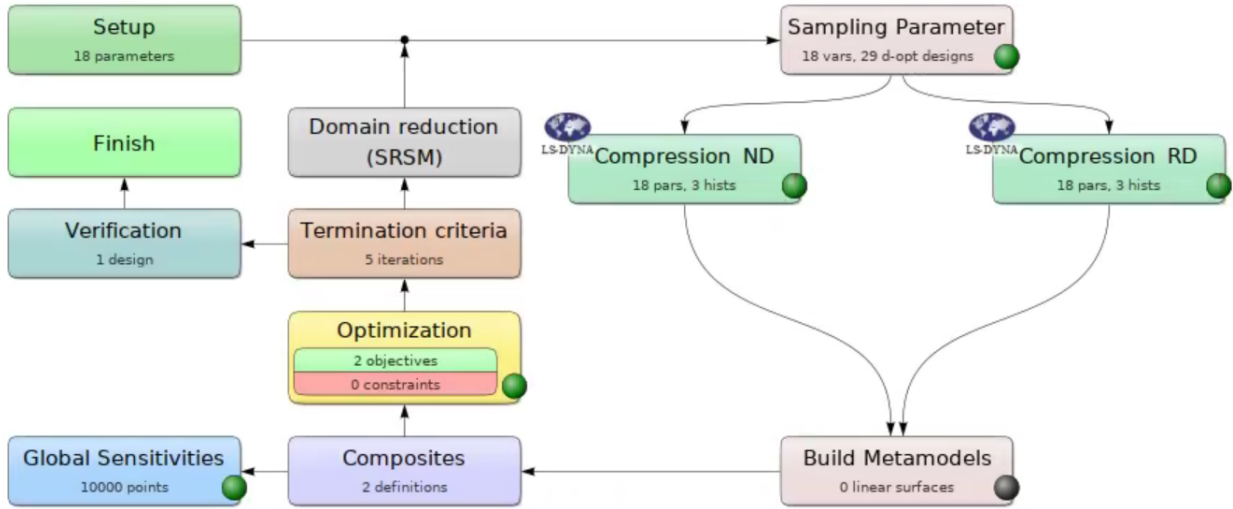


Figure 4.17: Schematic showing optimisation procedure to determine crystal plasticity model parameters for WE43-T6.

to vary the parameters detailed in Table 4.2 within the ranges shown; thermal softening was not invoked for these studies due to a lack of data. Three slip system families were considered for this material system, specifically the basal, prismatic, and 2^{nd} order pyramidal; 1^{st} order pyramidal slip was found to be relatively inactive [13, 36]. Pictorial representations of these slip systems are shown in Figure 4.7. $\{10\bar{1}2\}\langle 10\bar{1}1\rangle$ tension twins were the only twin type considered as Bhattacharyya et al., 2016, [36] showed that they are significantly active compared to others for this particular composition and loading condition. Table 4.3 presents the parameters that were fixed for this optimisation. As the optimisation was set to use D-optimal sampling, 29 CPFEMs were run for each loading condition. The objective of the optimisation was to minimise the mean-square-error, through a curve-matching algorithm, between the experimentally measured true stress-strain data and those predicted by the CPFEMs. The true stress from the CPFEMs were predicted for a given time-step (i.e. a given strain) using,

$$\sigma_{true} = \sum_{i=1}^N \frac{\sigma_i V_i}{V_{Domain}}, \quad (4.56)$$

where i identifies an element within a domain with a total number of N elements. The CPFEMs were constrained in the manner shown in Figure 4.18, where the hashed face represents a boundary condition that prevented translation and rotation around the direction of the displacement vector δu . They were also imparted a strong basal texture like that shown in Platts, 2019 [13]; Figure

Parameter	Minimum	Maximum	Initial	2 nd Initial *	Final *	Units
τ_c Basal	20.0	35.0	35.0	20.0	22.2	MPa
τ_c Prismatic	40.0	75.8	75.8	61.0	63.9	MPa
τ_c 2 nd order pyramidal	80.0	116.7	116.7	90.8	110.0	MPa
$\tau_c \{10\bar{1}2\} < 10\bar{1}1 >$ Tension Twin	5.0	13.0	13.0	8.7	5.7	MPa
H_0 Basal	10.0	1000.0	350.0	44.6	182.8	MPa
H_0 Prismatic	10.0	1500.0	758.0	1253.1	539.3	MPa
H_0 2 nd order pyramidal	10.0	2500.0	1167.0	82.5	812.8	MPa
τ^* Basal	1.05	10.0	1.5	3.88	5.3	-
τ^* Prismatic	1.05	10.0	1.5	3.86	1.9	-
τ^* 2 nd order pyramidal	1.05	10.0	1.5	1.44	1.6	-
q	1.0	1.5	1.4	1.26	1.06	-
m	0.015	0.025	0.02	0.019	0.017	-
h_{HP} Basal	1.0	50.0	25.0	20.1	21.5	MPa $\mu m^{1/2}$
h_{HP} Prismatic	1.0	75.0	37.5	68.7	34.1	MPa $\mu m^{1/2}$
h_{HP} 2 nd order pyramidal	1.0	750.0	375.0	456.5	194.6	MPa $\mu m^{1/2}$
$\dot{\gamma}_0^{\text{twin}}$	10.0	200.0	50.0	17.7	38.6	s ⁻¹
f_g^{PTS}	0.05	0.3	0.06	0.19	0.12	-
τ_g^{PTS}	10.0	25.0	20.0	24.5	11.8	MPa

Table 4.2: Table identifying the variable parameters of the WE43-T6 optimisation, as well as the limits of their search domains, and their optimum settings; the values of τ^* are scaled by τ_c for their respective slip system. Columns denoted * will be discussed later in the text and should not be consulted on first reference to this Table.

4.19 compares pole figures generated using experimentally measured data sampled from hot-rolled WE43-T6 to those generated numerically for use in the CPFEMs. Finally, the optimisation was set to complete after five iterations, with the optimal fit achieved being shown in Figure 4.20.

Even though the optimiser was able to converge on a set of parameters that yielded something close to the experimentally measured mechanical behaviour (MSE of 60.1 and 55.7 for RD and ND, respectively, with a slight deviation observed at the onset of plasticity for ND compression), this was done using a structured raster mesh representation of a polycrystalline structure that may not satisfy the criteria for it to be considered an RVE. Therefore it should be noted that the optimised behaviour may just be specific to the CPFEM realisation and

Parameter	Value	Units
$\dot{\gamma}_0$	1	μs^{-1}
c/a ratio	1.624	-
S^{PTS}	12.89	%
$f_{\text{twin}}^{\text{PTS}}$	1.0	-
PTS Threshold	0.005	-

Table 4.3: Table identifying the fixed parameters of the optimisation.

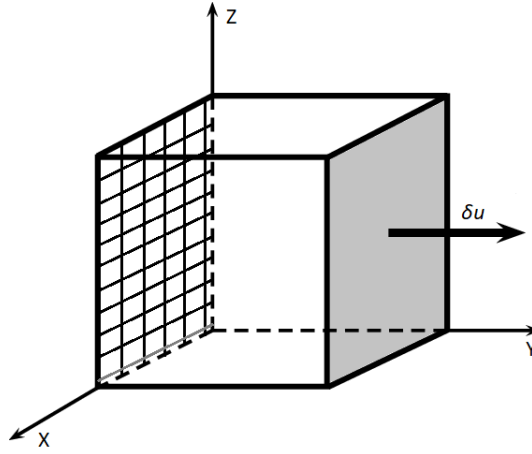


Figure 4.18: Example of prescribed motion boundary condition applied to domains; the hashed face represents a boundary condition that prevented translation and rotation around the direction of the displacement vector δu .

not reflective of homogenised WE43-T6. Therefore, to ensure it is, an RVE sizing study was deemed necessary. Furthermore, the observed deviation could be due to experimental error, or it could be indicative that the converged upon parameters may not reflect that occurring physically, and that the optimiser converged upon a local and not global minima; crystal plasticity-based constitutive models with parameters that are not uniquely defined and are determined through a least squares error minimisation optimisation have been shown to incorrectly predict the stress in individual grains [101]. Consequently, a second optimisation was conducted following the RVE sizing study to be detailed.

To determine the settings required for a structured raster mesh representation of a polycrystalline structure to be considered an RVE, a study was conducted using the converged upon parameters detailed in Table 4.2 (see column 2nd Initial). First, to determine the domain size

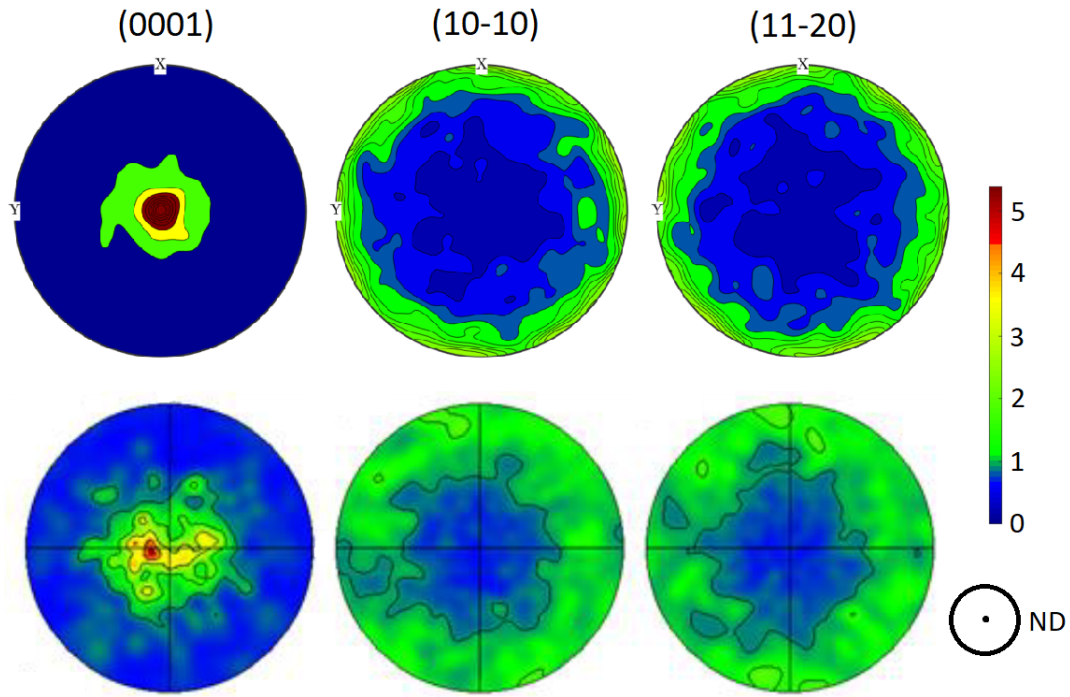


Figure 4.19: Comparison of (top) numerically generated pole figures against (bottom) those generated from experimentally sampled hot-rolled WE43-T6 plate [13].

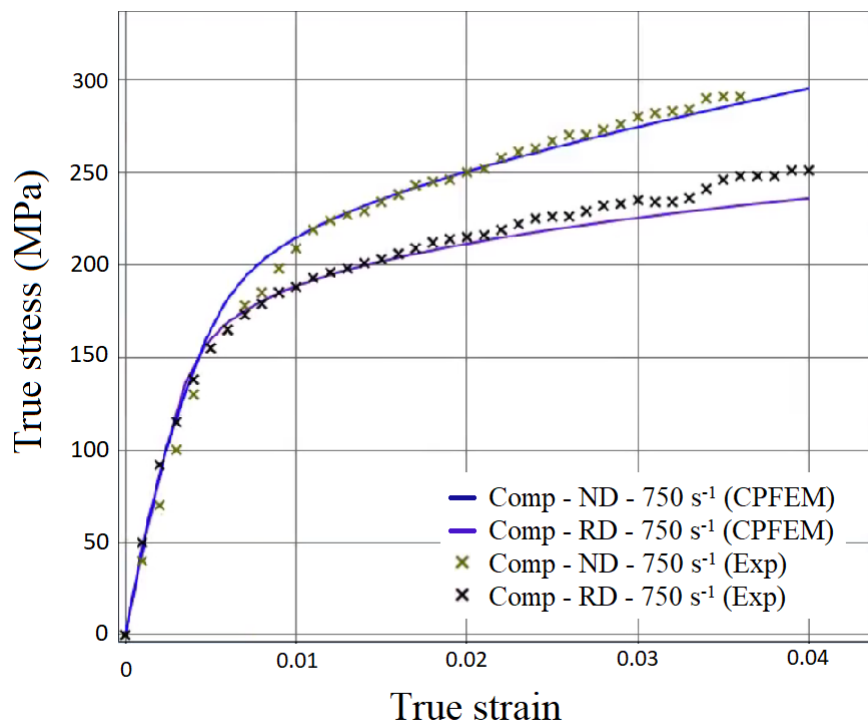


Figure 4.20: CPFEM fits, as per an optimisation after five iterations, to experimentally measured true stress-strain curves reflecting the ND and RD compression of WE43-T6 plate. The MSE prior to any RVE sizing was 60.1 and 55.7 for RD and ND compression, respectively. The parameters that generated these fits were then used to size the CPFEMs into RVEs. The deviation seen during the onset of plasticity for ND compression could be due to parameters being converged upon that do not reflect that occurring physically therefore a follow-up optimisation was deemed necessary.

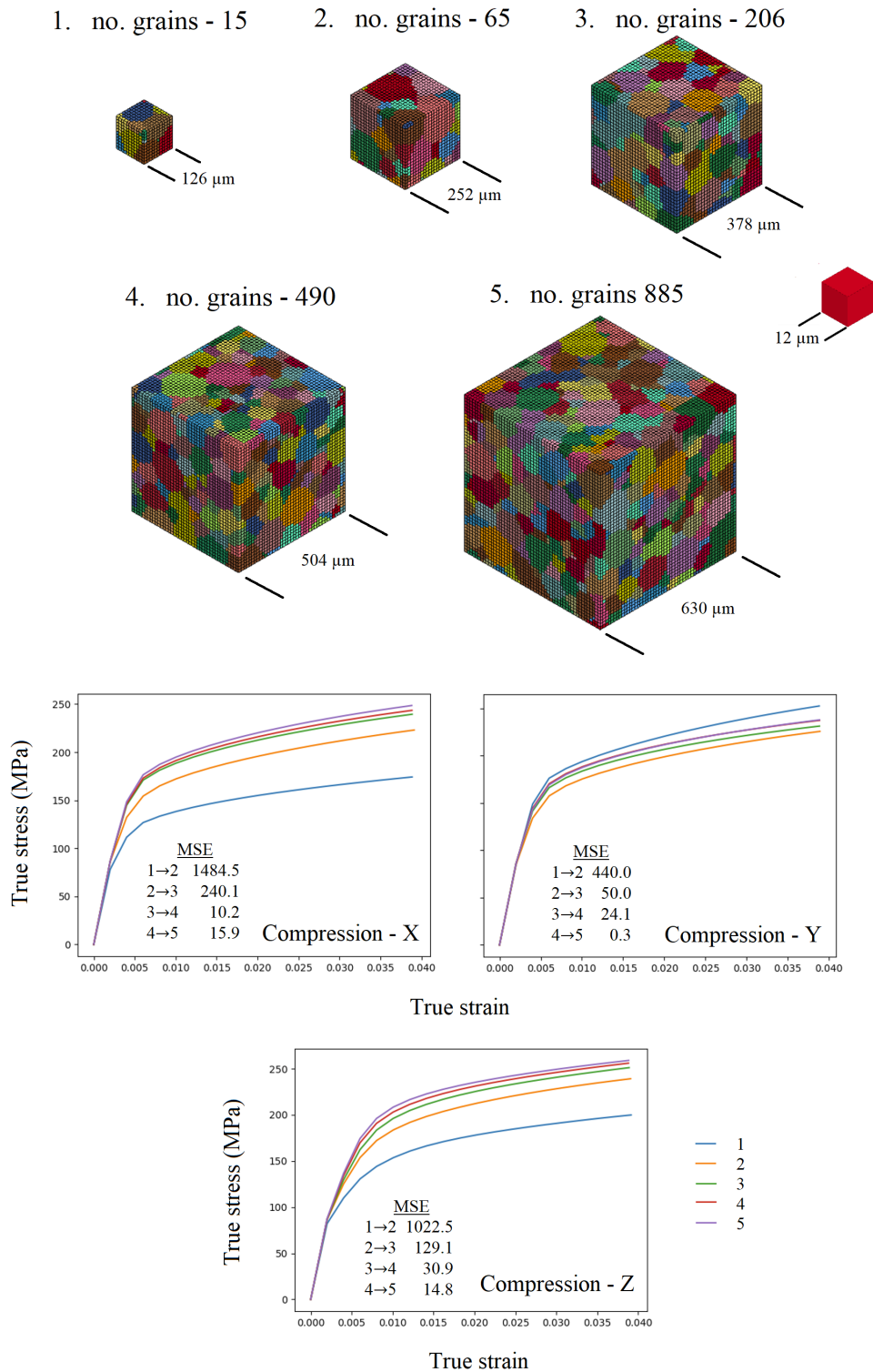


Figure 4.21: Study to determine domain size to constitute a RVE for a CPFEM with a fine mesh ($\sim 12 \mu\text{m}$). Uni-axially loaded CPFEMs of incrementally increasing size had their true stress-strain behaviour plotted and the MSE between adjacently numbered CPFEMs calculated. Convergence was deemed when the MSE for all three load cases was less than 20. Model 5 was regarded as appropriately sized to constitute an RVE.

required, a tessellation realisation was used to seed the generation of CPFEMs that had the same element density as the optimiser's model (~ 578703 per mm^3 , equivalent to cubic element with edge lengths $\sim 12 \mu\text{m}$), but incrementally increasing in size. These CPFEMs were then uni-axially loaded and their true stress-strain responses compared as shown in Figure 4.21. The following condition was then applied to gauge for convergence on the criteria to be considered an RVE,

$$\text{MSE}(\epsilon^x) \leq \text{Threshold} \mid x(\text{size}) \in (\text{Microstructure realisation}), \quad (4.57)$$

where MSE is the mean-square-error between incrementally sized models. Sufficient convergence was deemed when the MSE fell below 20 for all three load cases, which was observed to occur for CPFEMs designated 4 and 5. However, as the runtime for CPFEM 5 was nine hours when run using 8 cores on ARC, mesh sensitivity studies were conducted to see if this could be reduced. Using the converged upon domain size, the element density was then incrementally varied and the resulting true stress-strain curves compared (alongside runtimes) as shown in Figure 4.22.

It was clear that stress-strain behaviour was fairly insensitive to element density (2.4 being the maximum MSE between adjacently numbered models), with lower element densities exhibiting marginally stiffer behaviour toward higher strains; believed to be due to a reduction in degrees of freedom. These results show that this FE-based homogenisation approach was fairly insensitive to the need of detailing highly accurate FE representations of the mesostructure. This was confirmed by the fact that the largest MSE between the curves of the models with the highest and lowest element densities was 53.4 across all three load cases, which was considered low in comparison to the domain size study. However, this was because element sizing that considered the smallest grain size was used. If this was not considered, and the mesh was made too coarse then the CPFEM could violate the conditions required for it to be considered an RVE. Drawing on observations from the sizing study, it was expected that if mesh coarsening resulted in the CPFEMs detailing fewer than 490 grains (through lack of resolution), MSEs against the finest meshed model could be in the order of hundreds. Ultimately though, a significant reduction in runtime was observed between models 7 and 8 (~ 9 hours to 1 hour 31 minutes) for a trade-off in MSE of a maximum 1.8.

One consideration to note is that even though coarsening the mesh resulted in faster runtimes for models that made similar predictions of homogenised behaviour (at the expense of slightly over-predicting stiffness), if models that enable precise insight into the approximated stress

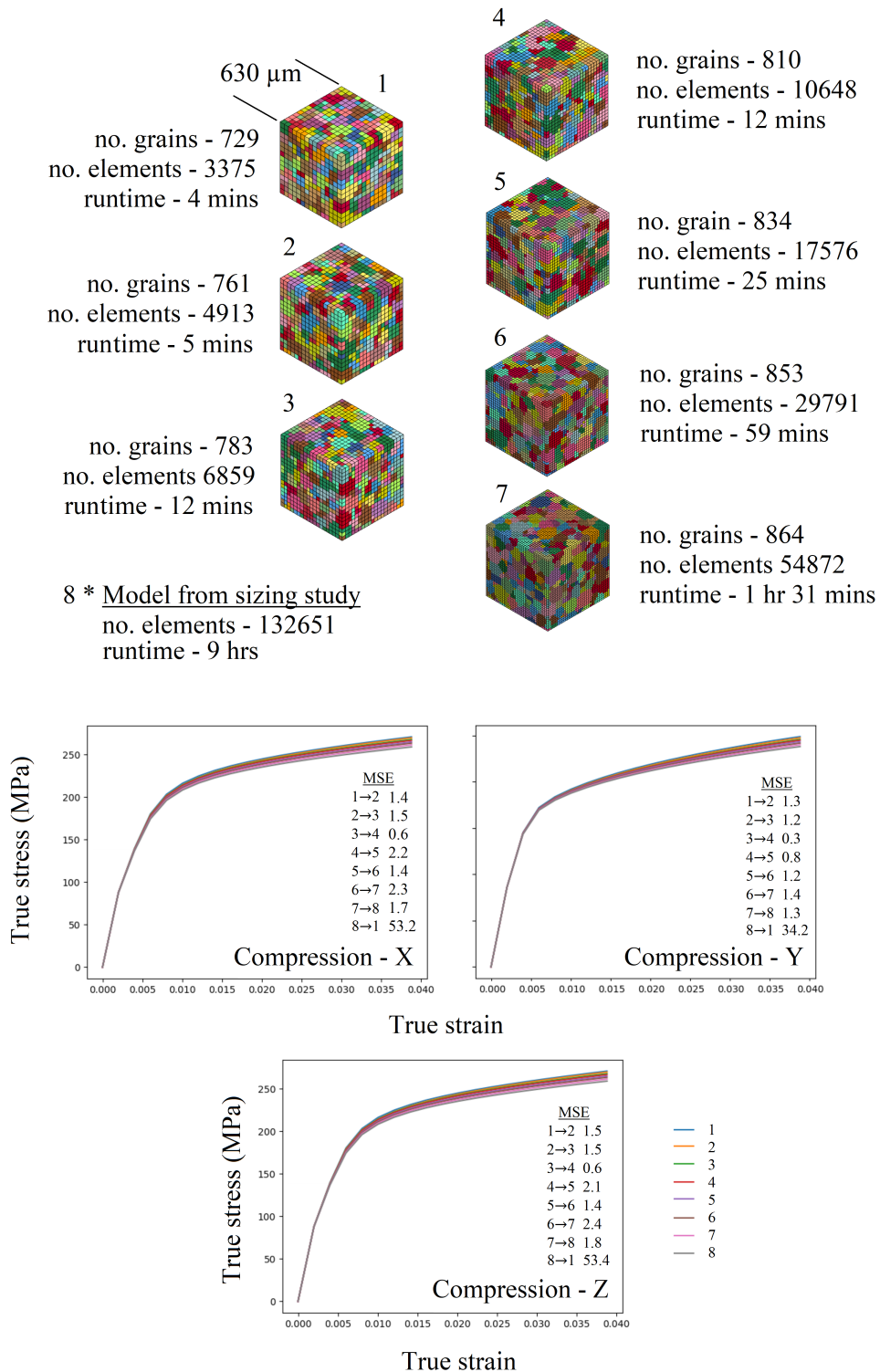


Figure 4.22: Study to determine element density to improve computational efficiency of CPFEMs with cubic domain and 630 μm edge length. Uni-axially loaded CPFEMs of incrementally increasing element density had their true stress-strain behaviour plotted and the MSE between adjacently numbered CPFEMs calculated. All calculated MSEs were less than 2.4, thus showing low sensitivity to element density. However, the MSEs between the CPFEMs with the lowest and highest element densities was notably larger at ~ 50 . Nevertheless, this in comparison to the domain size study was considered low.

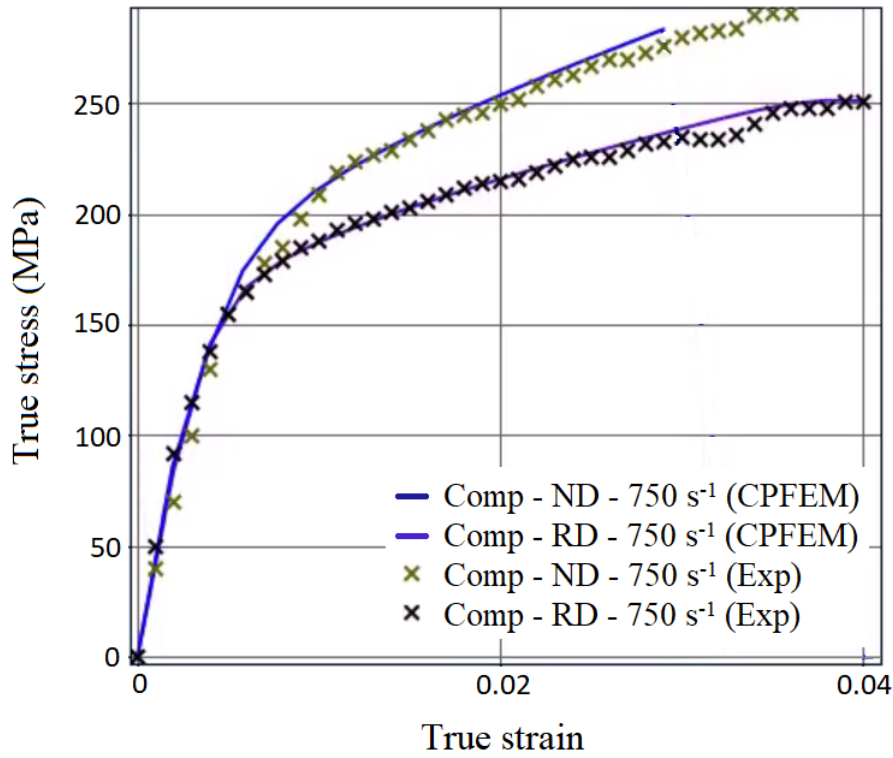


Figure 4.23: RVE-sized CPFEM fits, as per 2nd optimisation after five iterations, to experimentally measured true stress-strain curves reflecting the ND and RD compression of WE43-T6 plate. The MSE was 13.0 and 55.5 for RD and ND compression, respectively.

field heterogeneity are required (e.g. stress around grain boundaries) then a finer mesh would be preferred. As all the programs currently utilised have been made to work on the high-performance computing cluster, ARC, the settings of model 7 in the element sizing study were used moving forward. This was because it maintained the best representation of the generated numerically-based tessellation and because the ability to massively parallelise any subsequent runs meant an extra 1 hour 6 minutes (difference in runtime between models 5 and 7) was not deemed too costly. Now that optimal model settings for the CPFEM to be considered an RVE have been determined, the optimisation was re-run to see if the fits initially converged upon could be improved. The resulting parameters are presented in Table 4.2 (see column Final) and the fits achieved are shown in Figure 4.23. An improvement was observed with the MSE reducing to 13.0 from 60.1 and 55.5 from 55.7 for RD and ND compression, respectively.

The performance of the optimiser was dependent on the accuracy of the meta-model, and as such, approximation error indicators (see Figure 4.24) were used to assess it. The strong positive correlation observed gave confidence that the meta-model provided a good approximation. On-top of converging upon parameters to achieve a fit to a curve, the optimiser

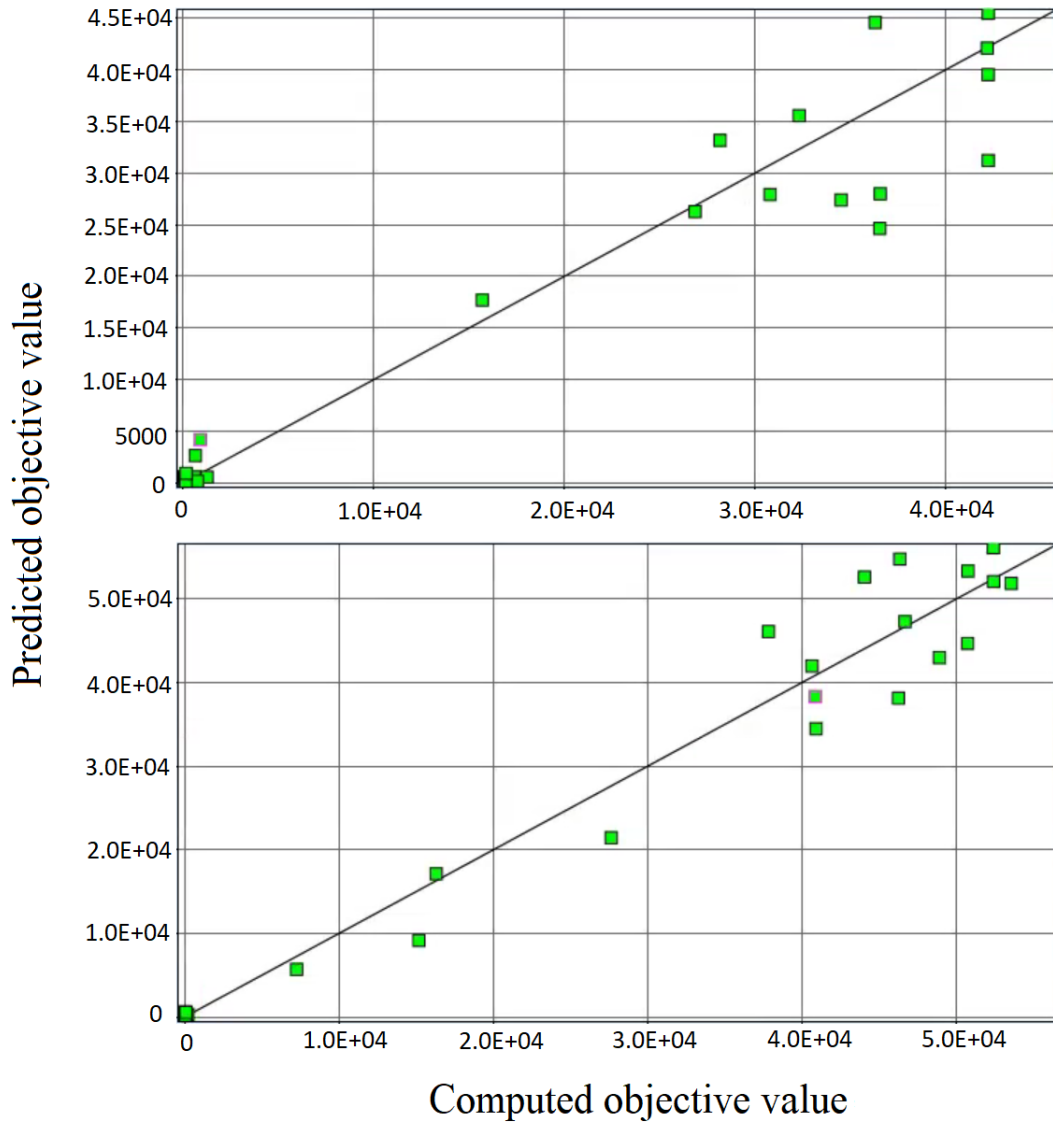


Figure 4.24: Assessment of meta-model accuracy via comparison of computed and predicted composite values for rolling (top) and normal (bottom) directions. The strong positive correlation indicated good accuracy.

can also provide insight on the sensitivities of the parameters (see Figure 4.25). It is this information that could be used by material scientists to aid with designing a material for a specific application as these parameters reflect the interaction of different solutes and precipitates to various plasticity mechanisms (e.g. It was clear that H_0^{Basel} contributes the most to mechanical behaviour for both loading conditions). Now that parameters have been converged upon that yield homogenised constitutive behaviour consistent with those experimentally measured, the insights offered by full-field CPFEMs are presented.

Figure 4.26 shows the heterogeneity in the von Mises stress fields that develop within the

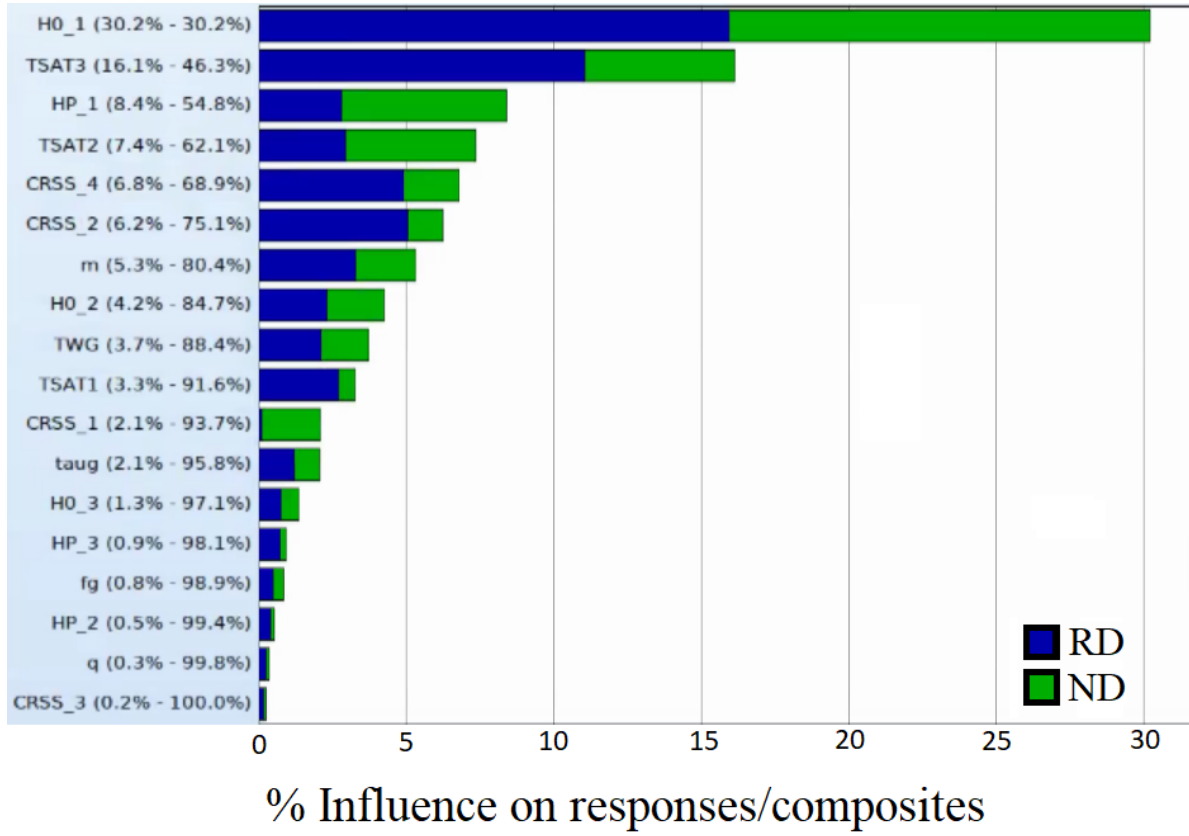


Figure 4.25: Bar chart showing the sensitivities of the parameters of the crystal plasticity-based constitutive model (as assessed by the optimiser) to achieve the fit shown in Figure 4.20.

CPFEMs. As observed, various grains have orientations, shapes, and sizes that can either build or relax stress. One capability that was implemented into the crystal plasticity-based user-subroutine was the ability to track the relative activity of the various deformation mechanisms within the elements. This was done by implementing the relative activity tracker [51],

$$\text{relative activity}_{\kappa} = \frac{\dot{\gamma}_{\kappa}}{\sum_{\kappa+\alpha} \dot{\gamma}} \quad (\text{slip-based}) \quad (4.58)$$

$$\text{relative activity}_{\alpha} = \frac{\dot{\gamma}_{\alpha}}{\sum_{\kappa+\alpha} \dot{\gamma}} \quad (\text{twin-based}) \quad (4.59)$$

that was based on shearing rates. Figure 4.27 shows the evolution of this activity with engineering strain for an arbitrarily selected grain. For the normal direction compressed CPFEM, the basal slip system family was found to be dominant. Whereas, for the rolling direction compressed CPFEM, first pseudo slip that contributes to the prediction of the twin volume fraction was dominant, after which basal slip then became dominant. However, once the volume fraction reached the threshold value for twin nucleation, basal slip in the

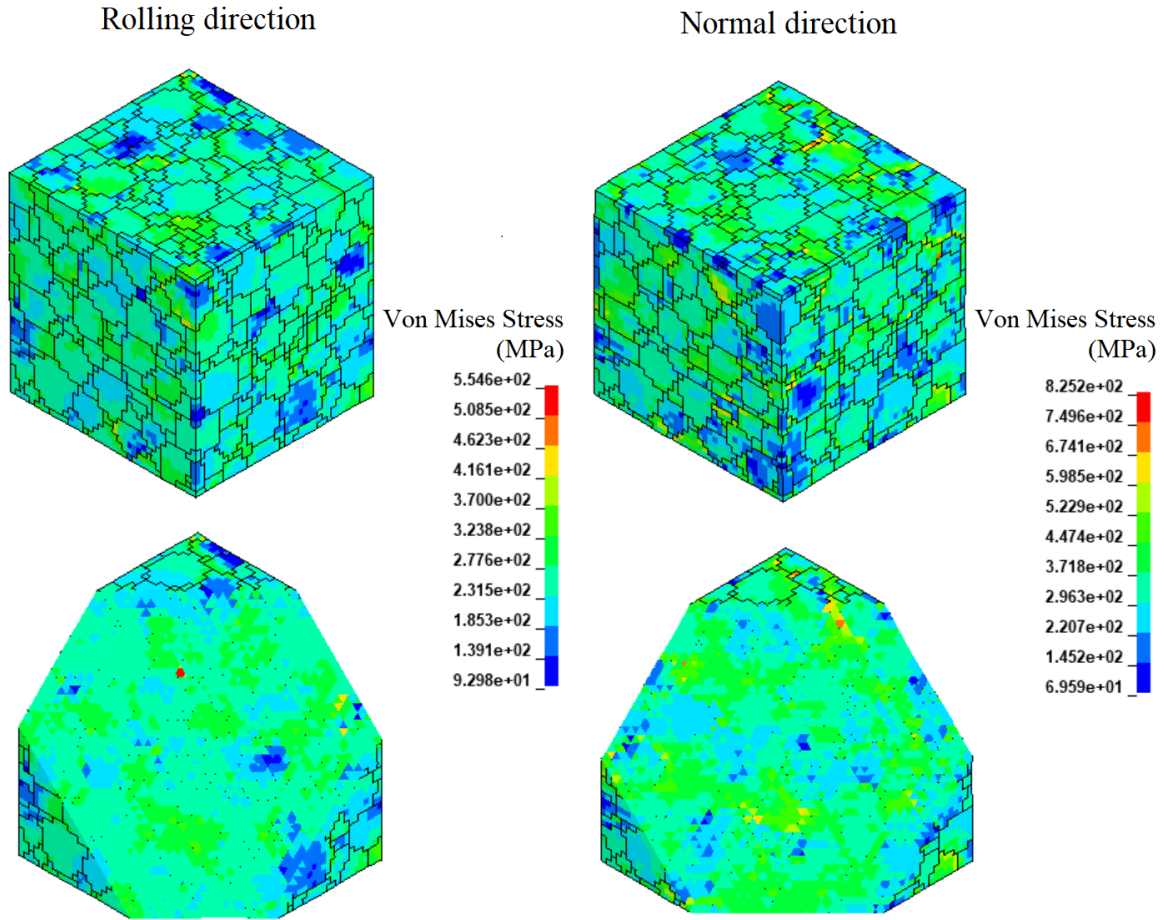


Figure 4.26: Examples of heterogeneity in von Mises stress fields for converged upon CPFEMs after $\epsilon_{\text{eng}} = 4\%$.

twinned domain became dominant.

Figure 4.28 shows the predicted twin volume evolution for the same grain, and as expected tension twin activation was not predicted for normal direction compression, whereas it was for rolling direction compression (this activation was expected due to Poisson related effects). Confidence was gained in the model's twin volume fraction predictive capabilities as they are close to those experimentally measured by Feather et al., 2019, [9] for equivalent loading conditions (see Figure 4.28). Figure 4.29 then proceeded to show the formation of these twins, as well as those in every other element of the CPFEM, through texture evolution as told by pole-figures (formation of contours in the centre of the hemispheres above and below the initial basal poles indicate tension twins); similar tension twin activation is expected with transverse direction compression. Even though the shearing rate due to slip was predicted through a power-law (giving it rate-dependence), and that the pseudo slip rule used to predict twin volume

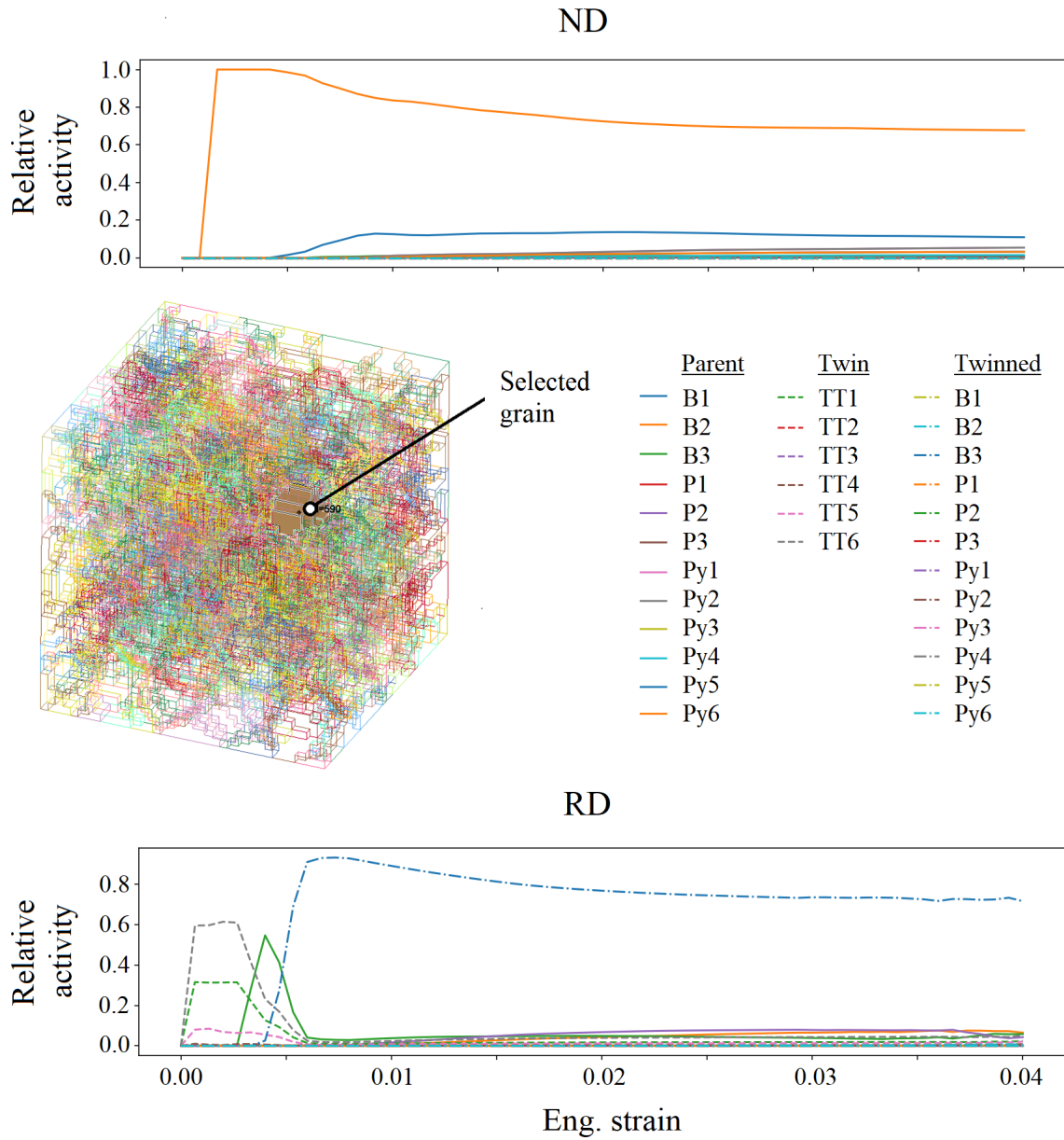


Figure 4.27: Plots showing the relative activity of the available deformation mechanisms in selected grain for RVEs loaded under compression along the normal (top) and rolling (bottom) directions. Deformation mechanisms have been given different line-styles depending on whether they are in the parent or twinned domain. Twin activity has also been given its own line-style.

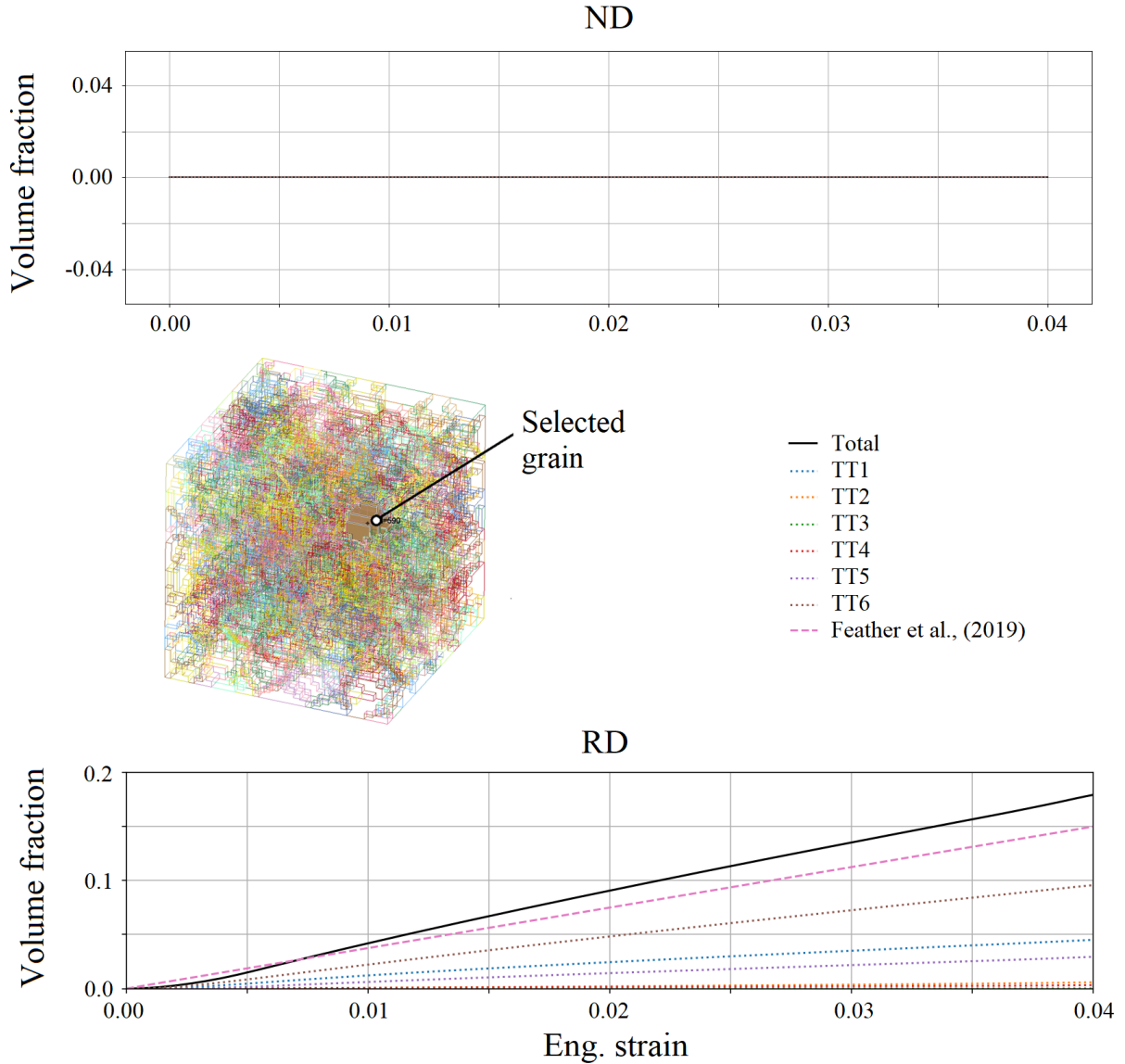


Figure 4.28: Plots showing the prediction of tension twin volume fractions in selected grain for CPFEMs loaded under compression along the normal (top) and rolling (bottom) directions. The total tension twin volume fraction was compared against that measured in Feather et al., (2019) (linear fit from (0, 0) to the first measured value for equivalent load cases), and good agreement was observed.

fraction growth only considered the RSS over the CRSS ($\frac{\tau^\alpha}{\tau_c^\alpha}$) (thus being rate-independent), Figure 4.30 showed that the CPFEM compressed in the rolling direction exhibited more rate-sensitivity, even though tension twins were activated for only this load case. This sensitivity was expected to be due to the basal slip systems in the twinned domain being positioned in such a way that the stress field projected onto them resulted in a higher Schmid's factor, and thus a higher shearing rate. As it was difficult to discern the extent of experimentally measured rate-dependence from Figure 1.2, it was not possible to verify the accuracy of the

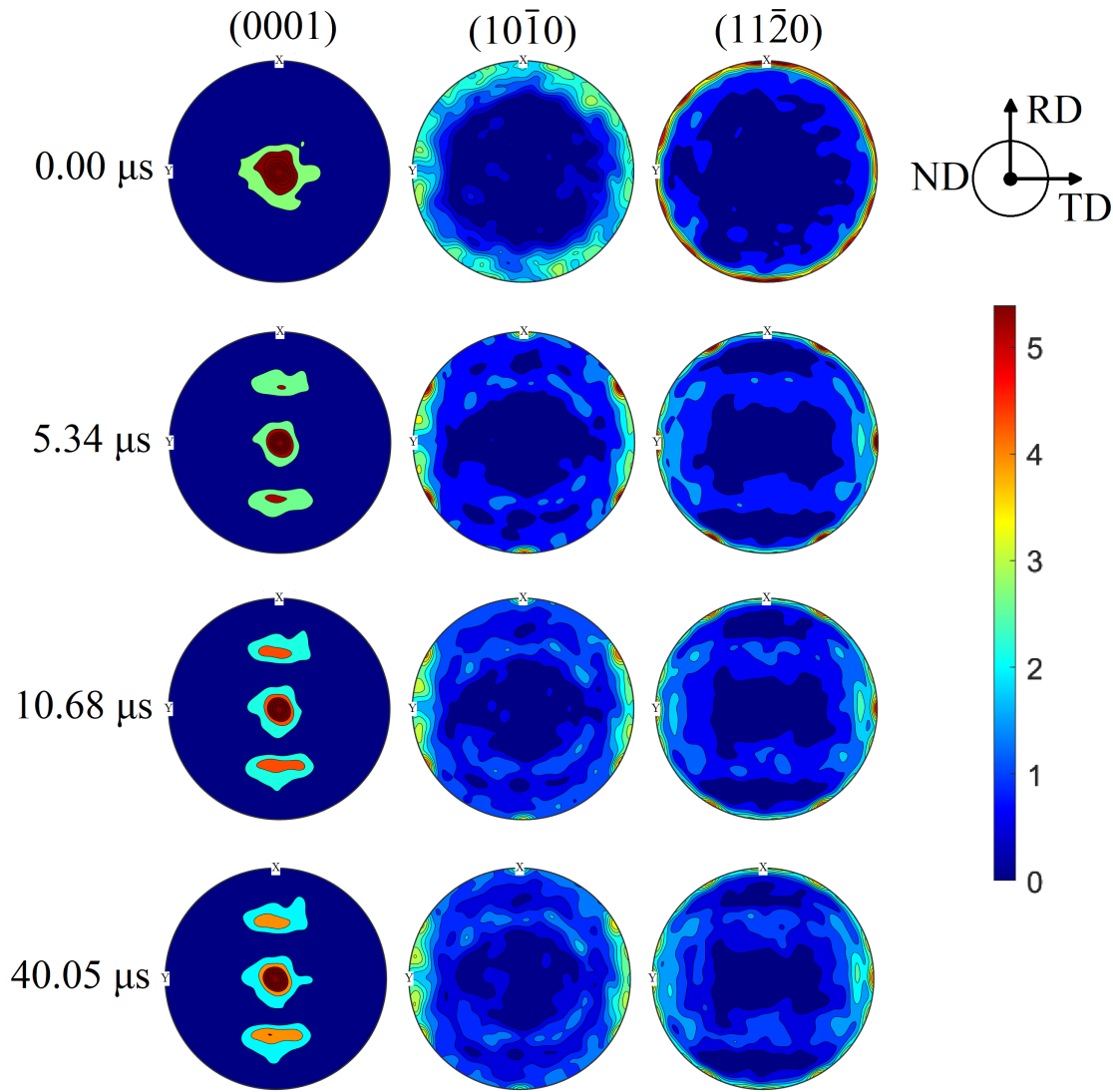


Figure 4.29: Texture evolution as told through pole figures of CPFEM loaded in compression along the rolling direction. Twin nucleation is identified through the formation of contours in the centre of the hemispheres above and below the initial basal poles.

CPFEM's rate-dependence predictive capability. However, the expected general trend does seem to be observed (flow stress increases with strain-rate).

In addition to the power-law hardening exhibited by the CPFEMs, appropriately modelled CPFEMs should also be able to predict the up-turn in flow stress observed for in-plane compressed magnesium alloy AZ31B-O sheet (as shown in Figure 1.1). This up-turn exhibited the majority of this material system's rate-dependence for in-plane loading and offers the ability to verify whether twin formation is rate-independent as stated by Kurukuri et al., (2014) [8]. To facilitate this, the following section details the development of AZ31B-O-based CPFEMs. Another capability that was developed into the user-subroutine, that was not activated due

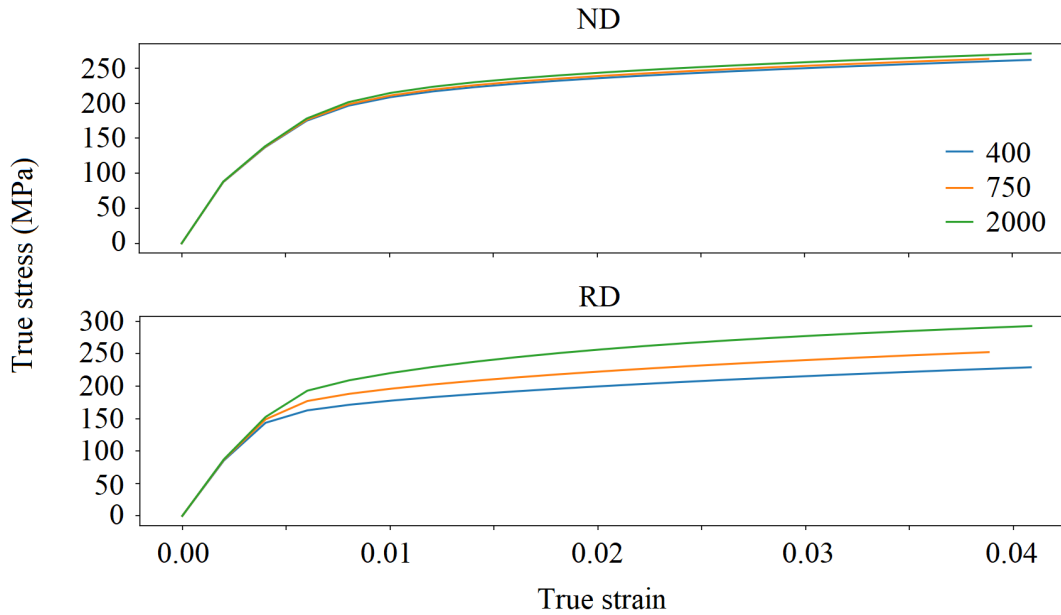


Figure 4.30: Plots showing the variation in flow-stress with strain-rate for CPFEMs compressed in the normal (top) and rolling (bottom) directions.

to a lack of data, was thermal softening. In spite of this, CPFEMs with it considered were run to check whether the correct general trends were predicted. The results from these are discussed in the chapter concerning future work (Chapter 6).

4.5.2 Application of homogenisation scheme to sheet AZ31B-O

The methodology detailed in the previous section was used to generate statistically equivalent tessellations representative of a micrograph of rolled AZ31B [102]. Figure 4.31 highlights the key results of this, and as shown, both quantitative (error never exceeded 2%) and qualitative likeness was achieved. One matter to note is that the grain areas from the EBSD were used to infer the radii of the spheres used in the packing by the tessellation, therefore resulting in equiaxed grains. The consequence of this is that the capacity to model the elliptically shaped grains seen to manifest in Figure 4.31 (1) was lacking; these grains are seen to predominantly have their major axis preferably oriented along a single direction. To consider grains with such shapes, the tessellation could be stretched. However, this was not deemed a priority and was not attempted. Having now determined the input parameters for VorTeX to produce statistically equivalent tessellations of AZ31B-O sheet, attention turned to determining the settings required for the CPFEM to constitute an RVE.

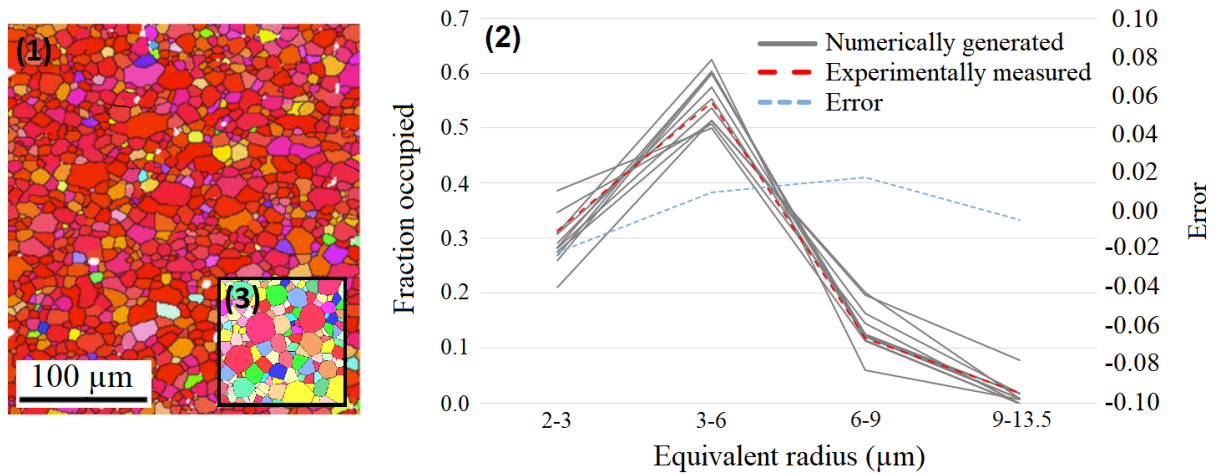


Figure 4.31: Figures highlighting process to generate statistical equivalent tessellations of rolled AZ31B. (1) EBSD micrograph of AZ31B-O [102]. (2) Comparison of equivalent grain radii measured from regularly spaced slices of a numerically generated tessellation (each line represents a slice) to that measured from (1). The error compares the average of those generated numerically to that experimentally measured. This was not seen to go above 2%. (3) Numerically generated tessellation compared to (1) to highlight likeness achieved.

With the knowledge that the constitutive behaviour of CPFEMs are fairly insensitive to element density, a coarse finite element representation of the tessellation (comprising more than 10 grains per edge) was used for the optimisation, with the same inputs to produce the strong basal texture for the WE43-T6 CPFEM also being used. The curves used as the objectives are those shown previously in Figure 1.1, and due to symmetry, only the specimens loaded in tension and compression in the rolling direction, and in compression in the normal direction were studied. To limit the number of stages, a strain-rate of 1000 s^{-1} was only considered. Figure 4.32 presents the fit, with Table 4.4 detailing the parameters to achieve it.

As shown, parameters were converged upon that could reproduce the shapes of the flow stress for each load case indicating that the formulated crystal plasticity-based constitutive model possessed all the necessary physics. However, as the objective curves only captured the plastic flow regimes, the prediction of the onset of yield to early plasticity was seen to deviate, especially for the tensile loaded and rolling direction compressed specimens. It was expected that a better fit would be achieved if the entire stress-strain response (including elastic deformation) was used; the elastic properties shown in Table 4.1 were used in this instance and may not reflect those experimentally measured. Additionally, the deviation of the rolling direction compressed CPFEM just post yield to the re-hardening regime was expected to be due to a combination of the slip systems' strain-based hardening law and the adopted homogenised-twin formulation.

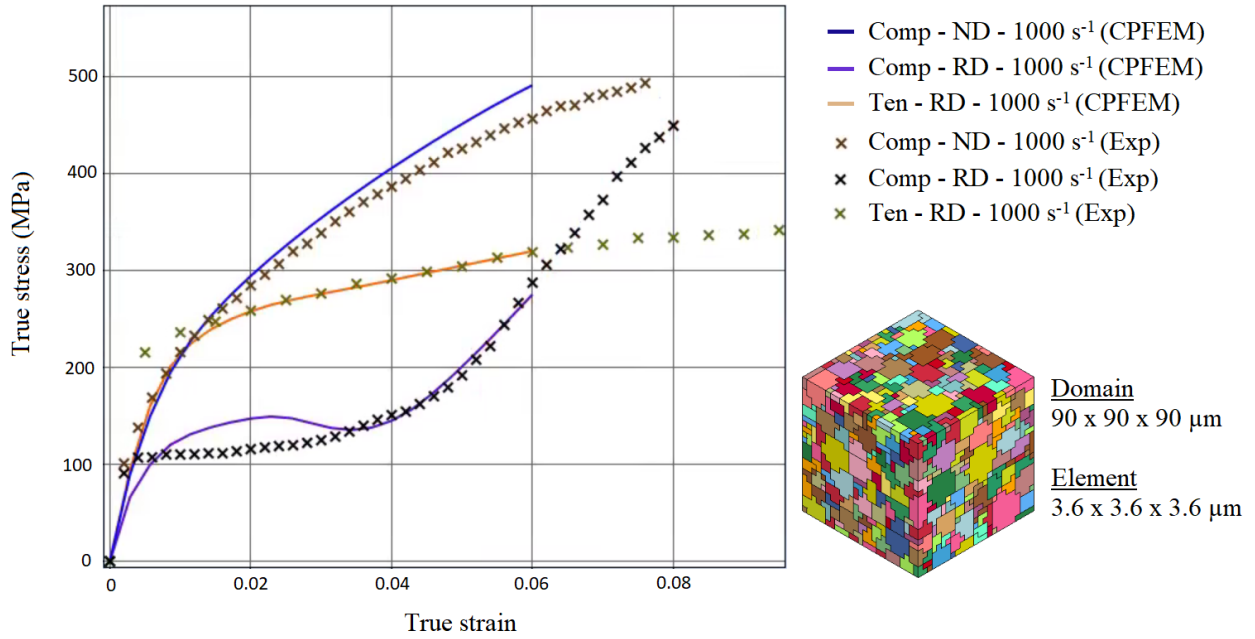


Figure 4.32: CPFEM fits, after six iterations, to experimentally measured true stress-strain data for AZ31B. MSEs of 85.1, 248.6, and 126.9 were reported for ND compression, RD compression, and RD tension-based CPFEMs, respectively.

Figure 4.33 presents the activity of the various deformation mechanisms for an arbitrarily selected grain. It shows that twinning coincided with yielding, with basal slip in the twinned domain driving the plateau in the flow stress. Once the twinned domain became saturated (sufficiently hardened), twinning was again activated, thus growing the twins and causing the Hall-Petch hardening of the slip systems in the parent grain, which is seen as the up-turn in flow stress; it should be noted that this reflects only one grain (not the entire CPFEM) and so these levels of relative activity should be used for indicative purposes. The rounded profile at the onset of yielding was due to the homogenised twin implementation adopted. A flatter plateau could be realised if twins were made to localise more acutely, thus resulting in the observed sharp yielding. This would then subsequently see the basal slip systems in the twin domain more suddenly favourably orientated for their sole activation, hence extending the plateau.

Now that a parameter set has been converged upon that yields the measured mechanical behaviour for the three load cases, the CPFEM underwent a sizing study to determine the settings required for it to be considered an RVE.

Since fewer runs were required for determining RVE settings compared to the optimisation, a CPFEM with a higher mesh density (compared to that of the optimisation) was used as the

Parameter	Minimum	Maximum	Final	Units
τ_c Basal	1.0	20.0	1.7	MPa
τ_c Prismatic	2.0	61.0	60.7	MPa
τ_c 2 nd order pyramidal	10.0	90.8	66.2	MPa
τ_c {10 $\bar{1}2$ }<10 $\bar{1}1$ > Tension Twin	1.0	8.7	1.5	MPa
H_0 Basal	10.0	2000.0	223.9	MPa
H_0 Prismatic	10.0	2500.0	1367.0	MPa
H_0 2 nd order pyramidal	10.0	3500.0	1850.7	MPa
τ^* Basal	1.05	10.0	8.9	-
τ^* Prismatic	1.05	10.0	1.1	-
τ^* 2 nd order pyramidal	1.05	10.0	7.3	-
q	1.0	1.5	1.1	-
m	0.015	0.025	0.018	-
h_{HP} Basal	1.0	50.0	29.7	MPa $\mu m^{1/2}$
h_{HP} Prismatic	1.0	75.0	65.9	MPa $\mu m^{1/2}$
h_{HP} 2 nd order pyramidal	1.0	750.0	239.8	MPa $\mu m^{1/2}$
$\dot{\gamma}_0^{\text{twin}}$	10.0	200.0	179.7	s ⁻¹
f_g^{PTS}	0.05	0.3	0.12	-
τ_g^{PTS}	10.0	25.0	12.0	MPa

Table 4.4: Table identifying the variable parameters of the AZ31B-O optimisation, as well as the limits of their search domains, and their optimum settings; the values of τ^* are scaled by τ_c for their respective slip system.

impact of longer runtimes was less; element edge length decreased from 3.65 μm to 2.75 μm . As for the WE43-T6 study, multiple simulations (for the concerned loading conditions) with fixed element density but increasing domain size were run and their true stress-strain responses compared to assess convergence on the criteria to be considered an RVE. As illustrated in Figure 4.34, the mean-square error between curves 4, 5, and 6, which represent domain widths of 60, 75, and 90 μm , respectively, were sufficiently low (<10.6) to indicate an RVE. Using the 90 μm wide domain CPFEM, an element size sensitivity study was then conducted (cubic elements with edge lengths 2.75, 3.2, 3.65, 4.1, 4.55, and 5.0 μm considered), whose results are presented in Figure 4.35. These models were subjected to the same loading conditions as the domain sizing study. As shown, the CPFEMs were fairly insensitive to element density for

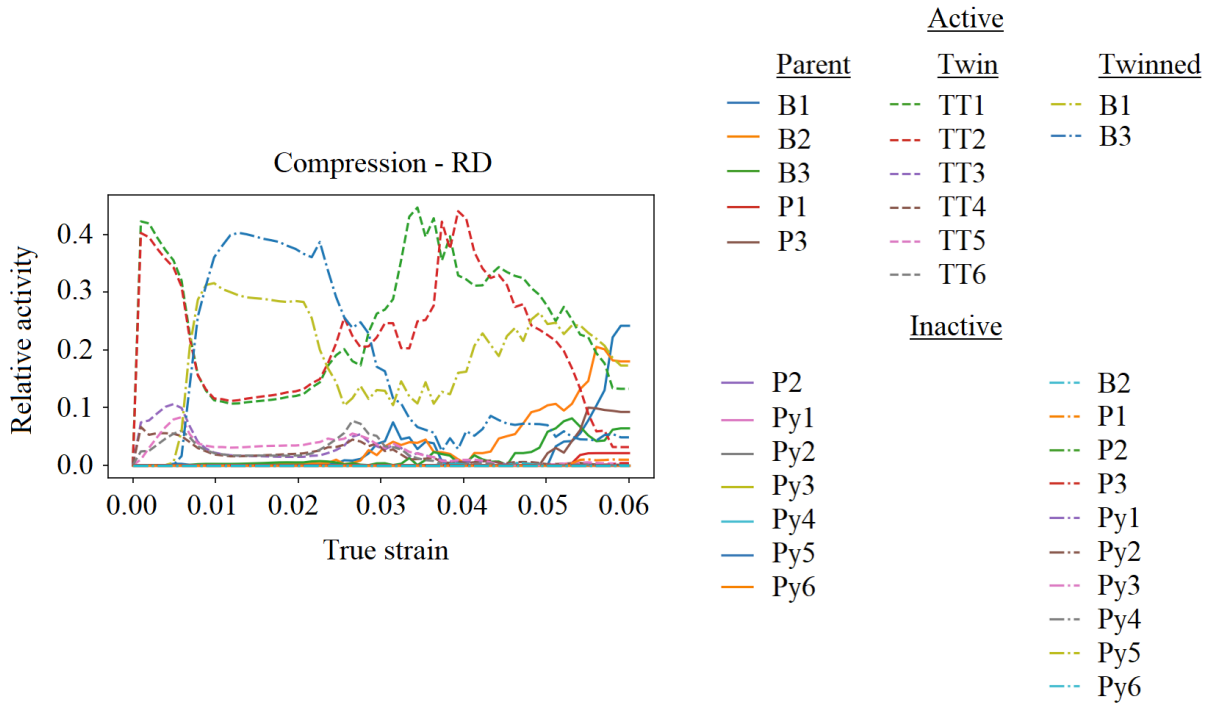


Figure 4.33: Plot showing the relative activity (see Eq. 4.58) of the various deformation mechanisms for an arbitrarily selected grain within the RD compressed CPFEM. Twinning was initially most active (0.0→~0.007 strain), after which basal slip in the twinned domain became dominant (~0.007→~0.025 strain). Twinning was then again observed to become the primary deformation mode (~0.025→~0.055 strain), with it then being overtaken by basal slip in the parent domain.

the element sizes studied. Because of this, the optimisation was not rerun as it was believed that the converged upon settings were adequate.

The strain-rate dependence of the CPFEMs were assessed by varying the rate at which the loading was applied, with the results for 500 s^{-1} and 1000 s^{-1} being presented in Figure 4.36. The expected general trends were not observed for the converged upon parameter set. For example, the up-turn in flow stress for the lower rate RD compressed specimen was observed to occur earlier at a lower strain than expected, and its gradient increased instead of decreased. Furthermore, ND compressed and RD tensioned CPFEMs exhibited minimal strain-rate dependence. It was believed that this did not reflect a problem with developed formulation, but instead with the parameter set converged upon during the optimisation which only considered one strain-rate. Therefore, to remedy this, it is recommended that any further optimisations should consider various strain-rates as part of its objective.

An opportunity offered by fully realising mesostructural stress fields is that the uncertainty arising from their aleatoric nature could be quantified (as each realisation is unique). In doing so,

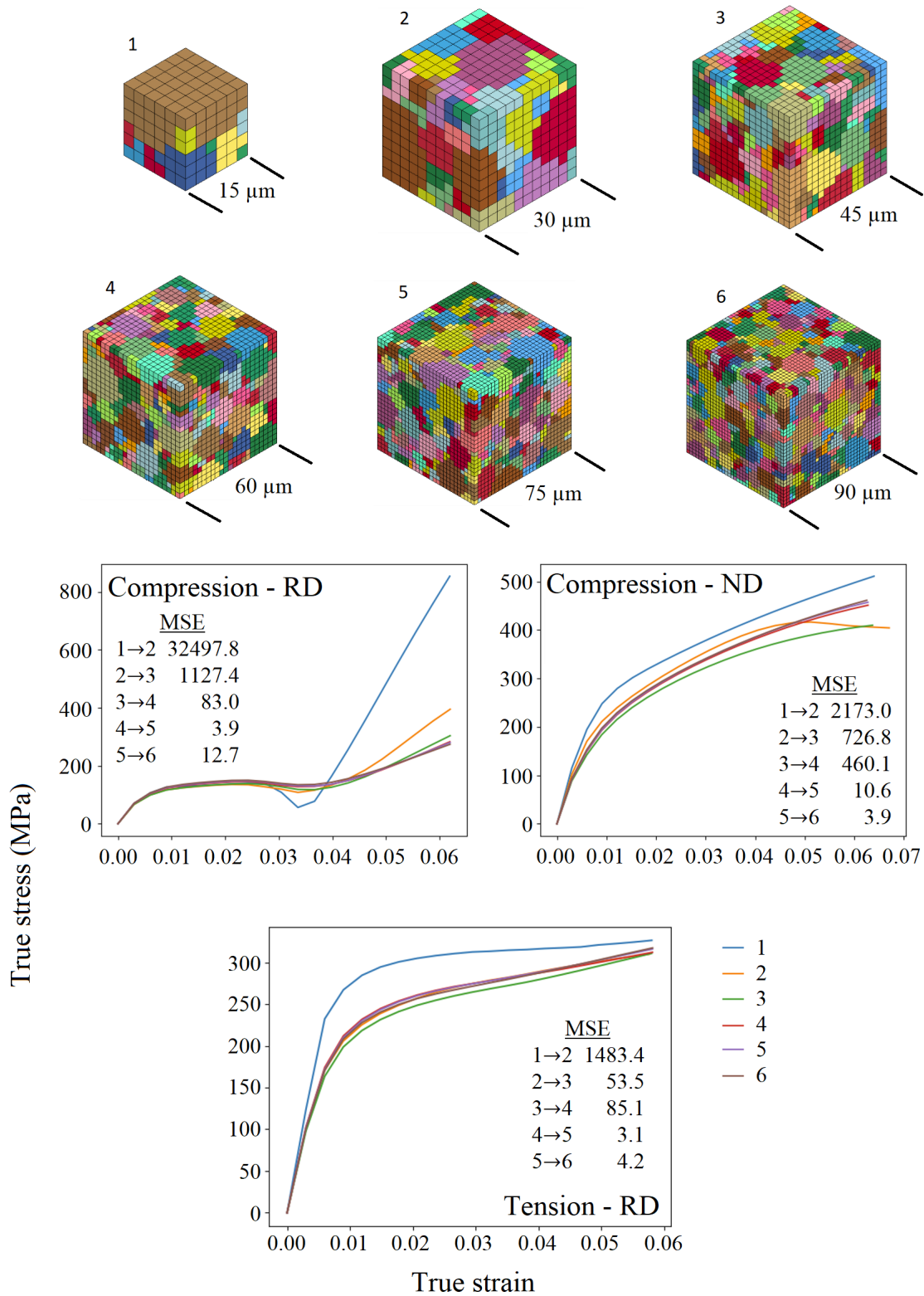


Figure 4.34: Study to determine domain size to constitute an RVE for CPFEMs of AZ31B-O using an element size of $2.75\mu\text{m}$. (Top) Designation of models used in study alongside their respective edge lengths. (Bottom) Comparison of true stress-strain curves for considered loaded cases. The MSE between adjacently numbered curves were computed and presented to gauge convergence. The threshold was set at 50.0 and was satisfied for all load cases from model 4 onward.

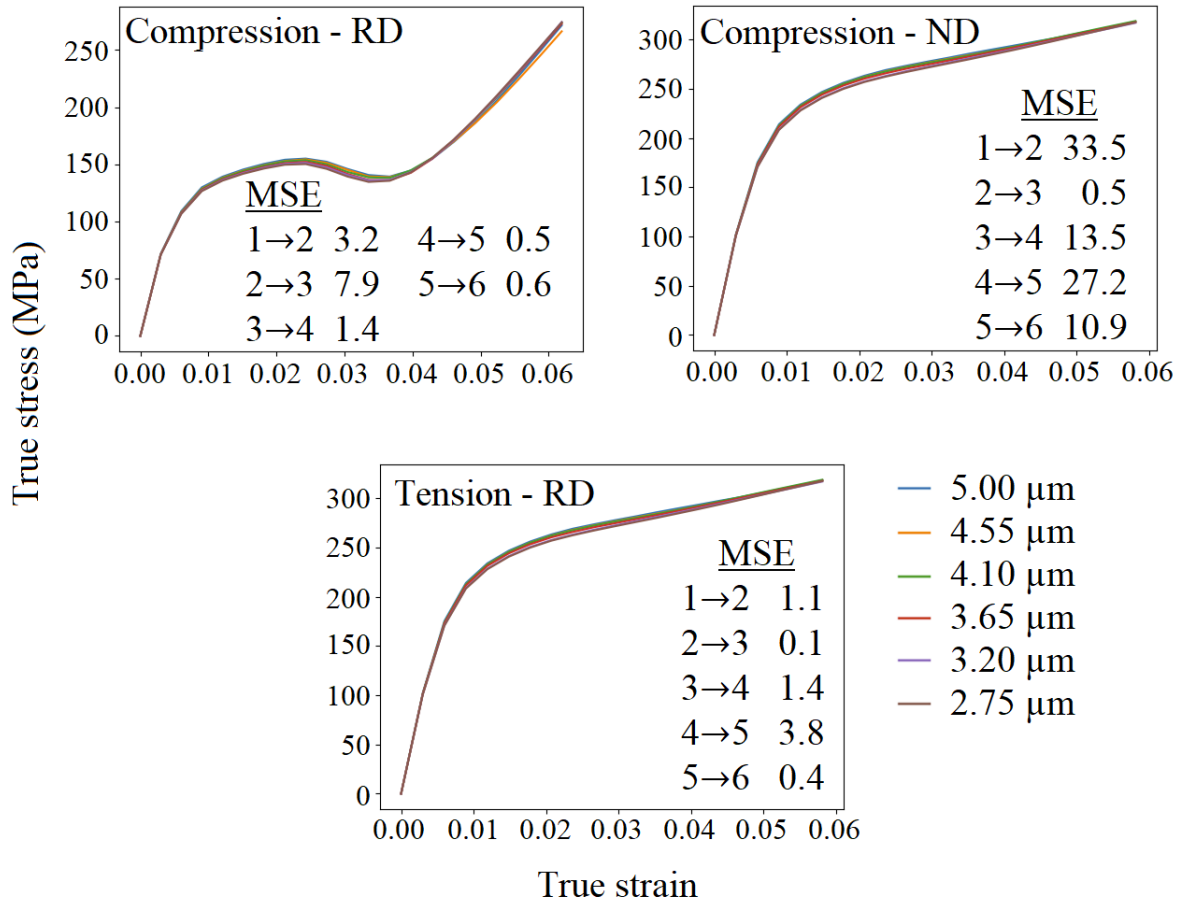


Figure 4.35: Study to determine mesh sensitivity of AZ31B-O cubic domain CPFEM with edge length $90 \mu\text{m}$. The element densities considered were (1) $\frac{18}{90} = 0.2 \mu\text{m}^{-1} \rightarrow$ (6) $\frac{33}{90} = \sim 0.37 \mu\text{m}^{-1}$. The MSE between adjacently numbered curves was sufficiently low (<50.0) for all those calculated to determine the CPFEM was insensitive to element density for the range considered.

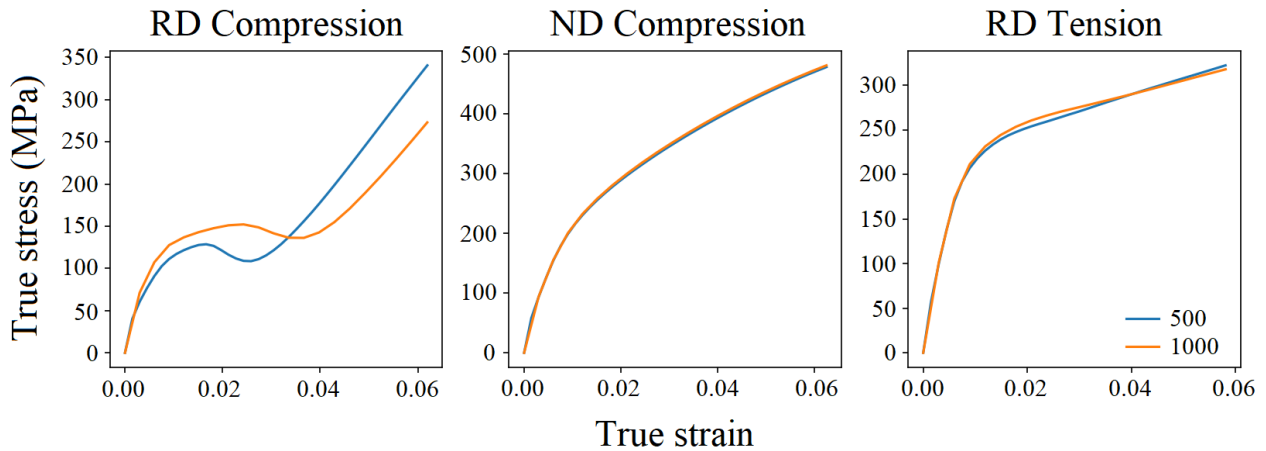


Figure 4.36: Study to assess rate-dependence of AZ31B-O-based CPFEMs. The expected general trends with strain-rate were not observed. For the lower strain-rate, the up-turn in flow stress for the RD compressed specimen was observed to occur earlier at a lower strain than expected, and its gradient increased instead of decreased. Furthermore, ND compressed and RD tensioned CPFEMs exhibited minimal strain-rate dependence.

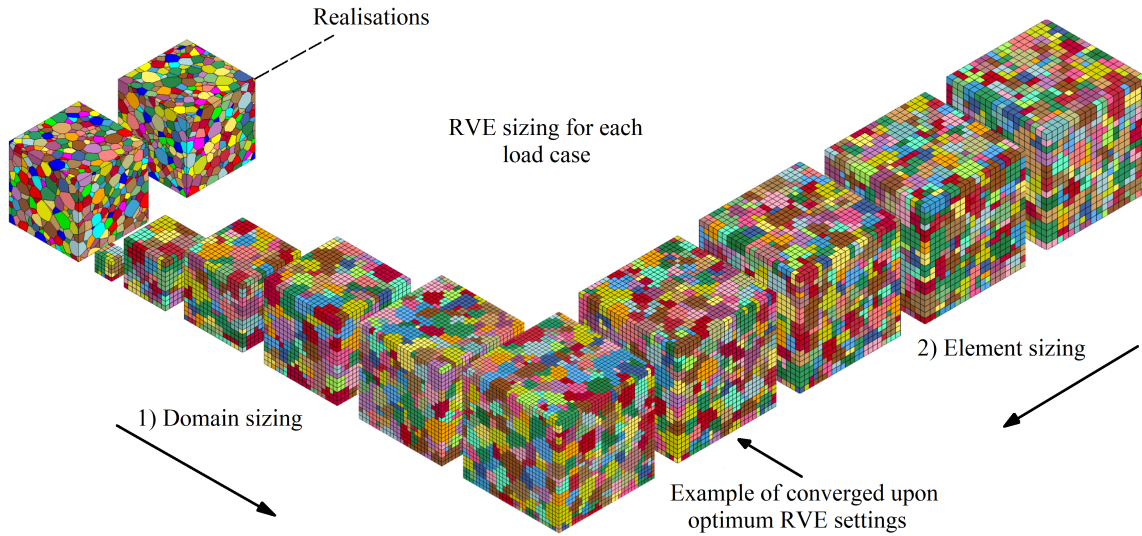


Figure 4.37: Pictorial representation of automated RVE sizing for each mesostructure realisation's load case. It starts with a tessellation from which CPFEMs of increasing domain size are derived. The true stress-strain behaviour of these are then compared to assess convergence ($MSE < 50.0$). With the converged upon domain size, the sensitivity to element density is then assessed. The optimum RVE settings was considered the model that showed convergence for the lowest number of elements.

a distribution of parameters could be made available from which the component-level constitutive models developed in Chapter 3 could sample from, thus facilitating stochastic-based analyses. How the first part of this was achieved is discussed in the following section.

4.5.3 Uncertainty quantification of the aleatoric nature of mesostructure through a Monte-Carlo method

To quantify the aleatoric nature of mesostructure, a sufficiently large population first required generating (the group being referred to as an ensemble). To aid with this, the author of this thesis made VorTeX system independent so that it could be run on both Windows and Unix-based systems. As such, the RVE sizing activity could be automated and run on ARC, greatly increasing parallelisation, and the number of simulations run; Figure 4.37 attempts to visualise the number of simulations required per load case for each realisation. Presented in the following is this uncertainty quantification for both WE43-T6 and AZ31B-O-based CPFEMs, starting with WE43-T6.

As each mesostructural realisation has a unique stress field deriving from its specific topology and texture, the homogenised mechanical behaviour of their CPFEMs sized into RVEs subtly

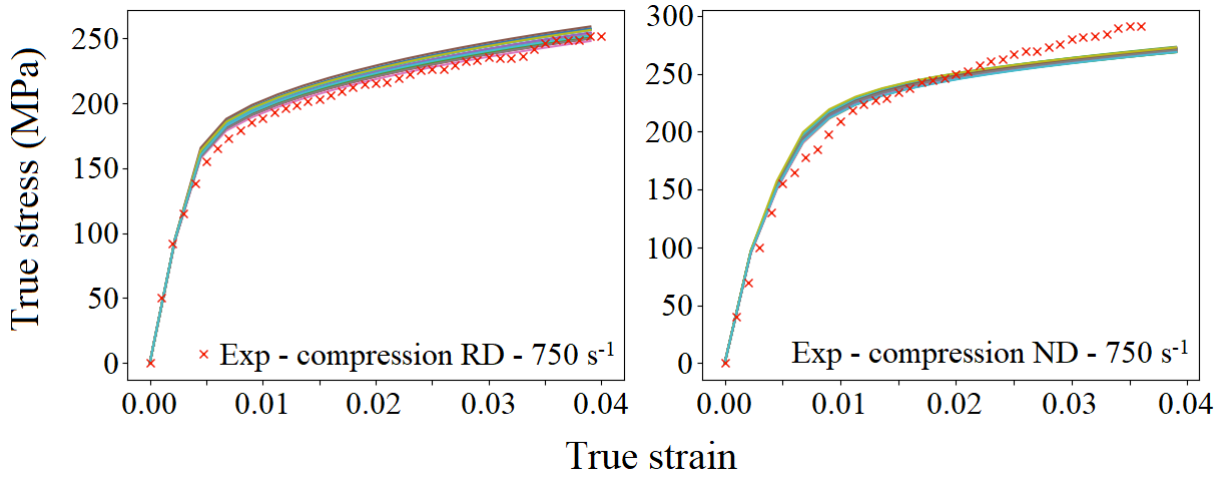


Figure 4.38: True stress-strain curves of ensemble of CPFEM RVEs representative of WE43-T6 plate loaded in RD (left) and ND (right) compared against those experimentally obtained. The stiffer response for rolling direction compressed CPFEMs was attributed to a coarser mesh being used compared to that of the first optimisation (element edge length $12.29 \mu\text{m} \rightarrow 30.24 \mu\text{m}$). The slight difference in yield behaviour for normal direction compression was believed to be due to the domain being larger (domain edge length $504 \mu\text{m} \rightarrow 756 \mu\text{m}$).

varies when compared to others. To quantify the extent of this variation, a Monte-Carlo study was conducted which saw numerous sets of RVE realisations generated and subjected to a defined loading analysis until convergence in measures quantifying uncertainty were achieved. The spreads in the predictions of true stress-strain behaviour for the rolling and normal direction compressed CPFEMs were compared against those experimentally measured and are presented in Figure 4.38. It should be noted that the parameter set converged upon during the second optimisation (see Figure 4.23) resulted in crashes, so the decision was made to revert to those initially determined (see Figure 4.20). Nevertheless, fits that were deemed sufficient for this study were observed for both load cases. The stiffer response for rolling direction compression was attributed to a coarser mesh (element edge length $30.24 \mu\text{m}$ instead of $12.29 \mu\text{m}$) being used in this study compared to that in the optimisation, and the slight difference in yield behaviour for normal direction compression was believed due to the domain being larger (cubic domain edge length $756 \mu\text{m}$ instead of $504 \mu\text{m}$). This highlighted the need to size the CPFEMs into RVEs for the optimisation, and that errors associated with element density can accumulate. As plate WE43-T6 exhibits transversely isotropic characteristics due to its strong basal texture, any in-plane loading was expected to yield similar mechanical behaviour (CPFEMs loaded in the rolling and transverse directions should be equivalent), and as such, transverse direction compressed CPFEMs were not run.

Convergence in measures quantifying uncertainty were assessed by fitting the flow stresses of fifty RVE-sized CPFEMs through a least square regression to the following expression that reflected the thermally-independent strain and strain rate hardening portion of the Johnson-Cook model,

$$\sigma_Y = (A + B(\varepsilon_{\text{eff}}^p)^n)(1 + C \ln(\varepsilon^*)). \quad (4.60)$$

As the CPFEMs were loaded to a single strain-rate, the rate-dependent part became a constant when the experimentally-based value of $C = 0.0046$ was used. This fitting enabled the variation in constitutive behaviour observed across the RVEs for each load case to manifest through parameters A , B , and n . Figure 4.39 presents the resulting distributions in the parameter spaces. The fact that there was a range in mechanical behaviour and that a distribution existed identified that each realisation reflected a unique RVE. The sufficiency of the population size to quantify uncertainty was then assessed by plotting the coefficient of variation against the number of realisations for each parameter space (see Figure 4.40). The plateauing observed for the various parameters indicated convergence in measures of second order statistics, and that a population size of fifty was adequate. Normal distributions were then fit to the distributions presented in Figure 4.39, thus quantifying the uncertainty arising from the aleatoric nature of topology and texture. Surprisingly, given the spread that was observed in Figure 4.38, the standard deviation of the RD parameters were slightly lower than those of the ND. This however was attributed to the larger means of the RD's B and n parameters.

Repeating the process for AZ31B-O plate, the uncertainty in the parameter spaces of the two expressions used to describe component-level in-plane flow stresses (see Section 3.3.4) were quantified (compressive and tensile in-plane flow stresses being described by Eqs. 3.80 and 4.60, respectively). Additionally, for investigative purposes, uncertainty quantification of the compressive out-of-plane flow stresses was also completed even though this could not be used to parameterise the component-level model. Figure 4.41 shows the spread in the predictions of true stress-strain behaviour of fifty CPFEMs compared against their experimentally measured counterparts. Good overall agreement was observed, with the behaviour being more consistent with the optimisation than that of the WE43-T6 plate study. The reason for the discrepancy between the optimised fits and those of the uncertainty quantification for the WE43-T6 study have already been discussed. The success in maintaining the behaviour

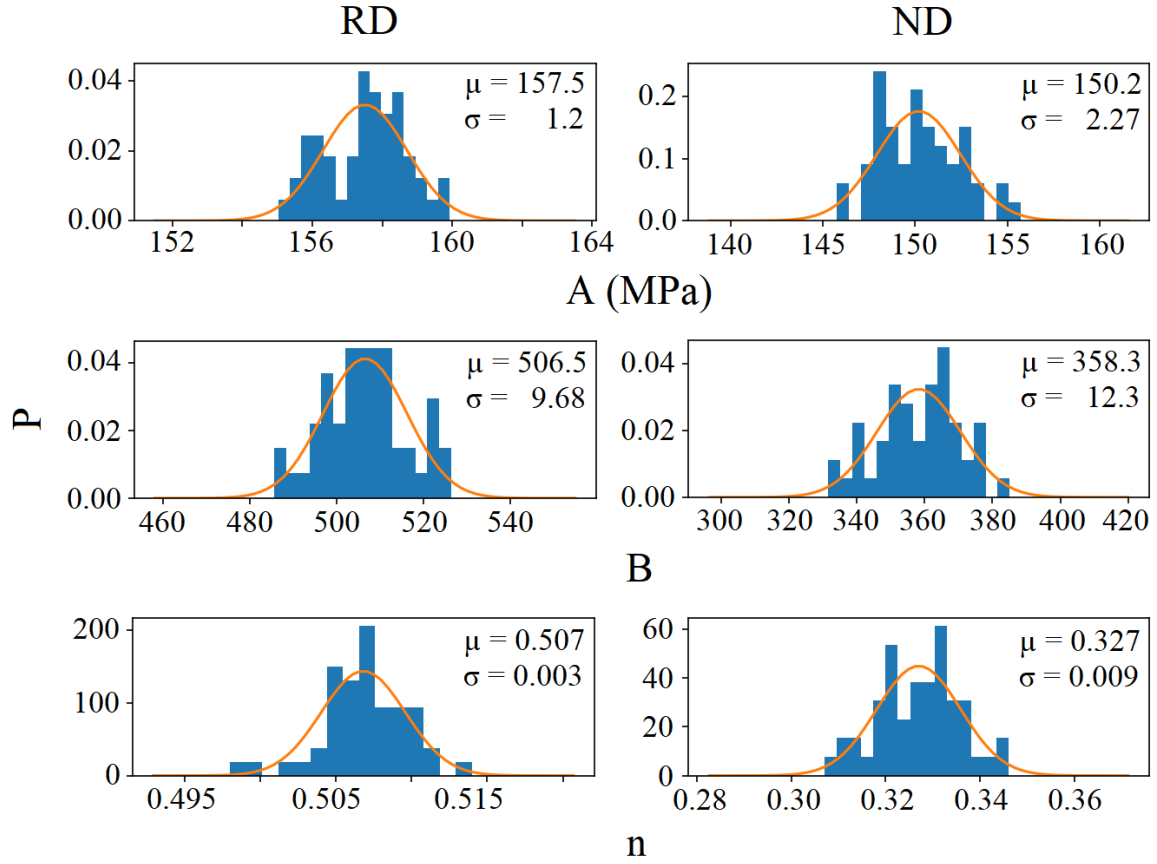


Figure 4.39: Distribution in A , B , and n parameter spaces of Eq. 4.60 arising from characterisation of CPFEMs with unique realisations. Normal distributions have been superimposed alongside their mean and standard deviation.

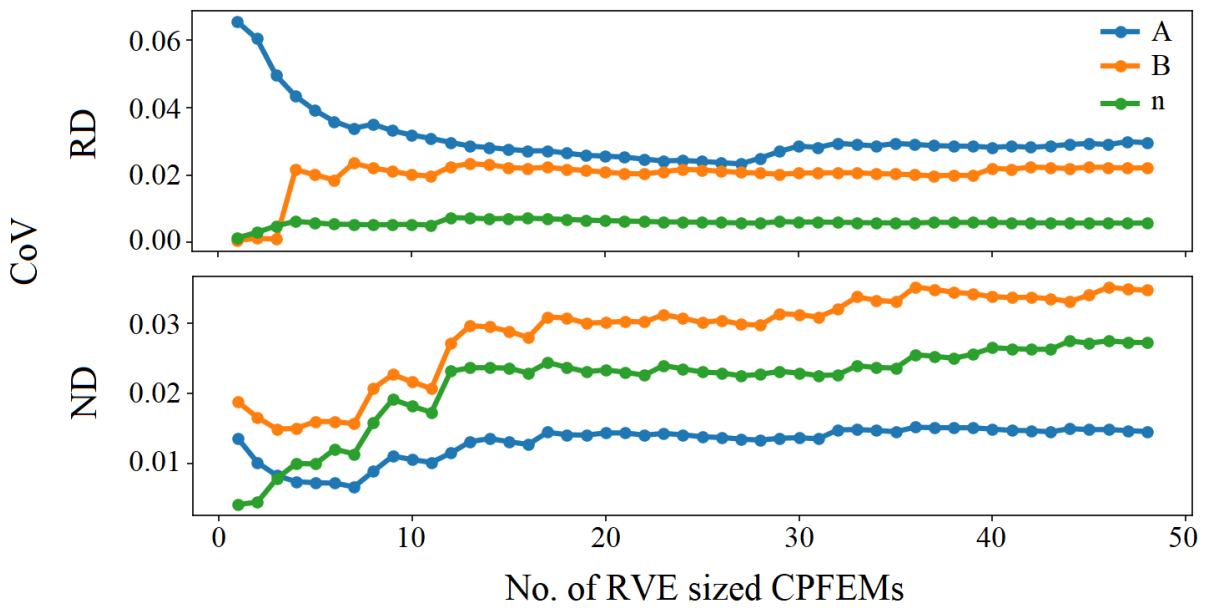


Figure 4.40: Coefficient of variation of parameter spaces A , B , and n for rolling and normal directions with number of runs. Convergence indicates sufficient population size.

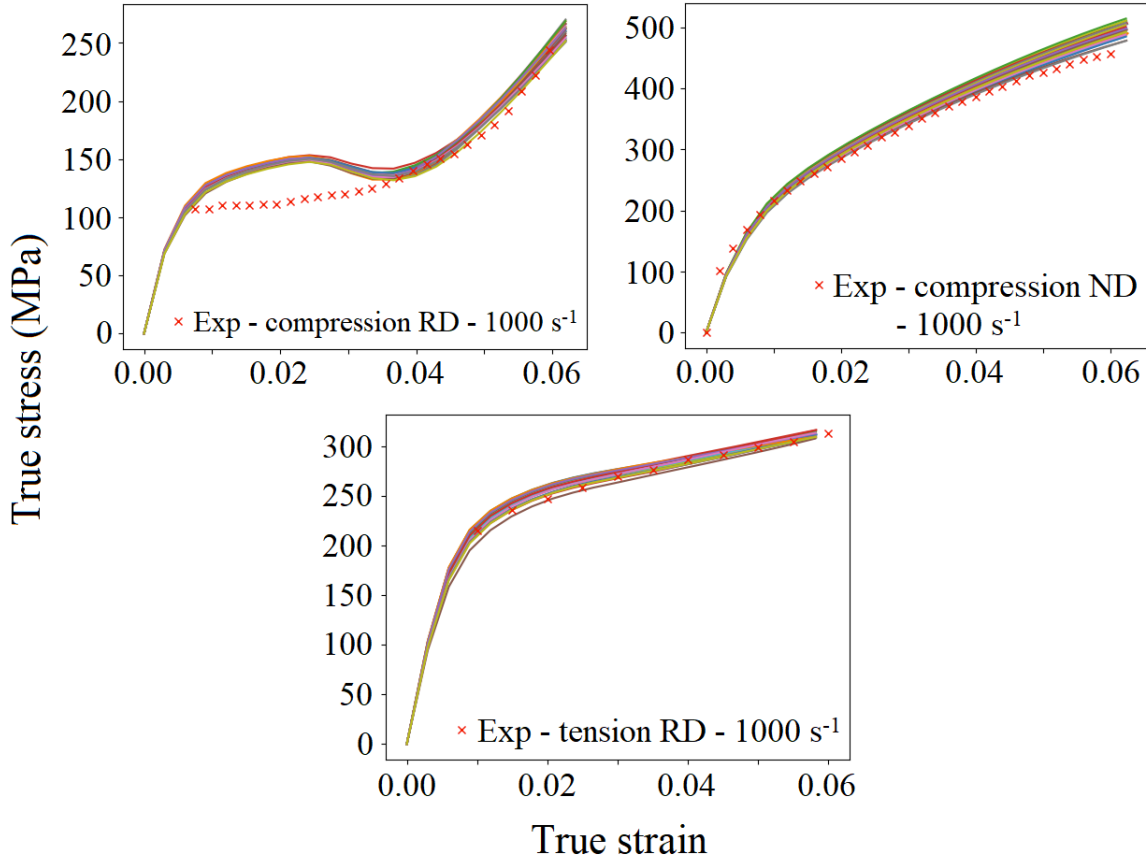


Figure 4.41: True stress-stress curves of fifty RVE-sized CPFEMs loaded in compression RD (top left), compression ND (top right), and tension RD (bottom) compared against those experimentally obtained. As the domain and element sizes of these model were similar to those of the optimisation, the predictions made were consistent with them.

between the optimisation and uncertainty quantification for the AZ31B-O study highlighted the importance of determining efficient RVE settings before the optimisation and to then maintain them for the uncertainty quantification.

In order to quantify uncertainty, Eq. 4.60 was again used to characterise responses exhibiting power-law hardening behaviour (the ND compressed and RD tensioned CPFEMs), but this time with $C = 0.1$. The rolling direction compressed hardening was characterised using Eq. 3.80. However, to maintain the position of the plateau seen in the experimentally measured data, parameters K_1 , K_2 , K_3 , and K_6 were fixed to those experimentally determined [8], and only parameters K_4 and K_5 parameters were permitted to vary. The population size was assessed to ensure it was large enough to constitute a distribution using the same method as before. Figures 4.42 and 4.43 show the distributions in the parameter spaces and the convergence of the coefficient of variation with number of runs, respectively. Again, a sample size of fifty was

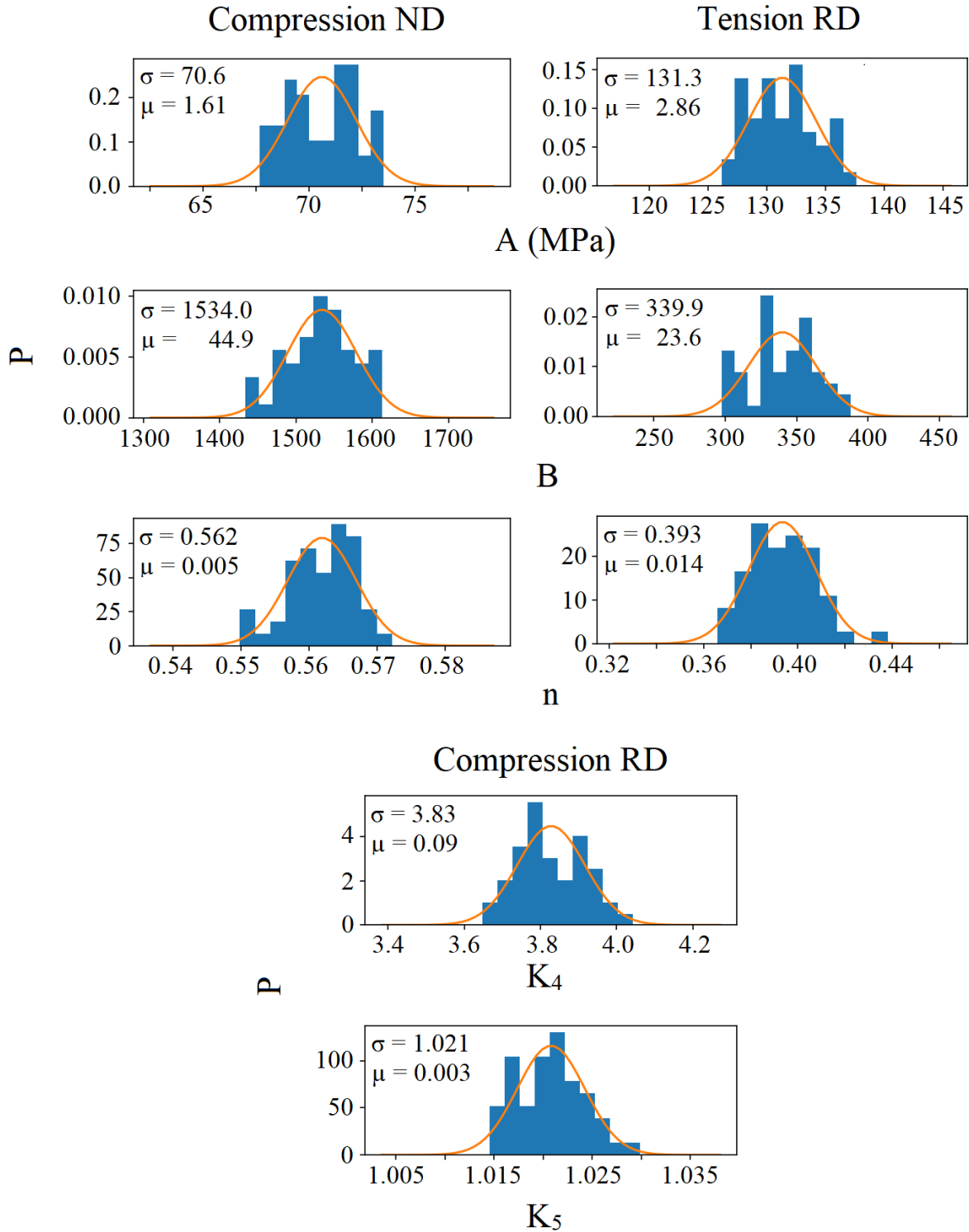


Figure 4.42: Distribution in A , B , and n parameter spaces of Eq. 4.60 for ND compression and RD Tension, and distribution in K_4 and K_5 parameter spaces of Eq. 3.80 for RD compression, arising from characterisation of CPFEMs with unique realisations. Normal distributions have been superimposed alongside their mean and standard deviation.

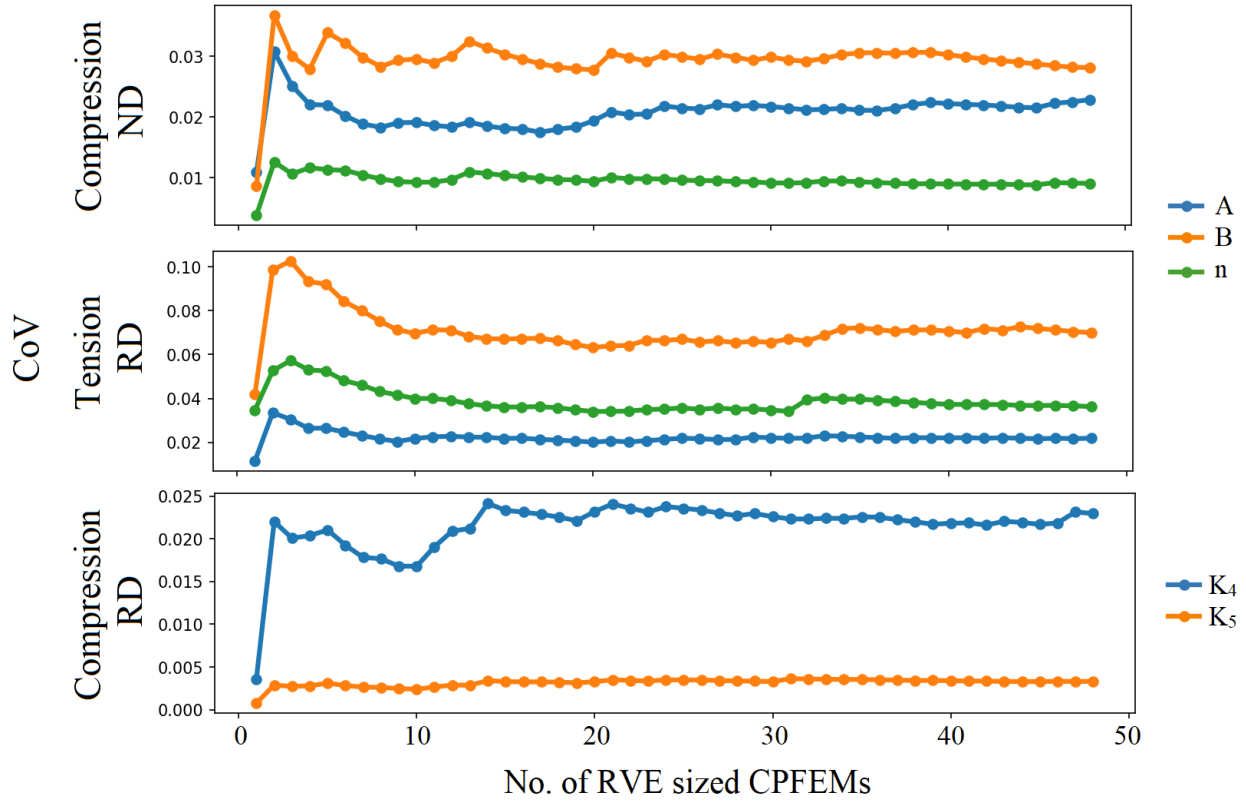


Figure 4.43: Coefficient of variation of parameter spaces A , B , and n for ND compression and RD tension, and K_4 and K_5 parameter spaces for RD compression with number of runs. Convergence indicates sufficient population size.

deemed sufficient as adequate convergence was observed. Normal distributions were fit and superimposed on-top of the distributions shown in Figure 4.42, thus quantifying uncertainty. Having now developed and presented a methodology that homogenises full-field statistically representative CPFEMs of WE43-T6 plate and AZ31B-O sheet, and subsequently quantifies the uncertainty arising from their specific topologies and textures (through use of macroscale hardening laws), the following chapter (after this chapter's conclusion) details how these datasets were used to facilitate component-level stochastic-based analyses.

4.6 Chapter conclusion

The objective of this chapter was to answer the questions,

- Is it possible to generate approximations of the full-field stress heterogeneity that develops at the mesoscale from bulk mechanical characterisations of a material using lower length-

scale models?

- Could a hierarchical link between these and component-level constitutive models be established where the effect of altering micro- and meso-scale features (such as solutes and precipitates, texture, grain size distribution, etc.) influence bulk mechanical properties?
- Would it be possible to design these micro- and meso-scale features to improve the performance of a component for its specific application?

In doing so, explicitly time-integrated CPFEMs were developed which saw,

- The module StaTeX being added to VorTeX to enable the generation of numerically-based tessellations that reflected polycrystalline structures statistically. To do this, the module took tessellations, serially sliced them, determined the area of intersected grains, and compared these to those experimentally measured. This in turn facilitated an iterative approach for converging on desired statistics through alteration of the input.
- A crystal plasticity-based constitutive model being formulated and integrated into the in-house developed FEM solver DEST. This model predicted plasticity through the thermally activated deformation mechanisms dislocation glide and twinning which in turn were both based on shearing rate-based phenomenological models. Furthermore, a phenomenological hardening law known as the generic hardening model was used to predict strain-based hardening, with twinning being homogenised for the sake of computational efficiency. This consequently necessitated the use of a rate of mixtures rule, the predominant twin reorientation philosophy, and a physically-based Hall-Petch hardening law to enable consideration of twin shear, and slip in both parent and twinned domains. Ideally, the strain-based hardening law would have been dislocation density-based but this was not deemed instrumental for scale-bridging and so was not pursued. Additionally, the model was implemented with a handle on thermal softening that was not utilised due to a lack of data; nevertheless, its use was evaluated in Chapter 6. Finally, it should be noted that in order to run the crystal plasticity model in DEST, fully integrated elements were formulated and implemented as excessive hourglassing was observed which could not be controlled with the available controls.

- The need to port the developed crystal plasticity-based constitutive model into LS-Dyna to facilitate the high model-throughput required by optimisation toolkits to converge upon parameters that made RVE-sized CPFEMs yield experimentally measured bulk-level mechanical behaviour, and the uncertainty quantification study whose results served as the basis for the stochastic-based hierarchical scale-bridging presented in the next chapter. This was necessary as DEST was not UNIX compatible, so could not be run on the high performance computing cluster, ARC. Whereas, LS-Dyna was, so could. To automate the RVE sizing activity required by the uncertainty quantification study, VorTeX was made system independent through extensive debugging, and a programme was scripted that massively parallelised the running of jobs.
- The development of a toolbox that enabled their interrogation. This toolbox could generate per grain relative activity plots of plasticity mechanisms, instantaneous pole figures (providing insight into texture evolution), per grain twin volume fraction plots, and plots showing how homogenised behaviour changed with boundary condition.

Bearing these in mind, the answer to the first question is yes, as it was shown that approximations of the full-field stress heterogeneity that develops at the mesoscale from bulk mechanical characterisations of a material could be generated using lower length-scale models. Discussed in the state of research section of this chapter was the recognition that bulk mechanical loading could generate mesoscale stress fields either by concurrent or hierarchical means. Even though concurrent-based methods would have been preferred (enables the consideration of mesostructural resolution directly from component-level analyses), it was deemed more appropriate to first pursue hierarchical ones due to the fact that the data from hierarchical models would be subsequently required by concurrent ones. Nevertheless, decisions were still steered toward furthering concurrent-based capabilities. For example, even though the crystal plasticity-based user-subroutine was implemented into an explicit time-integrated solver for the reason that they are better suited for rate-dependent problems. Another reason was that it could be used with an explicit-explicit subcycling algorithm to facilitate spatial concurrent-based modelling (specifics are discussed in the next chapter).

Digressing back on to the topic of the opted for hierarchical approach, approximations of the full-field stress heterogeneity at the mesoscale from bulk mechanical characterisations were generated by sizing CPFEMs, with polycrystalline topologies statistically equivalent to

those experimentally measured, into RVEs and using an optimiser to converge upon parameters that produced experimentally measured bulk-level mechanical behaviour; it should be noted that crystal plasticity-based constitutive models with parameters that are not uniquely defined and are determined through a least squares error minimisation optimisation have been shown to incorrectly predict the stress in individual grains [101], but, regardless of this, it was still believed that the adopted approach gave a good approximation of the predicted stress field. Furthermore, the uncertainty quantification study saw the characterisation of CPFEMs with statistically equivalent polycrystalline topologies predict similar bulk-level mechanical properties, thus showing that numerous approximated heterogeneous stress field configurations could yield the experimentally measured bulk-level material behaviour.

In answer to the second question, a hierarchical link was established between lower length-scale (CPFEMs) and component-level models where the effect of altering micro- and meso-scale features was shown to influence bulk mechanical properties. This was done through the consideration of the two magnesium alloy-based material systems, WE43-T6 plate and AZ31B-O sheet. Both materials share similar crystal plasticity mechanisms but yield (as shown) entirely different bulk-level mechanical behaviour stemming from variations in how these mechanisms activate and interact. Once statistically equivalent CPFEMs reflecting each material system were generated, their homogenised mechanical behaviour were able to reflect the differences in the experimentally measured behaviour of both these material systems through the available parameters. These parameters phenomenologically and to an extent in a physically-based manner controlled shearing to reflect characteristics of mechanisms occurring in the substructure of grains, and thus provided predictions of the materials' microscale high-rate deformation behaviour. As there are handles on micro- and meso-scale features that influence bulk-level mechanical properties, the second question was regarded as answered. Whether or not these features could be designed using the proposed CPFEM-based hierarchical framework was the focus of the third question and is discussed next.

The developed hierarchical framework could be used to design micro- and meso-scale features to improve component performance for its specific application, but this came with a caveat. As it was unknown whether the converged upon parameters reflected what was occurring physically, the ability to accurately realise changes in the microscale considered model through the crystal plasticity parameters could not be guaranteed as their sensitivities were unknown. This could

however be addressed by replacing the phenomenological strain-based hardening law with one physically-based, and conducting specifically tailored experiments (or running even further lower length-scale models) to parameterise it. Conversely, the ability to design texture was believed to exist due to how the stresses induced in the grains averaged and coupled with texture to yield the desired homogenised mechanical behaviour. Designing grain size distributions was, however, not believed possible as the invoked Hall-Petch hardening rule directly related to grain size, and as a result, the parameter controlling this behaviour suffered from the same uncertainty, regarding sensitivity, as the phenomenological strain-based hardening law.

Having now provided answers to the three questions posed, and generated datasets that quantified the uncertainty on bulk-level mechanical behaviour arising from the aleatoric nature of polycrystalline topology and texture, the next chapter focused on using this data to facilitate hierarchical scale-bridging from the mesoscale to the component-level. Furthermore, it then went on to discuss other potential modelling strategies the developed CPFEMs could facilitate, hence making relevant the following question initially posed in Chapter 1,

- could the datasets generated through the homogenisation and characterisation of CPFEMs be leveraged to facilitate novel, data-rich modelling strategies?

One matter that was not given due attention in this chapter was the development of the CPFEMs' strain-rate dependence, and as such, will be discussed in more detail in Chapter 6. What follows next is the chapter detailing meso- to macro- scale-bridging approaches.

5

Meso- to macro- scale-bridging opportunities

The previous chapter concluded with the generation of mesostructure-based datasets that when used to parameterise component-level constitutive models could enable stochastic-based predictions of performance. This capability will be presented in the following section through the blast-loaded plate analyses conducted in Chapters 2 and 3 for plate WE43-T6, with a test coupon-level model first being run to verify implementation. On completion of this study, the developed meso- to macro-scale-bridging methodology was deemed a success as a direct hierarchical link between mesostructure and component-level performance was demonstrated. As CPFEMs that reflect the homogenised behaviour of their concerned magnesium alloys have now been generated, the ability to run additional simulations to supplement experimental data now exists. This was presented through a study that sought to make available a component-level plasticity model that could predict the orientation dependent behaviour (under compression) of AZ31B-O sheet. This study led to the realisation that data-driven-based constitutive models may prove better suited than the developed modified ISML anisotropic Johnson-Cook plasticity model as they negate the need for a functional form to predict flow stresses. Furthermore, it was recognised that the developed full-field CPFEMs also provided a means of considering other mechanical phenomena such as fracture at the mesoscale, and as such this was further

investigated. Intergranular cracking was successfully implemented, but the requirement for an automatic subcycling capability became apparent due to instabilities. Subsequently, before running the prior study with one, attempts were first made to concurrently run the component-level plasticity model alongside the CPFEMs. This identified the need to develop a more sophisticated explicit-explicit subcycling algorithm due to the need to self sort and run numerous parallel time-stepping regimes at arbitrary non-integer time-step ratios. With the need to further investigate these opportunities, this chapter concludes and leads into the future work chapter.

5.1 Stochastic hierarchical parameterisation of the modified ISML orthotropic Johnson-Cook plasticity model

Taking the mesostructure informed datasets generated in Section 4.5.3, and using them as inputs to the modified ISML orthotropic Johnson-Cook plasticity model developed in Chapter 3, stochastic-based hierarchical scale-bridging is now presented for plate WE43-T6. This was done by seeding the A , B , and n parameters of the plasticity model (see Eq. 3.52) with the values predicted by the RVE-sized CPFEMs compressed at 750 s^{-1} along the rolling, normal, and ' directions. Additional ' direction compressed CPFEMs were ran to supplement the existing dataset, with parameter allocation ' $\equiv$ ''' and $11 \equiv '' \equiv 33$ being set to reflect the transversely isotropic mechanical behaviour of the plate; 11 and 33 reflect vectors orientated in-plane, and 22 in the normal direction (see Figure 5.1 for reference). Even though the WE43-T6-based CPFEMs had been shown to be rate-sensitive and as such could be used to make predictions of the rate-sensitive term (C) in Eq. 3.52, as it was not considered in the optimisation, the experimentally derived values of C (reported in Table 3.1) were used instead. The value for C' was derived through the linear interpolation, $C' = \frac{C_{11}+C_{33}}{2}$. Furthermore, even though the CPFEMs could exhibit thermal softening, the equivalent term in the Johnson-Cook model was set to not contribute as no experimentally measured data was available for calibrating this.

The analyses were made stochastic by enforcing the uniform sampling of sets of parameters from the dataset generated from the uncertainty quantification of WE43-T6, and then applying them arbitrarily to elements of the domain. As the parameter set already reflected a normal distribution, uniformly sampling it yielded an equivalent distribution over the domain. As the uniform sampling was conducted at the start of each run, a unique spread of the A , B ,

Sectioned view of armoured-plate for reference

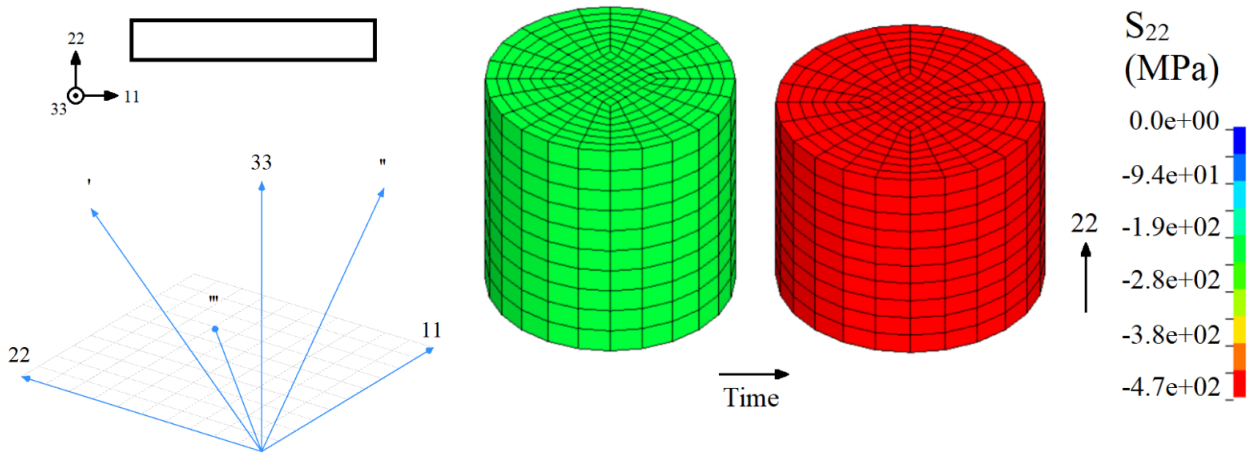


Figure 5.1: Example of test specimen used in scale-bridging verification analyses alongside sectioned view of armour plate as to convey orientations.

and n parameters were allocated across the domain within each execution. This hierarchical scale-bridging and its ability to pass on anisotropy is discussed next using 750 s^{-1} compressed $\varnothing 8 \times 8 \text{ mm}$ test specimen models that reflected the experiment that generated the data in the first place (see Figure 5.1).

The variation in stress-strain behaviour for the modelled compressed test specimens with rotation of the underlying substrate around the 11 and 33 axes (22 being orientated axially) are plotted against experimental measured data in Figure 5.2; the number designations for the lines denoted RVE reflect the angle between the specimen axial direction and the plate normal direction from which the specimen was prepared. As shown, the RVE parameterised Johnson-Cook model made highly plausible predictions in the spread in stress-strain behaviour with rotation. Slight deviations were seen in the elastic and early onset of yielding regimes for normal direction loading. The cause of which was believed to be due to non-representative values of the Young's modulus being used, and (as already discussed) less than ideal CPFEM parameters being converged upon during the optimisation. Further research is required to see if these predictions could be improved.

The effect of the hard-coded stochastic seeding was studied by running the same simulation five times for the normal direction, $'''$, and rolling direction orientations. Figure 5.3 shows that this resulted in no variation in predicted stress-strain behaviour. The reason for this was believed to be due to the fact that the load was distributed such that the contribution from each element was sufficiently averaged over the domain of the specimen thus resulting in the

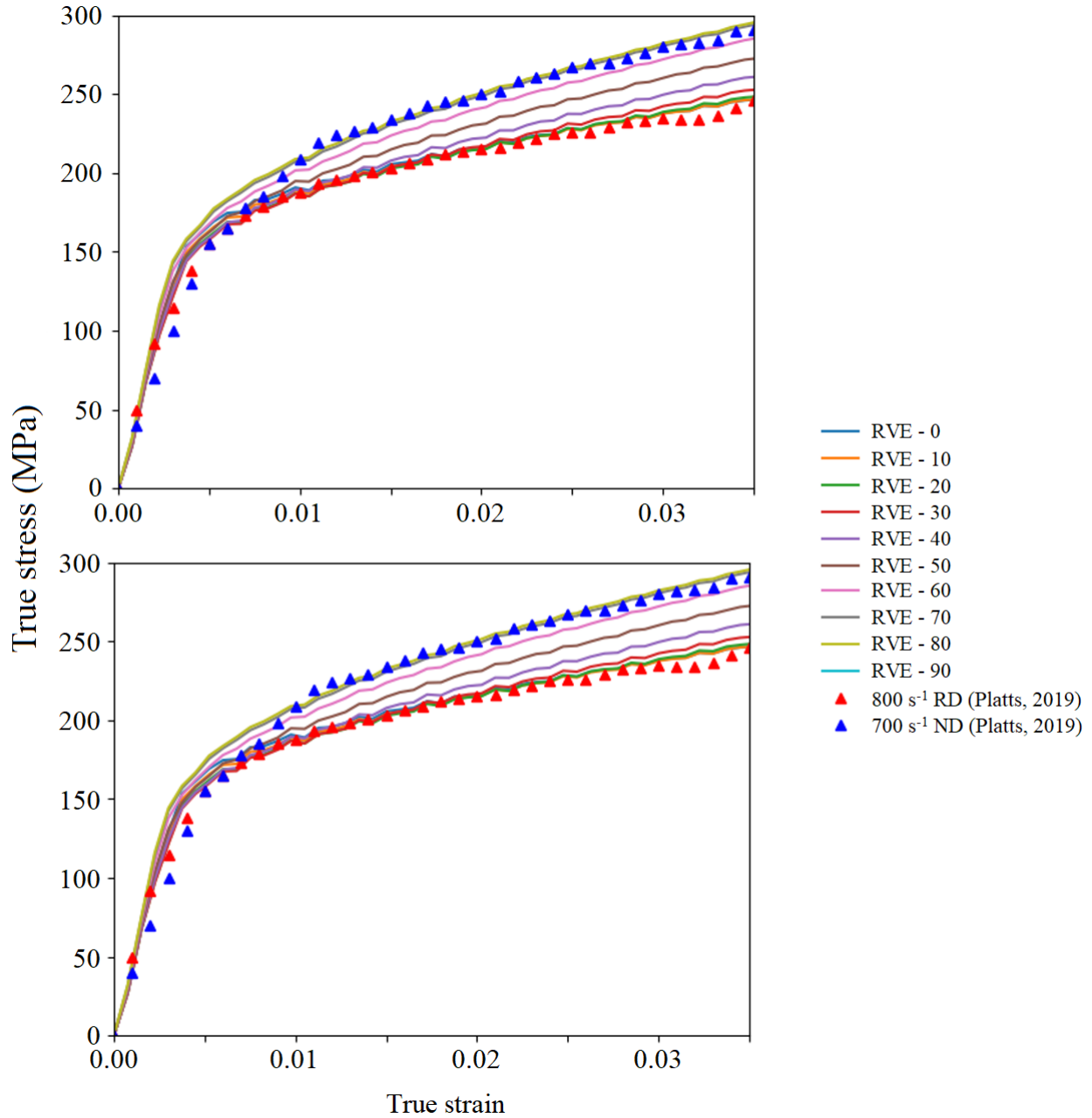


Figure 5.2: Variation in true stress-strain behaviour with rotation of substrate around (top) 11 and (bottom) 33 axes inside test coupons model allocated Johnson-Cook model seeded with RVE derived parameters. These predicted behaviours are then compared against those experimentally measured. The numbers associated with the curves designated RVE represent the orientation between ND and loading vector. As shown the model made highly plausible predictions in the spread of stress-strain behaviour with rotation.

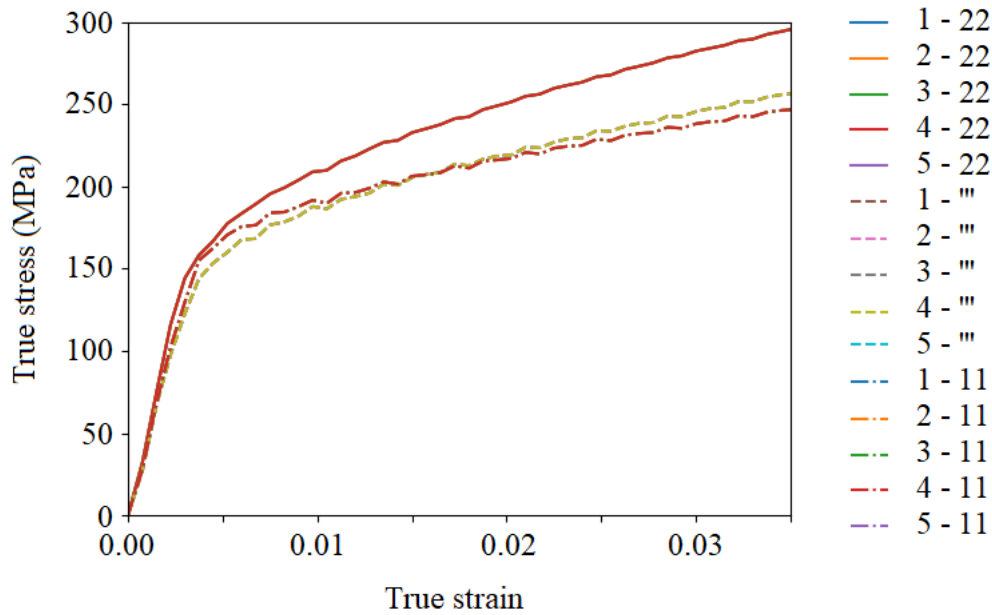


Figure 5.3: Study investigating the effect stochastic element seeding had on stress-strain behaviour for various orientations. Five simulations were run for each orientation, with the various linestyles reflecting the orientation (solid - 22 orientated, dashed - ' ' orientated, dash-dotted - 11 orientated). The fact the lines for each orientation type overlapped so perfectly implies that this type of analysis was insensitive to stochastic seeding.

same homogenised response being predicted. It was however expected that if stresses were to localise, stochastic behaviour would become more prominent. As such, the blast-loaded plate case-study was rerun with these settings as stresses were seen to localise more in these analyses.

The blast-loaded plate simulation was run three times with no user-prescribed changes being made in-between runs. Figure 5.4 shows the resulting von Mises stress fields at 0.6 ms. As can be observed, there are slight variations between all three. For example, if the periphery of the inside orange contour is followed and compared, different outlines are observed. The same can be seen for the red contour. Even though introducing stochastic effects in this manner resulted in variations, the overall impact was still rather insignificant. It is, however, believed that if this modelling approach was to be used on components with smaller features, then stresses would further localise, making the stochastic effects more obvious. Furthermore, this capability could be used to investigate the effect of introducing parameters reflecting unfavourable material characteristics (such as badly orientated grains) to areas in the proximity of these features. The next section now goes on to present attempts to try and get the modified ISML orthotropic Johnson-Cook plasticity model to reproduce the experimentally measured flow stress, with

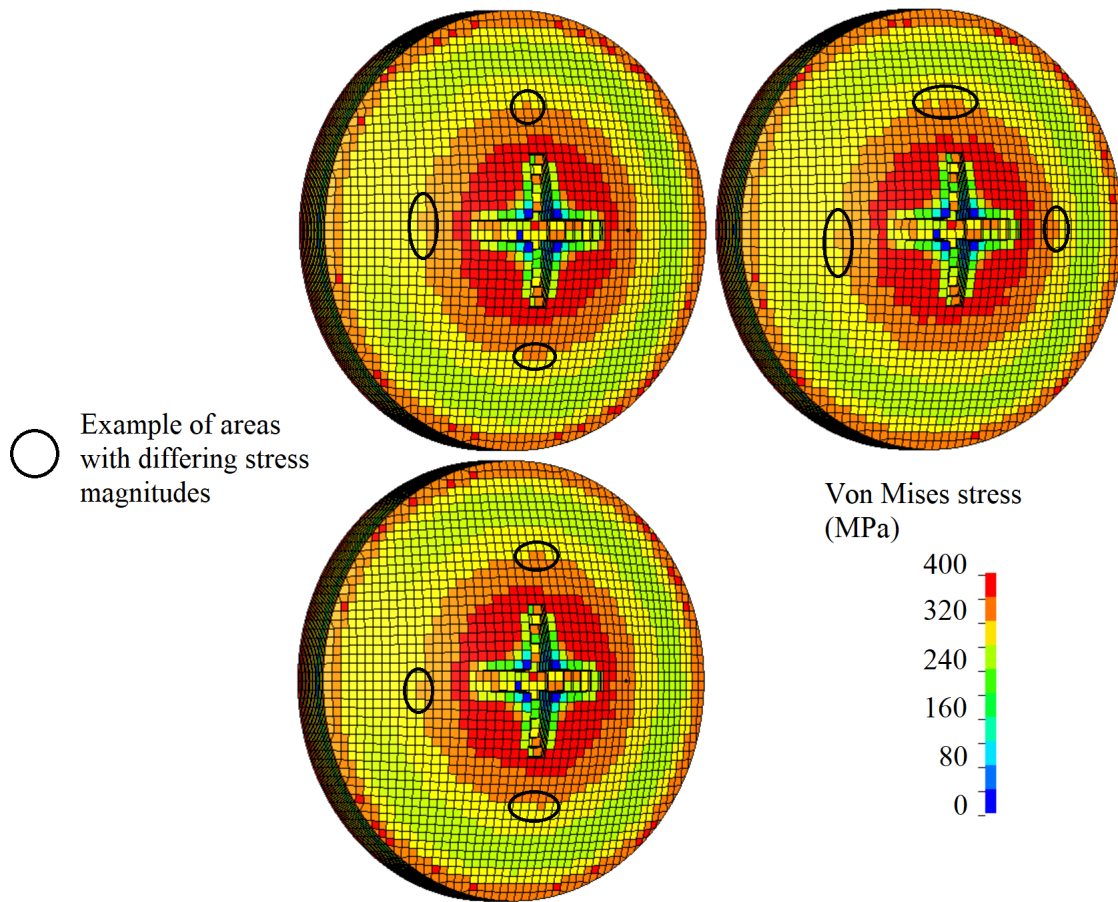


Figure 5.4: Von Mises stress fields at 0.6 ms for three separate blast-loaded WE43-T6 plate analyses. Slight variations in the stress fields were noted. The fact no user-prescribed changes were made in between these runs highlighted the hard-coded stochastic capability.

rotation, behaviour of compressed AZ31B-O sheet. This was done through exploration of its parameter spaces as additional CPFEMs could be run to supplement missing experimental data; it was stated in Section 3.3.3 that the currently developed model could not reproduce the in-plane to out-of-plane transition in flow stress behaviour of AZ31B-O sheet under compression.

5.1.1 Investigation into reproducing the compressed in-plane to out-of-plane flow stress of AZ31B-O sheet

It was presented in Section 4.5.3 that two hardening laws were required to characterise the variation in flow stress with orientation for AZ31B-O sheet under compression. Bringing these two expressions into one model presented a challenge as invoking hardening laws as a function of orientation is not as simple as invoking them as a function of uni-axial load type, as was done in Chapter 3. Consequently, an attempt was made to capture this orientation dependency using just

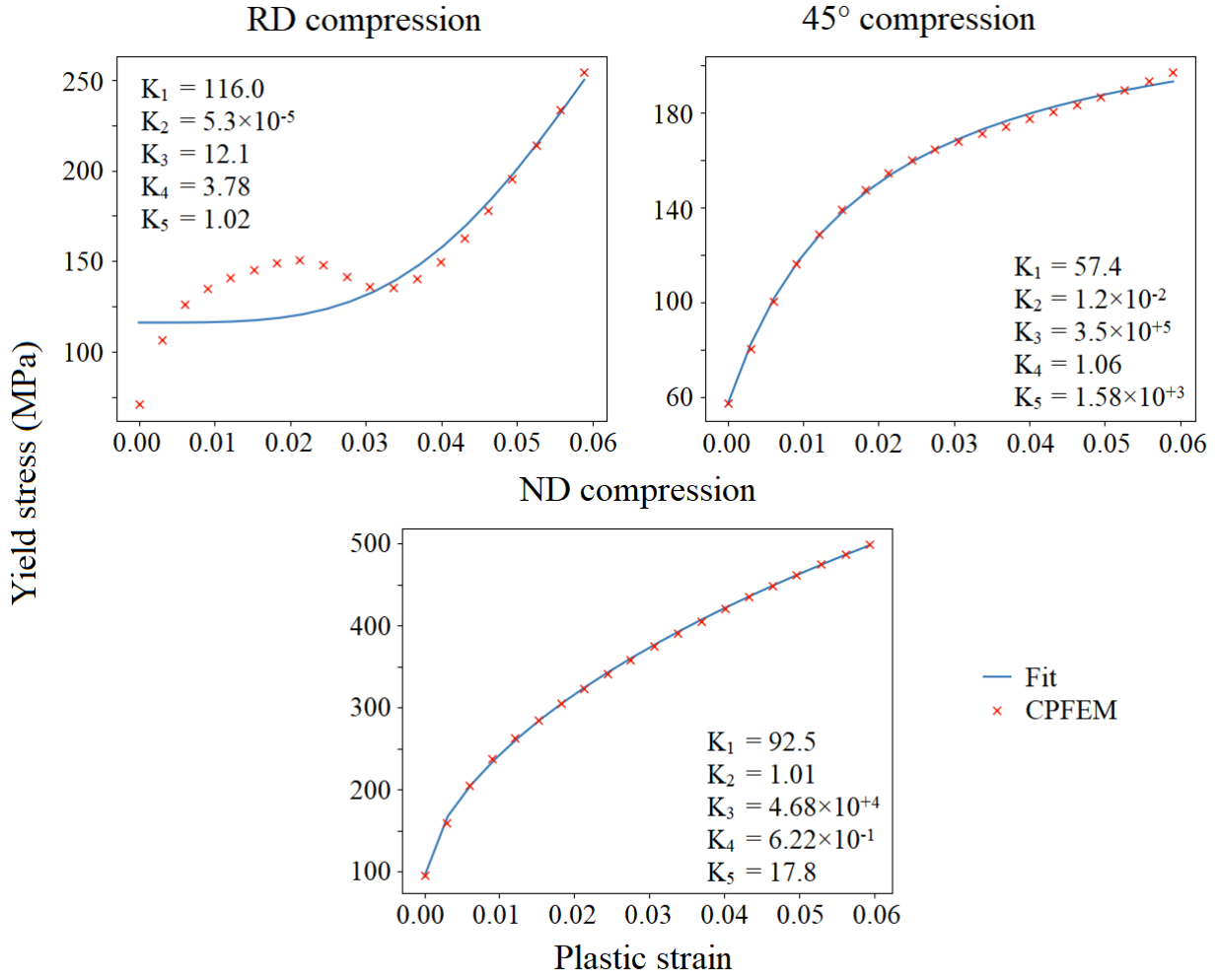


Figure 5.5: Determined parameters of Eq. 3.80, alongside fits, to reproduce CPFEM flow stress for the three orientations considered (RD, 45°, and ND). A good fit was observed for all three.

one hardening law. Use of power law-based hardening expressions were immediately dismissed as they were unable to predict the sigmoid flow stress behaviour seen with RD compression. Eq. 3.80 ($\sigma^Y = \frac{K_1 K_2 - \frac{K_3 (\epsilon_{\text{eff}}^p)^{K_4}}{1 - K_5 \epsilon_{\text{eff}} - K_6}}{K_2 + (\epsilon_{\text{eff}}^p)^{K_4}}$) was however considered ideal as this functional form could predict both experimentally measured shapes in flow stress behaviour. To map the change in flow stress with orientation between in-plane and out-of-plane orientations, an additional CPFEM was run that reflected a specimen loaded 45° in between the two. Figure 5.5 presents the fits to the flow stress predictions of the CPFEMs and reports the parameters required to achieve them. Good agreement for all three load cases was observed, bearing in mind the inability of Eq. 3.80 to reproduce the non-physical early flow stress behaviour predicted by the RD compressed CPFEM. This showed that if the hardening law was used in a rate-independent manner then it could very well be suitable for making orientation-dependent predictions.

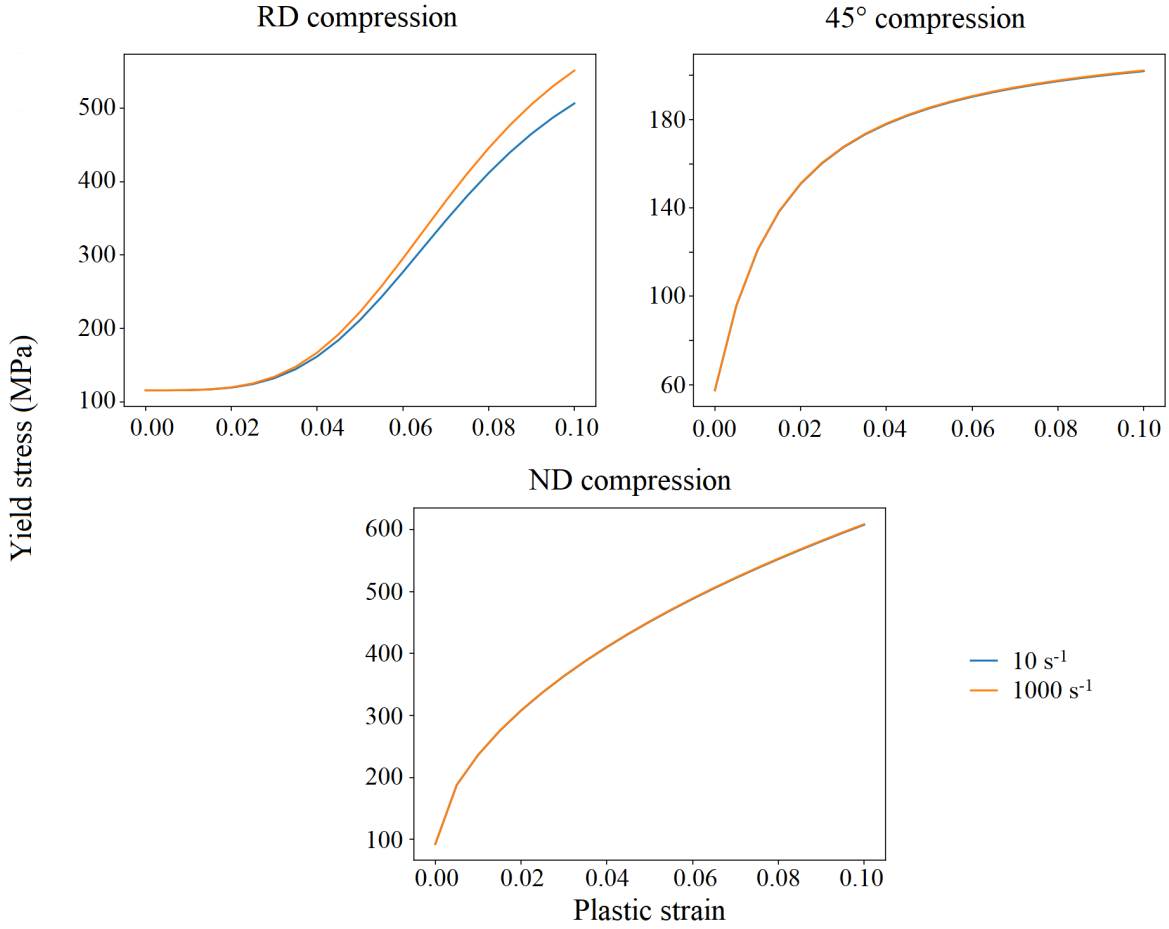


Figure 5.6: Effect of varying strain-rate as predicted by Eq. 3.80-based analytical model for the concerned orientations (RD, 45°, ND). The expected strain-rate sensitive was observed for the RD compressed orientation, whereas, it was not for the others.

Subsequently, the rate-sensitivity of the hardening law was investigated through use of an analytical model whose results are presented in Figure 5.6. As shown, the hardening law was not capable of predicting strain-rate sensitivity for a fixed value of $K_6 = 3.5 \times 10^{-4}$ for the 45° and ND orientations. The value of K_6 was thereafter varied and again no strain-rate sensitivity was observed for these orientations. K_5 was not varied as it was required to achieve the fits presented in Figure 5.5. Nevertheless, despite this shortcoming, the fact that the hardening law could predict the orientation-dependent behaviour of AZ31B-O sheet for the studied orientations warranted further investigation. As such, finite element models were set-up where the orientation of the underlying substrate was rotated in a sweep like manner, like that detailed in Figure 5.2, to study how the constitutive behaviour transitioned for intermediary orientations. Unfortunately, none were able to run, even with the time-step scaling being reduced to 0.01. The reason for this was believed to be due to the vast span observed in the

parameter spaces (e.g. K_2 ranged from 5.3×10^{-5} to 1.01, K_3 ranged from 12.1 to 3.51×10^5 , K_5 ranged from 1.02 to 1.58×10^3) making the aspect ratios of the 6-D hyper-ellipsoids unworkable. Consequently, the use of a functional form-based plasticity model was considered problematic for polycrystalline-based metals that exhibited a transition in flow stress with orientation similar to that of AZ31B-O sheet. Accordingly, other solutions to this problem were investigated, with data-driven being considered first. This is discussed next.

5.1.2 Toward mesostructure trained data-driven component-level constitutive models

From the above example it was apparent that finding a functional form that can describe the full anisotropic flow stress and path-dependent behaviours of a material system may be problematic (even for just one load type with orientation). Therefore, instead of relying on the need to develop material specific functional relations to describe plastic-based constitutive behaviour, data-driven approaches are identified as a potential solution. From those available, the soft computing form of artificial neural networks (ANNs) were preferred as they required less mathematical rigour when compared to others [103, 104]. ANNs were first used by Ghaboussi et al., 1991, [105] to predict the constitutive behaviour of concrete under plane stress, and later works such as Y. Hashash et al., 2004, [106] and Palau et al., 2012, [107] incorporated neural networks into finite element codes to govern constitutive behaviour. For example, in Palau et al., 2012, a feedforward neural network was trained using single-element tests that were seeded with J2 elasto-plasticity models and subjected to generic multi-axial loads. The resulting neural network-based constitutive model was then able to correctly predict complex-load-path constitutive behaviour that was not part of the initial training data. The main issue with only using stress-strain data to train an ANN is that it is in essence being treated as a *black-box*. Consequently, principles from material science and thermodynamics are not implicitly considered meaning that physical laws may be violated resulting in instabilities [108]. Additionally, the amount of data training required would be significantly large. Conversely, ANN-based hyperelastic constitutive models grounded in the use of invariants [109, 110] have been shown to remedy these issues as they are hard-coded with the theoretical knowledge of the material system. Such adaptations have been extended to metals, for example, Zhang et al., 2020, [111] used von Mises plasticity (J2) theory with isotropic hardening to train an

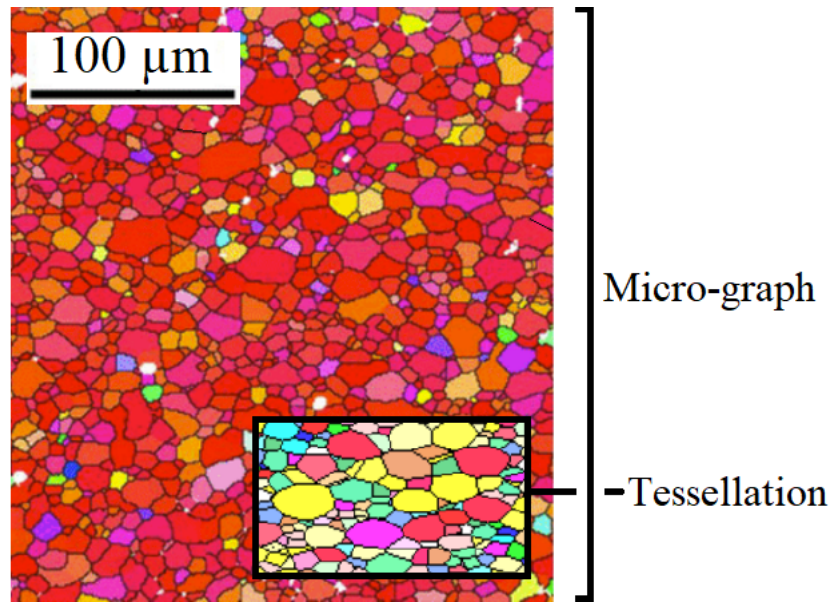


Figure 5.7: Comparison of (1.33:0.75:0.75)(RD:ND:TD) stretched tessellation-based model against EBSD micrograph [102]. Ability to better capture ellipsoidal grains was substantial shown.

ANN to predict the evolution of the elasto-plastic stiffness matrix. Liu et al., 2023, [112] then went further and developed a mechanistically informed ANN-based constitutive model whose anisotropic yield function was not known *a priori* but was arrived at through training of an ANN. In their work, two ANNs were used. One predicted the yield function of the material (to avoid explicit stated functions), while the other was used as the return-mapping algorithm.

In addition to negating the need for a functional form to describe anisotropic, path-dependent mechanical behaviour, ANNs offer the ability to make predictions on the effect micro- and meso-structure have on constitutive behaviour. For example, if the stress-strain behaviour of the homogenised full-field RVEs are coupled with vectors that characterise the mesostructure, then the mesostructure could be systematically varied and a dataset generated that could train an ANN. This ANN could then be used to make predictions on mesostructure characteristics that could improve the performance of a component for a particular application. Activities have been conducted that support this effort and are subsequently discussed next.

As stated in Section 4.5.2, the polycrystalline generating algorithm currently possessed the ability to only generate equiaxed grains. This was deemed to be inconsequential as it was shown that the 2D slices of the tessellation reflecting rolled AZ31B-O possessed close quantitative and qualitatively likeness to that of the experimentally measured micrograph. It was however noted that improvements in the reproduction of first order shape descriptors could be made through translational scaling; Figure 5.7 shows qualitatively the ability to generate ellipsoidal

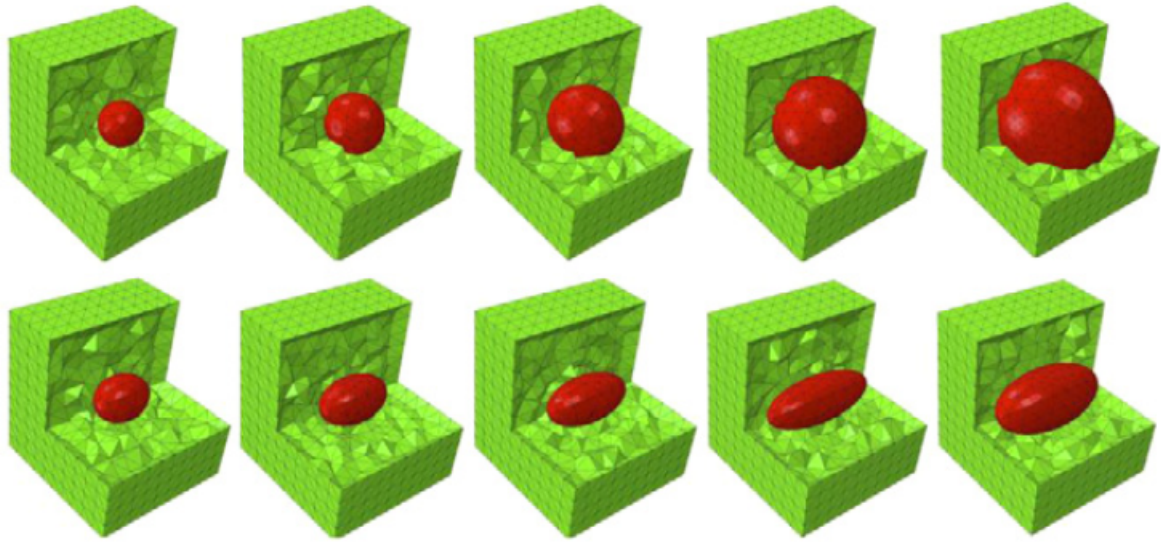


Figure 5.8: 10 examples of matrix-inclusion composite RVE materials as presented in Linka et al., 2022 [113].

grains (like those seen in the micrograph) through scaling ($4/3$ scaled in the rolling direction and $3/4$ scaled in the normal and transverse). These scaling factors in addition to the data used to generate the tessellation and the orientation distribution function used to impart texture could comprise the ANN input vector characterising mesostructure. Furthermore, information reflecting the manufacturing conditions such as cost, temperature, feed-rate, thickness reduction, and rolling strategy could supplement this vector and aid with converging on manufacturing conditions that yield optimum mesostructure to enhance a component.

Linka et al., 2022, [113] have made available their ANN code-base that is capable of predicting the constitutive behaviour of an matrix-inclusion composite RVE given the Neo-Hookean parameters of the matrix and inclusion, and the shape of the inclusion; examples of these RVEs are shown in Figure 5.8. It was believed that this code-base could be adapted to work with the proposed full-field homogenisation approach. However, to truly benefit from it, an ANN-based constitutive model that negates the need for a functional form to describe anisotropic, path-dependent yielding would be required to fully realise mesostructure to component-level design capabilities. This is because a new functional form may need identifying for each new RVE homogenisation, making the required user-input prohibitively large and inhibiting the automated scale-bridging. One factor to consider is that the material design exploration would be conducted in a virtual environment which would require the validity of some of the predictions to be assessed against experimental data, meaning that large experimental campaigns may be required.

An additional feature that RVE-trained ANN-based constitutive models could offer that conventional constitutive models like the Johnson-Cook plasticity model do not is that they can also infer constitutive behaviour that results from complex loading. To aid with this, a RVE testing environment has been developed that can characterise constitutive behaviour for a number of complex loads, and thus could be used to train an ANN. This capability is discussed further in Chapter 6.

Up to this point, successful meso- to component-level full-field hierarchical scale-bridging has been demonstrated for magnesium alloys that exhibit the power-law hardening behaviour typical of polycrystalline-based metals. With this capability, the opportunity to design mesoscale features such as texture to improve component performance now exists, and is discussed next.

5.1.3 Attempt to optimise texture to improve performance of blast-loaded plate

The intention of this section was to present the results of an optimisation that sought to improve the blast-resisting characteristics of the WE43-T6 plate through the optimisation of texture. Unfortunately, due to time constraints and the ARC scheduler being heavily utilised, this study could not be completed within the time-frame of this research project. However, the section was left in to emphasis to the reader the capabilities offered by the current scale-bridging approach.

Nevertheless, fracture, throughout the running examples of the blast-loaded plates, was represented by the deletion of elements when their respective effective plastic strain exceeded 0.2. It was recognised that this could be an oversimplification that resulted in a false representation of the plates' performance. Therefore, attempts to incorporate fracture into the CPFEMs, which in turn could be used to inform the length-scale above are discussed next.

5.2 Implementation of lower length-scale fracture mechanisms

Jamali et al., 2022, [61] characterised crack initiation locations for AZ31B-O and found that intergranular cracking comprised >57.2% of those observed for various RD orientated load cases, with the rest being transgranular. Falco et al., 2022, [100] proposed an intergranular cracking

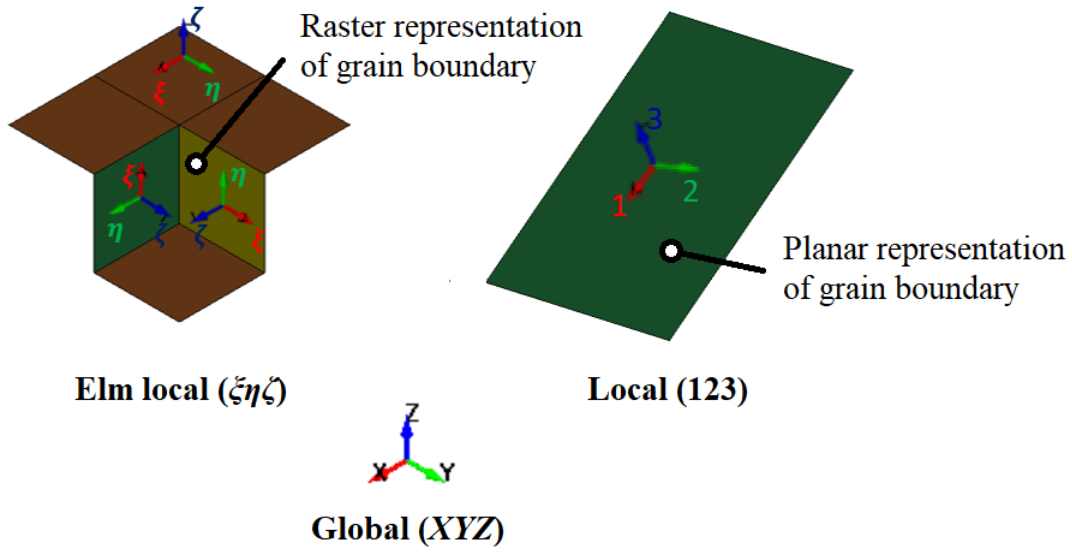


Figure 5.9: Comparison of planar representation of grain boundary to its equivalent raster representation. Coordinate systems required for transformations have been included for reference [70].

methodology for ceramic-based raster-meshed FE models to correctly represent grain boundary failure, while Marano et al., 2021, [114] presented a strain-gradient crystal plasticity-based constitutive model based on a quadratic energy contribution of the Nye tensor to simulate transgranular plastic slip localisation modes called slip and kink bands. Failure is promoted at these sites, and as such, could be implemented into the crystal plasticity-based constitutive model developed in Chapter 4. However, since intergranular cracking comprised the majority of crack initiation locations, attempts were first made to incorporate it into the developed CPFEMs using the methodology presented in Falco et al., 2022.

The intergranular cracking methodology, working in conjunction with VorTeX, utilised cohesive elements allocated a constitutive model to transform the stress state from the global coordinate system (XYZ) to a local one (123) defined by the normal unit vector of the grain boundary evaluated during the tessellation. An additional coordinate system was then imposed to identify the stress state in the cohesive element. The 1 and 2 basis vectors for the local coordinate system, and the ε and η basis vectors for the element lie on the in-plane spans. A demonstration of the orientation of these three coordinate systems is presented in Figure 5.9. As the grain boundaries were modelled as perfectly elastic-brittle interfaces, when displacements $(\delta_\varepsilon, \delta_\eta, \delta_\varepsilon)$ were applied, the user-subroutine calculated the normal components of force using the right hand-side branch of the procedure presented in Figure 5.10. These are the forces transferred through the grain boundaries. The other branch presents the procedure used to

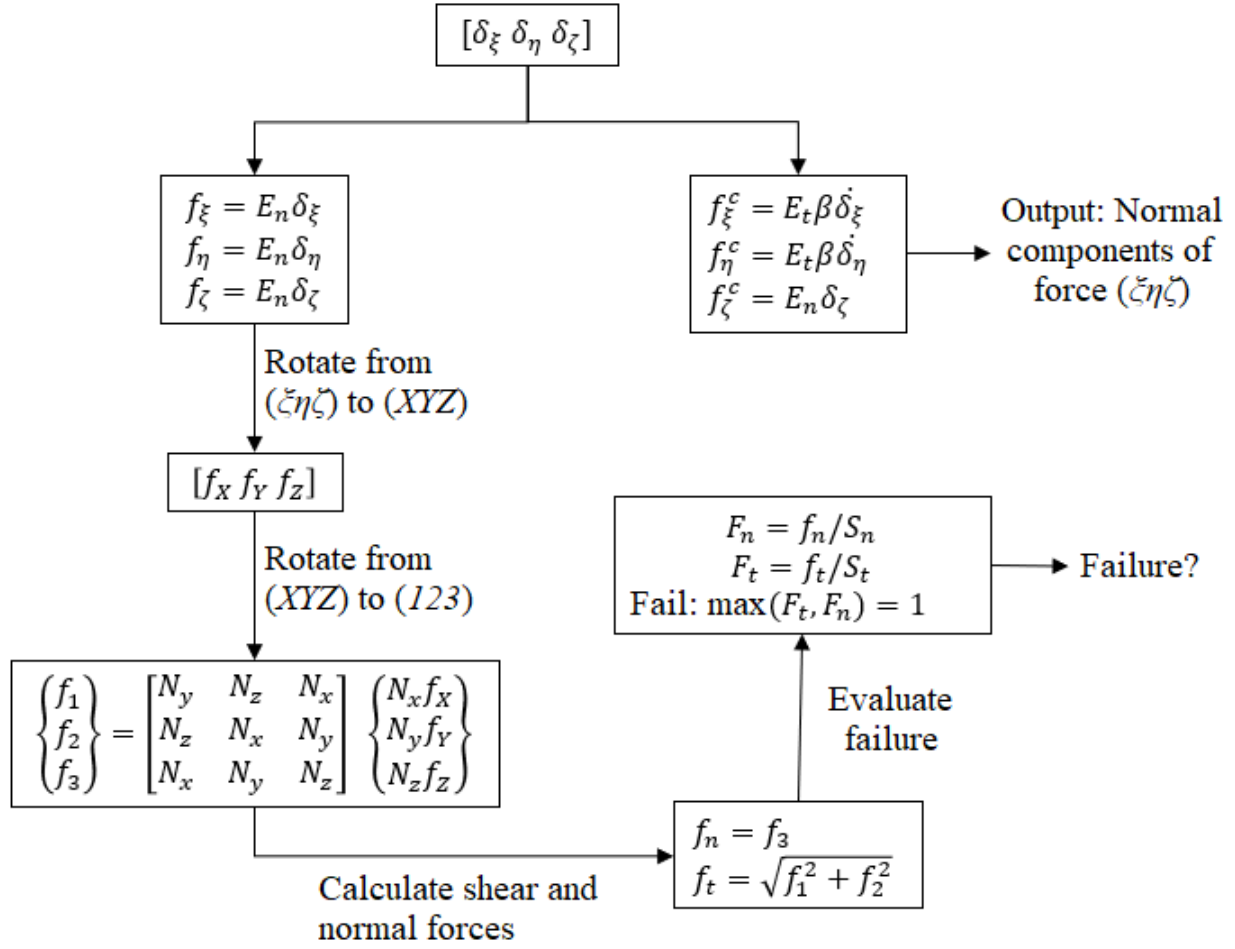


Figure 5.10: Flowchart presenting user-subroutine procedure that maps raster-mesh quantities onto a planar surface (representing the grain boundary) to facilitate assessment of fracture [70].

evaluate failure. Here, all components of force are considered. Falco et al., 2022, verified this implementation by comparing the stress state in the local coordinate system against that of a model where the cohesive element lay on the 12 span of the local coordinate system. Excellent agreement for both magnitude of the final strength and the onset of failure was noted. Presented next is the implementation of this methodology into a reduced domain, higher resolution representation of one of the WE43-T6 CPFEMs generated earlier.

As data was not available to calibrate the failure strain, a stiffness and failure strength that allowed the CPFEM to exhibit plasticity was chosen to showcase that the CP and fracture models were compatible. In this example, the normal and tangent stiffnesses (E), and failure strengths (S) were set equivalent ($E_n = E_t = 0.1$ GPa and $S_n = S_t = 250$ MPa, respectively), and the CPFEM was uni-axially loaded in the X -vector at 750 s^{-1} using the same boundary conditions as the earlier runs. Figure 5.11 presents the CPFEM alongside the cohesive elements

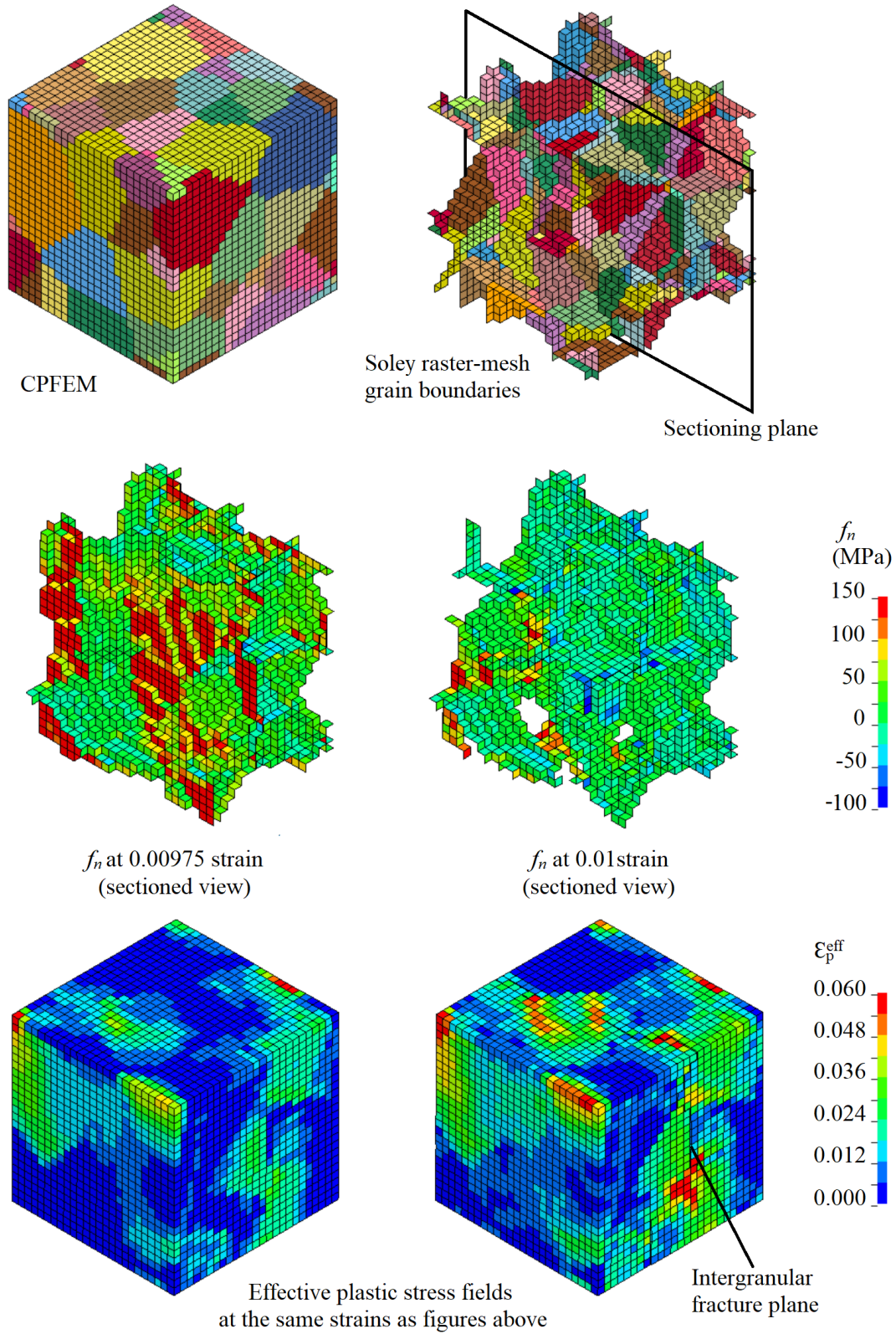


Figure 5.11: (Top, left) CPFEM used in intergranular cracking study. (Top, right) Cohesive elements of CPFEM. (Middle, left) Sectioned view of (top, right) model showing accumulation of f_n in cohesive elements of CPFEM strained to 0.00975. (Middle, right) Same plot but at 0.01 strain. Elements with high f_n have clearly been deleted. (Bottom) Effective plastic strain fields at the strains of the above images.

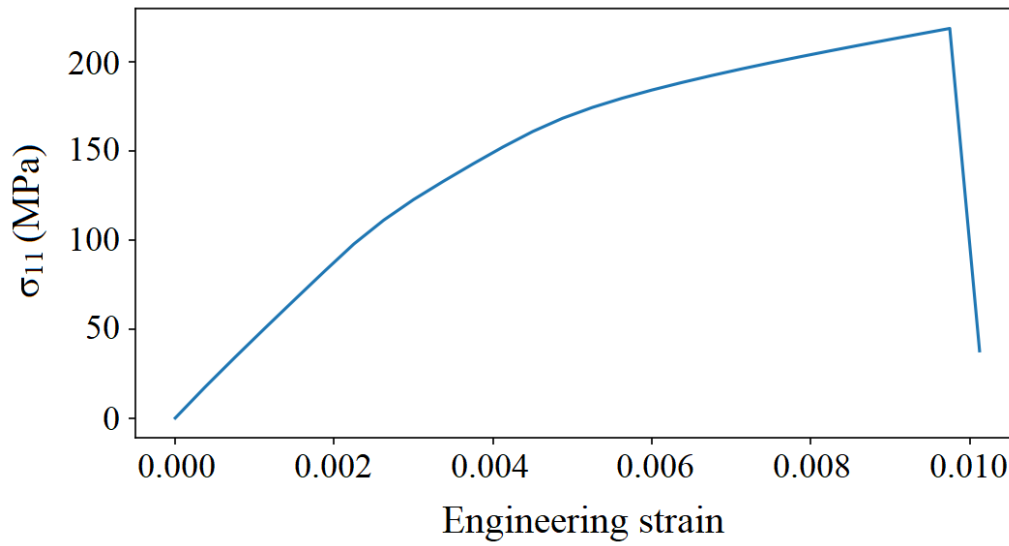


Figure 5.12: σ_{11} with engineering strain for 750s^{-1} X-vector uni-axially loaded CPFEM. Intergranular cracking resulted in material failure at near 0.01 strain.

that represent the grain boundaries. It also identifies the strain, the distribution of forces on the grain boundaries, and the effective plastic strain field just before and after element deletion. Figure 5.12 shows the engineering stress-strain behaviour and that failure occurred close to 0.01 strain. To get the crystal plasticity-based constitutive model to work together with the intergranular cracking user-subroutine, the time-step was reduced prior to the onset of fracture and throughout until element deletion was no longer reported; this required numerous runs. Figure 5.13 shows the input used to control the maximum time-step throughout the run. The fact that the period in time in which the time-step was reduced needed determining *a priori* massively increased the amount of user input, thus prohibiting its use with the automated RVE sizing algorithm. Additionally, it should also be noted that the amount of simulation time in the reduced time-step domain up to 1.45×10^{-5} s also accounted for $\sim 93\%$ of the runtime when it only comprised $\sim 10\%$ of the simulation time.

A potential solution to the problem of having to manually control the time-step would be to utilise an explicit-explicit sorting multi-time-stepping algorithm to manage the resulting instability (this could also improve computational efficiency). However, before using such an algorithm to aid with this instability, it was decided that its use to enable the concurrent running of the crystal plasticity-based constitutive model alongside the modified ISML orthotropic Johnson-Cook plasticity model would first be investigated. This is because these algorithms tend to sort time-steps by an element's characteristic length, which were similarly sized in the

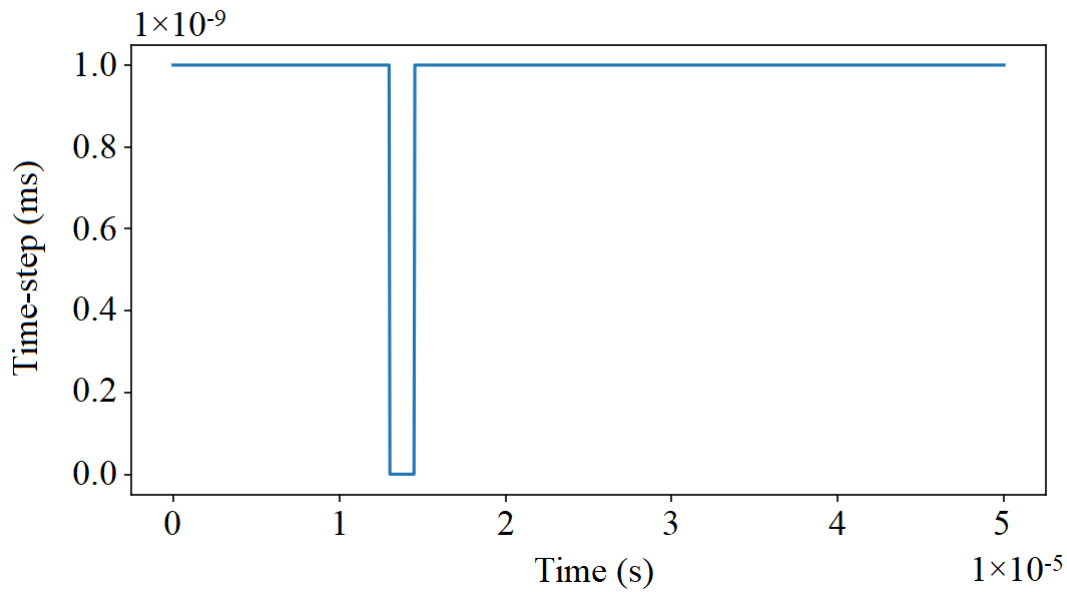


Figure 5.13: Input controlling the instantaneous maximum time-step throughout the run. The plateau of the trough lies on $1.0 \times 10^{-9} \mu\text{s}$.

intergranular cracking problem, but noted to vary substantially more in a concurrent-based spatial multi-scale model. The following section details this effort.

5.3 Concurrent modelling through use of an explicit-explicit multi-time-stepping subcycling algorithm

The critical time-step of an explicit time integrated FEA solver drives runtimes and is normally set by the characteristic length of the smallest element in a model. However, as shown in Section 5.2, it can also be reduced to improve stability. As such, this can often lead to large portions of a model unnecessarily running to a much smaller time-step, increasing computational cost. This section looks to explore the use of such an algorithm to facilitate the concurrent running of the developed crystal plasticity-based user-subroutine alongside the modified ISML plasticity model to enable mesostructural resolution in component-level analyses. This type of analysis would benefit from such a capability as the elements required to model mesostructure are much smaller than those required to model a component, such as the blast-loaded plate presented in Chapter 2. Typically, the areas to add mesostructure detail would not be known *a priori*, and it is foreseen that controls would be required to conduct on-the-fly adaptive mesh refinement in areas exhibiting high strain gradients, with mesoscale resolution being added when the element size fell

below a threshold value [32]. However, before pursuing this, and after a literature review, the two plasticity models were run concurrently using a pre-defined mesh and the subcycling algorithm available in LS-Dyna. Presented in the following is a review on the state of research in this field.

5.3.1 Review on the state of research of subcycling algorithms

Algorithms that enabled concurrent running of multiple time-steps were first developed in Belytschko et al., 1978 & 1979, [115, 116], and Hughes et al., 1979, [117, 118], who achieved this through nodal and element partitioning, respectively. Neal and Belytschko, 1989, [119] went on to couple explicit-explicit time resolved subdomains, and in later works with Lu et al., 1993 [120]. Coined *subcycling*, these algorithms have been well researched and can now allow for non-integer time-step ratios and the exchange of different kinematic quantities at the interface between areas within a domain [119, 121, 122]. Other such algorithms have been used to couple domains with relatively small time-step ratios [123–128], with their stability being assessed using either or both first and second order differential equations. Gravouil et al., 2001 & 2003, [129, 130] investigated combining *mixed* and *multi-time-stepping* algorithms to couple explicit and implicit non-linear schemes, where time-step ratios of 100 were noted. Prakash et al., 1991, [131] built on the implicit scheme featured in this work to develop the finite element tearing and interconnecting (FETI) method [132]. To do so, they relaxed the solution of the interface reactions to the maximum time-step, speeding up the solution by a factor of the time-step ratio. Other examples of work that focused on interfaces include; Mahjoubi et al., 2010, [133] who proposed a method that coupled domains with independent numerical dissipation parameters using multi-time-steps. In their work, Lagrange multipliers represented time-averaged constraint forces where stability was achieved via continuous displacement on the interface; Ghanem et al., 2013, [134] who utilised heterogeneous time-scales within an Arlequin method-based framework [135, 136] in which a gluing zone was enforced to maintain continuity of displacement; Combescure et al., 2014 & 2015, [137, 138] who developed the heterogeneous asynchronous time integrators (HATI) where both differing time integration schemes and discretisations were used. Here, subdomains took their own time integrator and timescale ensuring the continuity of velocity. Continuing the notion that each subdomain then can use its own time-step and integrator, Mota et al., 2022, [139] coupled subdomains using the Schwarz iterative process with a global time-stepper.

Bringing the focus on to works that implement subcycling algorithms into FEMs; Bao et al., 1998, [140] simulated the single step explicit propagation of elastic waves in large heterogeneous sediment filled basins; Cho et al., 2019, [141] more recently utilised a multi-time-step integration method to compute the discontinuous stress wave propagation in heterogeneous solids that enforced the continuity of tractions and accelerations, as opposed to previous methods that use velocities; Grunwald et al., 2021, [30] conducted a concurrent two-scale simulation of shocked quasi-brittle heterogeneous materials. A macroscale velocity was applied at the interface between the two domains, where the staggered approach was implemented in an updated Lagrangian formulation.

In addition to continuum-continuum coupling, notable work has been completed on the topic of particle-continuum spatial multi-scale coupling that commonly necessitates the need for separate time-scales. For example, in the bridging domain method [142], Xiao et. al utilised a multi-time-step Verlet algorithm to couple continuum and molecular models (if a single time-step was used, the critical time-step would depend on the Courant condition of the atomic spacing). Another key example as shown in Liu et al., 2016, [143] and more recently, Li, 2022, [39] was Discrete Element Modelling and Finite Element Modelling (DEM-FEM) coupling. Here, integer step ratios were used to allow for the DEM and FEM to run on two different time-steps with a transmission of displacement and velocity to particles and nodes, respectively.

Having established the state of the art in subcycling algorithms, the two developed plasticity models were implemented into an attempted spatial multi-scale FEM, and run concurrently using the subcycling algorithm available in LS-Dyna.

5.3.2 Utilisation of subcycling algorithm available in LS-Dyna

LS-Dyna (the FEA code the crystal plasticity-based user-subroutine and high performance computer-cluster utilising full-field homogenising capability have been developed around) has an explicit-explicit subcycling control available that enables elements to be run at differing time-steps through sorting of their characteristic length. It can however only sort elements by the ratio between the largest and smallest time-step (to an upper limit of 64), and needs to be user set. To assess its performance, the 2.5D FEM (3D elements, one element thick) shown in Figure 5.14 was run with and without subcycling, with a time-step ratio of 16 being set when it was utilised. Spatial coupling of conforming meshes was achieved through the use of a gradient

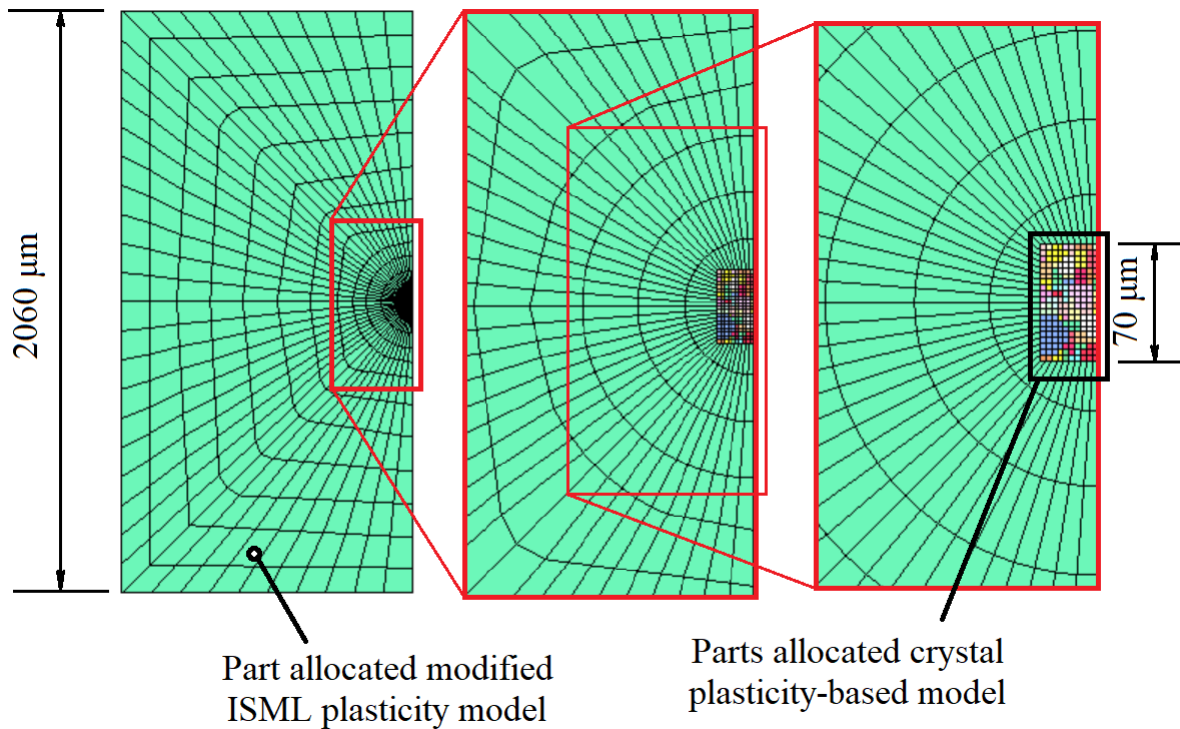


Figure 5.14: Attempted spatial multi-scale 2.5D FEM (3D elements, one element thick) used in subcycling study. This model ran the component-level modified ISML plasticity model concurrently with the crystal plasticity-based constitutive model. This model strove to increase the size of the elements from those used in CPFEMs to those typically used in component-level analyses. A gradient in element size was necessary as spurious wave reflection occurs if the difference in element size for adjacent elements is too drastic.

in element size from the crystal plasticity-allocated elements to the component-level. This was necessary as spurious wave reflection occurs if the difference in element size for adjacent elements is too drastic. This occurs due to the equilibrium conditions required by the solver, and the inability of the larger elements to carry high frequency waves. Consequently, any wave that possesses high frequency content that propagates from subdomains consisting of small elements into ones with large may see this content reflected back. Figure 5.15 shows how the boundary conditions were prescribed in this model, and the resulting Z-strain field at an arbitrary time. It is evident from the plot that the model was able to predict the homogenised behaviour of the component-level model, the heterogeneity arising from the granular resolution, and to at least start to increase the element size from that required by the crystal plasticity-allocated elements to those typically used at the component-level. The expected speed-up in runtime when the model was run with the subcycling algorithm was however minimal. Nevertheless, this study helped identify features for a better suited, more efficient algorithm.

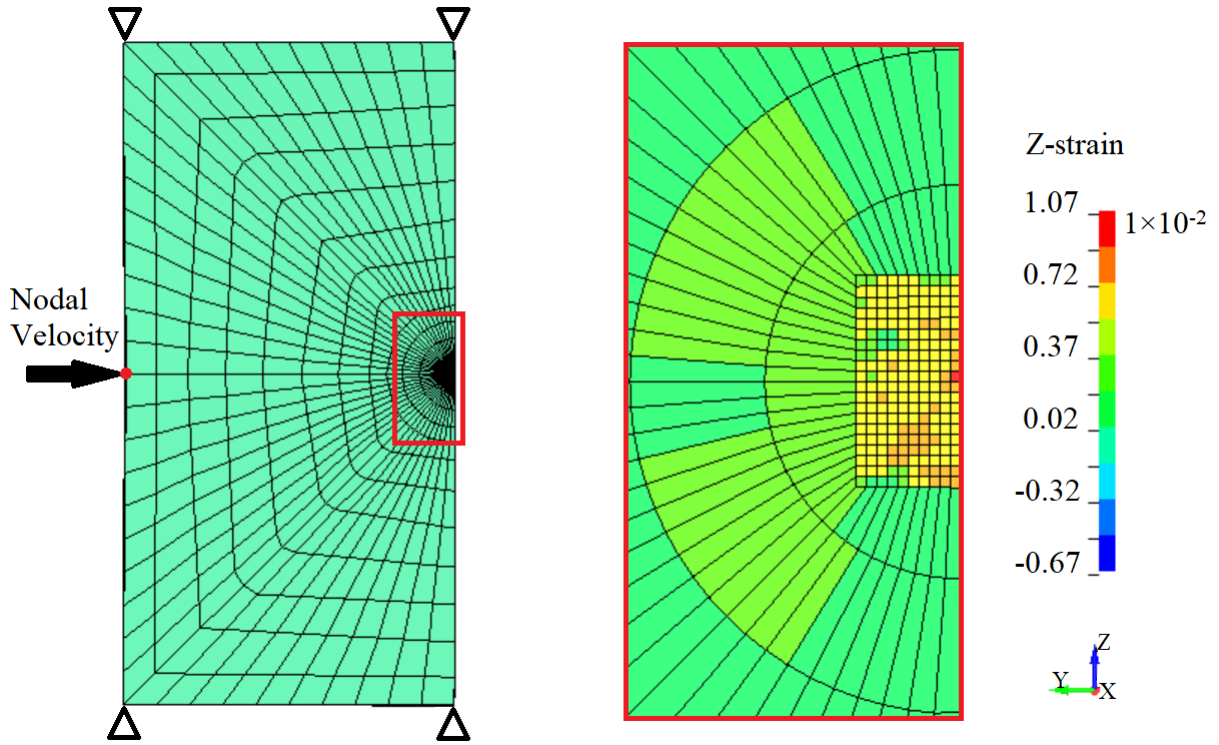


Figure 5.15: (Left) Schematic showing allocation of boundary conditions and (Right) plot presenting the resulting Z-strain field at an arbitrary time. The expected behaviour was observed, with the component-level model exhibiting a typical homogenised response, and the crystal plasticity-based model displaying granular resolution.

An improved algorithm would ideally negate the need for a user set constant time-step ratio, and potentially facilitate the parallel running of more than just two time-stepping regimes. This would be beneficial if the intergranular cracking methodology detailed in Section 5.2 was included in the presented spatial multi-scale FEM as the elements allocated the component-level plasticity model, the crystal plasticity-based model, and the intergranular cracking model could each be run at their own time-stepping regime. Furthermore, groups of elements allocated the component-level plasticity model, depending on their size, could also be run with their own time-stepping regime to compensate for the required gradient in element size. As time-step ratios also have the ability to vary suddenly over the course of a large time-step due to element distortion or material behaviour, further time-stepping regimes may also need generating on-the-fly. Consequently, a subcycling algorithm that determined for itself, depending on the instantaneous requirements of the model, the number of time-stepping regimes and their non-integer time-step ratios, was foreseen as desirable. Such a capability was being developed in the ISML at the time this thesis was being written whose description is detailed in Chapter 6.

5.4 Chapter conclusion

The objective of this chapter was to leverage the data generated through the homogenisation and characterisation of CPFEMs (see Chapter 4) to facilitate novel, data-rich modelling strategies, and to a large extent this was achieved. This chapter started with the utilisation of the dataset generated in Section 4.5.3 (Quantified the uncertainty of the effect the aleatoric nature of WE43-T6 mesostructure had on bulk-level mechanical behaviour) to seed component-level models with parameters based on approximated predictions of lower length-scale phenomena, thus achieving meso- to macro- hierarchical scale-bridging. Not only was this shown, but stochastic-based modelling was also made possible through the continuous sampling of the parameter space distributions and the arbitrary allocation of these to elements comprising a domain. To verify the scale-bridging methodology, a test coupon verification study was first conducted whose results were compared to the experimentally measured true stress-strain data used as part of the optimisation to determine the parameters of the crystal plasticity-based model. The model was able to reproduce this behaviour, with only slight deviations being observed in the elastic and early onset of yielding regimes for normal direction loading (believed to be due to non-representative values of the Young's modulus being used, and the CPFEM parameters of the 2nd optimisation not being used). Highly plausible predictions of behaviour with loading orientation were also observed.

The hard-coded stochastic capability was investigated by re-running the test coupon FEM numerous times (each run resulted in a unique realisation of parameter allocations). No variability was predicted, which was believed to be due to the fact that the contributions from the parameters were sufficiently averaged over the domain. Consequently, it was thought that in order for this stochastic seeding approach to yield variability, models that localised stress would be required. Subsequently, the blast-loaded plate analyses were re-run, but this time with the allocated plasticity model being parameterised through the new seeding approach. These models yielded subtle variations in the von Mises stress field, thus highlighting that stochastic-based predictions were made to an extent.

Further investigations were then conducted to try and get the the modified ISML plasticity model to reproduce the orientation-dependent mechanical behaviour of AZ31B-O sheet under compression. This is because it currently lacked this ability (shown to only predict sigmoid flow stress behaviour for all orientations), and the AZ31B-O-based CPFEMs developed in Chapter 4

could be used to infer the mechanical behaviour of orientations not experimentally tested (such as 45° in between the RD and ND). To reproduce the experimentally measured transition in flow stress behaviour seen with in-plane to out-of-plane rotation (sigmoid to power-law-shaped), attempts to find parameters for the hardening law defined by Eq. 3.80 were made as it was shown to have the ability to exhibit both flow stress shapes. Even though parameters were identified that produced the desired orientation dependence for a fixed strain-rate, it was analytically shown that they incorrectly predicted strain-rate dependence. Nevertheless, attempts to utilise the parameters within a FE-based model were made. These were unsuccessfully run, with the reason potentially being due to the wide parameter spaces for the various orientations making the 6-D hyper-ellipsoids (see Chapter 3) unfeasible. Consequently, data-driven component-level constitutive models were discussed as a likely solution.

ANNs-based constitutive models were considered desirable as they eliminate the need to develop material specific functional relations to describe flow stress behaviour. However, their use was not pursued further. Nonetheless, it should be noted that the use of ANNs also offer exciting new avenues for material design as they have the ability to make predictions on the effect micro- and meso-structure have on bulk-level mechanical behaviour. For example, if the stress-strain behaviour of the homogenised CPFEMs are coupled with vectors that characterise the mesostructure and information such as manufacturing conditions, then the mesostructure of the CPFEMs could be systematically varied and a dataset generated that could train an ANN to make predictions on characteristics that could enhance a material for its component's specific application. Regardless, as the use of ANNs were dismissed, attention was directed to trying to design mesostructure characteristics, like texture, through an optimisation. Such a study could not be completed within the time-constraints of this thesis and instead attempts to incorporate other mesoscale-level phenomena into the full-field CPFEMs, such as intergranular cracking, were made.

Intergranular cracking was implemented into the CPFEMs first, as this fracture mechanism was found to be most prevalent in experimentally tested AZ31B-O specimens [61]. This was achieved through the use of cohesive elements and a user-subroutine that assessed forces against failure criteria. As there was a lack of experimental data for calibration, values were selected that enabled the showcasing of this capability. Intergranular cracking was shown after a degree of plasticity, however, to get the CPFEM to fully fracture, the time-step needed to be significantly

reduced over the time domain element deletion occurred. This time-step control needed to be determined *a priori* through numerous runs, making the user-effort extensively large which made it prohibitively difficult to work with the developed CPFEM homogenisation methodology. As such, subcycling algorithms were pursued as a potential solution to this issue.

Before even considering running the subcycling algorithm with intergranular cracking-implemented CPFEMs, its use to improve the computational efficiency of a spatial multi-scale FEM, that concurrently ran the modified ISML and crystal plasticity-based constitutive models with a conforming mesh, was first investigated. This was because these algorithms tend to determine the time-stepping regimes each element belongs to through their characteristic length, which were noted to be similar for the intergranular cracking-implemented CPFEM, but to vary substantially more for the spatial multi-scale model. This model was able to make predictions of homogenised behaviour typically seen at the component-level model, the heterogeneity arising at the mesoscale, and to at least start to increase the element size from that required by the crystal plasticity-allocated elements to those typically used at the component-level. The expected speed-up in runtime when the model was run with the subcycling algorithm was however minimal. Nevertheless, the study helped identify that a better suited, more efficient algorithm should self-sort and run numerous parallel time-stepping regimes at arbitrary non-integer time-step ratios. This was the extent of the work completed on this topic. However, at the time this thesis was written, there was on-going work in the ISML to develop such an algorithm whose description is presented in Chapter 6.

These activities showcased how the data generated through the homogenisation and characterisation of CPFEMs was leveraged to facilitate novel, data-rich modelling strategies, and even though further work was required to fully realise some, it was believed that a good account of the capabilities offered was made. Detailed in the next chapter is a discussion on the work expected to follow-on from the work presented in the thesis thus far.

6

Future work

A multi-scale approach to the development of high-rate-based microstructure-aware constitutive models for the magnesium alloy-based material systems, WE43-T6 plate and AZ31B-O sheet, has been presented that homogenises and characterises explicitly time-integrated CPFEMs. The characterisation of the CPFEMs saw the generation of parameter space distributions that were used to seed component-level constitutive models, thus providing a hierarchical link between approximations of the mesostructural stress field and the homogenised stress at the bulk-scale. Opportunities to then leverage this data to facilitate more complex modelling strategies were then explored.

This chapter starts with a discussion on how other mechanistic properties (e.g. strain-rate, temperature), that the currently proposed homogenisation approach has the capability to predict but did not have verified or utilised, could be considered in future iterations. It then goes on to present methods on how to make the approach more physically-based, and recommendations on why component-level plasticity models should be made data-driven. It then moves on to detailing how it expects more complex modelling strategies would be developed, which it then followed by a description of the efforts made to encourage a user-base. Lastly, it discusses anticipated publications in academic journals.

6.1 Inclusion of further mechanistic behaviour into proposed homogenisation approach

Even though the proposed approach possesses the ability to predict the required relative activity of microstructural mechanisms to yield experimentally measured bulk-level mechanical material behaviour, some of the implemented dependencies, such as strain-rate or thermal softening, were not verified and subsequently used. For example, the parameters of the WE43-T6 CPFEMs were optimised upon using a single strain-rate, meaning that they did not predict exactly experimentally measured strain-rate behaviour. It should however be noted that the expected general trend was observed (flow stress increases with strain-rate). Moreover, when the same process was repeated for AZ31B-O, incorrect trends were observed. Therefore, the first task to be completed would be to re-run the optimisation but with the additional consideration of strain-rate. Furthermore, thermal softening was not utilised due to a lack of appropriate experimental data for its calibration. Nonetheless, assessment of its capabilities is evaluated in the following.

Figure 6.1 presents the evolution of state variables, of an arbitrarily selected element from one of the RD loaded WE43-T6 CPFEMs of the uncertainty quantification study, that the thermal softening implementation was dependent on; Eq. 4.52 defines thermal energy as a function of plastic strain, therefore when plastic strain increased, so did the thermal energy of the element. Table 6.1 reports the values allocated to the thermal softening-dependent parameters. The temperature of the element was observed to increase with thermal energy up to a limit defined by the material's melting point. This rise in temperature was subsequently met, as shown, with the decrease of a value evaluated by a function (defined in Eq. 4.50) that scaled back the CRSSs of all the slip systems, thus reflecting thermal softening. A problem with the implementation was that it was observed to be overly sensitive as the temperature was believed to increase too quickly resulting in excessive thermal softening, as such, it was thought that some other thermal dissipation mechanisms had been overlooked. This identified the need to verify the model's predictions of temperature against experimental results. The next section now goes on to discuss how other supplementary experimental campaigns could be used to improve the design capabilities of the proposed homogenisation approach through the implementation of even more physically-based considerations.

Parameter	Value	Unit
T_{ref}	293	K
T_{melt}	923	K
z	0.9	-
n	1.3	-
C_p	1.02×10^{12}	J /Kg K

Table 6.1: Allocation of values to parameters of the thermal softening model.

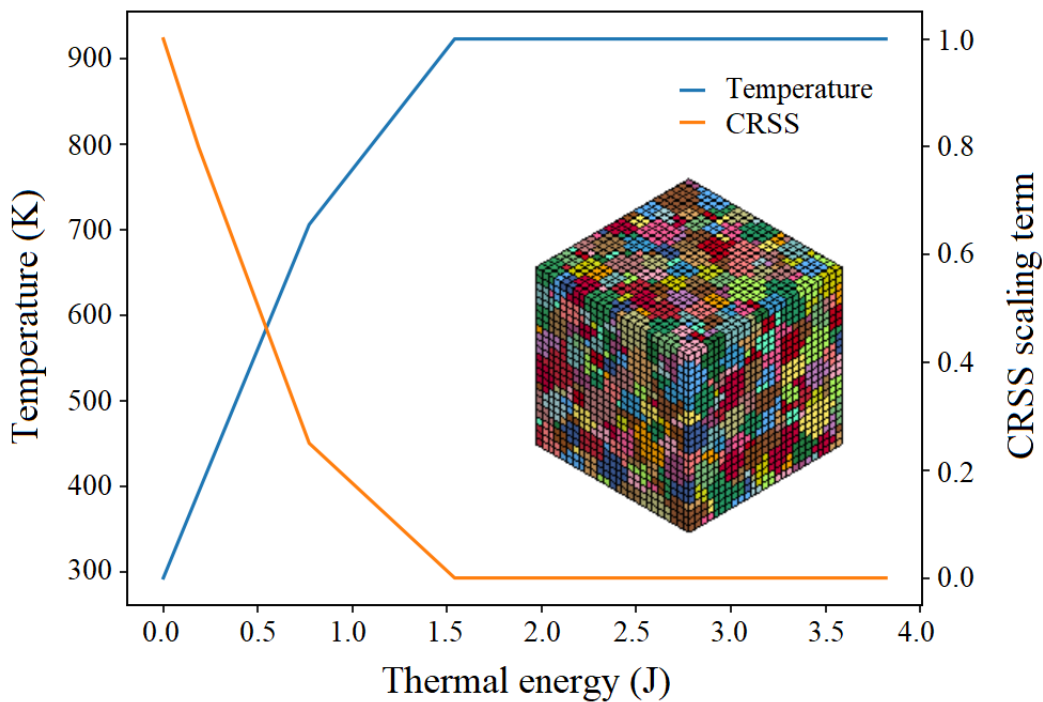


Figure 6.1: Evolution of state variables, of an arbitrarily selected element from one of the RD loaded WE43-T6 CPFEMs of the uncertainty quantification study (shown), that the thermal softening implementation was dependent on. Temperature was observed to increase with thermal energy (which itself depended on plastic strain). With this increase in temperature a handle that controlled the CRSSs of all the slip systems decreased, reflecting thermal softening.

6.2 Implementing even more physically-based considerations

The parameters of the RVE-sized CPFEMs were determined through a least squares error minimisation optimisation to experimentally measured data reflecting uni-axially loaded test specimens. Castelluccio et al., 2017, [101] however, showed that this was problematic for

models with parameters that were not uniquely defined, and subsequently went on to suggest that this problem could be addressed through the use of specifically targeted experiments or supplementary lower-length-scale models, such as those dislocation or molecular dynamics-based. Digressing back to the developed crystal plasticity-based constitutive model, Mecking and Kocks, 1981 [96], derived a dislocation density-based hardening law, and Dunne et al., 2007 [23], a physically-based shearing law, that could be incorporated directly into it (implementation of the dislocation density-based hardening law was attempted). Such laws would provide a means for considering experimentally-measured characteristics of a material system, thus aiding with making the solution uniquely defined.

Another approach could see the parameters of the strain hardening-based phenomenological model being determined through specifically designed experiments. For example, Stander et al., 2015, [144] proposed high-rate single crystal micro-pillar compression tests be used to target individual slip systems whose characterisation could parameterise their modelled counterpart. More sophisticated tests would, however, be required to establish the extent of latent hardening. Furthermore, as the Hall-Petch term included in the additively comprised expression for τ_c^α (see Eq. 4.45) is in fact already physically-based (it has terms for the mean-free-path and twin separation), the value for h_{HP}^κ (see Eq. 4.46) could be calibrated through specifically designed experiments where the resulting hardening arising from grain size effects and twins are characterised. Subsequently, with h_{HP}^κ being experimentally determined, the opportunity to design the grain size distribution becomes plausible (discussed in Section 6.4). While loosely on the subject of twins, the manner in which they were considered is challenged in the following.

The adopted homogenised-based twinning formulation was acknowledged to give predictions of bulk-level mechanical behaviour not truly reflecting that of the material system as it was shown that the flatness of the plateau observed in the experimentally measured flow stress behaviour of in-plane compressed AZ31B-O sheet was not reproduced (see Figure 4.32). This deviation was believed to be due to the non-local twin implementation used in the current work, and so it is expected that modelling the twins explicitly would rectify this. It should however be noted that homogenised-based approaches were chosen over explicit-based ones as they are more computationally efficient due to them not needing additional subroutines outside of the constitutive model. Furthermore, the converged upon RVE settings resulted in meshes too coarse to be able to precisely model twin laths, and if the element density was to be increased to enable

their consideration, this would be met with (as shown in Figure 4.22) substantial increases in runtime. Nevertheless, it is hoped that the representativeness of the implemented homogenised-based twinning formulation could be improved via the introduction of conditions into the user-subroutine that reflect localisation. Revisiting of the homogenised-based twin implementation also provides the opportunity to explore path dependency and as such is discussed next.

Currently, the presented full-field homogenisation approach (as it is) only characterises uni-axially loaded CPFEMs, which was sufficient to enable hierarchical parameterisation of the modified ISML plasticity model. This model is however only suitable for analyses where reverse loading is negligible, which is in part due to how specific portions of the yield surface in principle stress space evolved at different rates (see Figure 3.3). For example, if an element allocated the model was initially loaded in tension, it would harden with plastic strain following the anisotropic Johnson-Cook law (see Eq. 3.52). However, as the measure of plastic strain increased, the yield surface associated with compression (see Eq. 3.80) still evolved, even though the criteria to activate the mechanisms that lead to the observed sigmoid flow stress behaviour were not met. Another shortcoming of the developed plasticity model was that it could not reproduce the orientation-dependent behaviour of AZ31B-O sheet under compression (transition from sigmoid to power-law-shaped flow stress behaviour with in-plane to out-of-plane rotation). These issues highlight the limitations of plasticity models that use a functional form to describe anisotropic, path-dependent yielding, and to overcome them the use of ANN-based plasticity models was proposed (future work discussions on this topic are discussed in the following section). If it was taken for granted that the passing of mechanical behaviour from the CPFEMs to the component-level model was guaranteed, then more effort could be directed toward incorporating path-dependent behaviour at the CPFEM-level (e.g. twinning/detwinning, intergranular cracking, transgranular slip and kink bands etc. [36, 70, 114]). Furthermore, to facilitate the consideration of even higher-rates, mechanisms beyond the thermally activated regime, such as phonon drag [145], could also be explored and implemented. Nonetheless, the incorporation of path-dependent mechanisms would require extensive efforts to facilitate their parameterisation, and subsequently so would the characterisation of the CPFEMs to train ANN-based plasticity models. The following section proceeds to detail how the latter of these was foreseen to be developed.

6.3 Toward data-driven component-level constitutive models

As already discussed in Section 5.1.2, ANNs could be trained to predict yielding or to make predictions on micro- or meso-structure characteristics that could improve the performance of a material system for its component's particular application. Through use of the code-base made available in Linka et al., 2022, [113], the mechanistically informed ANN-based constitutive model proposed by Liu et al., 2023, [112] whose anisotropic yield function was not known *a priori* but was arrived at through training of an ANN, the proposed homogenisation approach, and a unit-cell test environment [100], it is believed that a data-driven component-level plasticity model with anisotropic, path-dependent traits reflecting that of a CPFEM could be trained. It is envisioned that once a CPFEM with all the necessary mechanisms has been parameterised, a dataset to train an anisotropic yield function would be generated by subjecting the CPFEM to various loading conditions as defined by the unit-cell test environment. Examples of loading conditions include, uni-axial compression and tension, pure shear, cyclic, multi-axial loading at various ratios (e.g. 11 + 22), and uni-axial with shear at various ratios (e.g. 11 + 12), with Figure 6.2 visualising what the various load combination ratios might look like. Assuming that this is sufficient to develop a mechanistically informed ANN-based constitutive model, a further activity would then be to use the code-base made available in Linka et al., 2022, again, but this time to train an ANN to make predictions on micro- or meso-structure, or even manufacturing processes, that might give a material system desirable traits (these could range from flow stress considerations to those concerning manufacture or cost). This would be achieved through the vectorisation of values characterising the micro- and meso-structure, and homogenised mechanical behaviour of the CPFEMs, and supplementing it with information such as temperature, feed-rate, thickness reduction, rolling strategy, or cost.

In addition to using the homogenisation approach to find desirable material system traits through ANN-based methods, it could also be used to set up an optimisation that could design a material system for a structural component's specific application, thus improving performance. As it is, the homogenisation approach is currently bottom-up, but through the use of component-level analyses to seek advantageous lower length-scale material characteristics the approach could become top-down. What is required to develop this capability is discussed in the following.

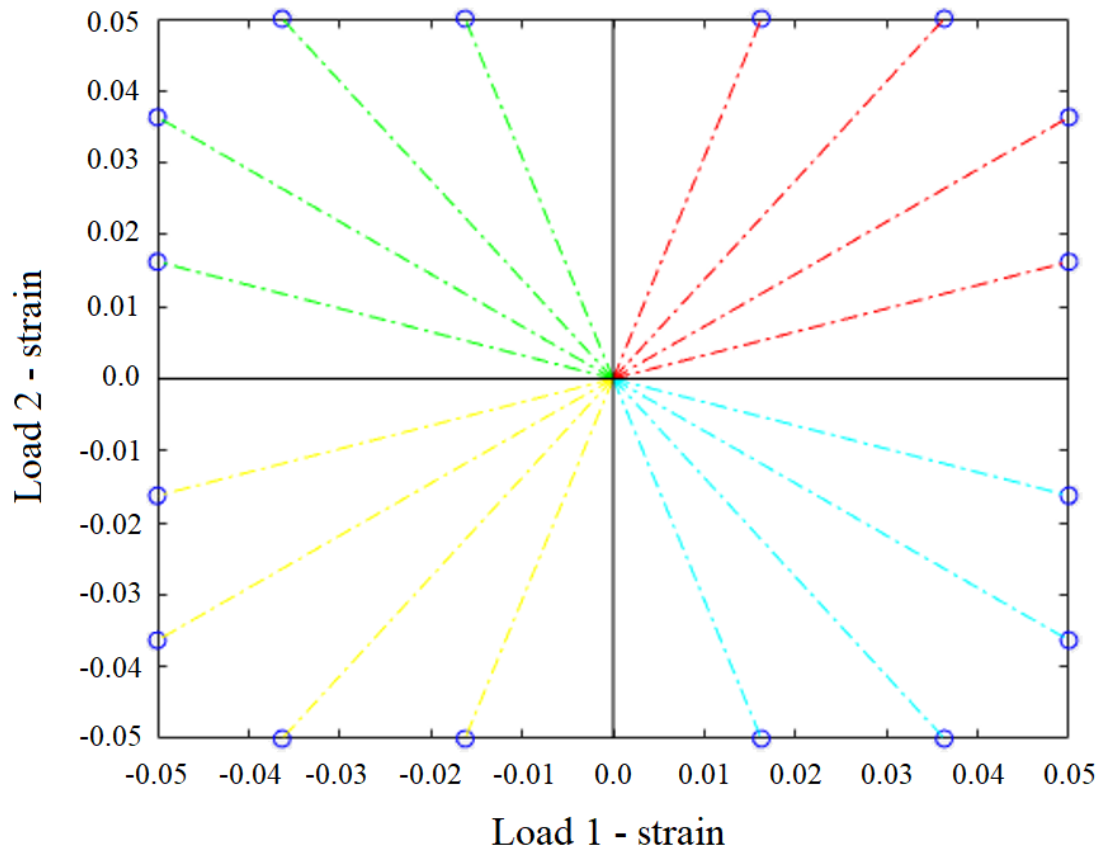


Figure 6.2: Example of what various load combination ratios might look like. Each line originating from $(0.0, 0.0)$ represents a loading case.

6.4 Toward more complex modelling architectures

As detailed in the preceding section and Section 5.1.3, the proposed homogenisation approach could be used in an optimisation where the texture of a material system could be designed to improve the performance of a component. Furthermore, if the parameters are made physically-based and thus unique, as detailed in section 6.2, the opportunity to then possibly even design the shape and size of grains, and potentially their substructure (precipitates and solutes), becomes plausible.

Another capability offered by the homogenisation approach was the ability to generate stochastic-based component-level models (see Section 5.1). This ability arose due to the fact that the aleatoric nature of mesostructure could be quantified through the characterisation of the full-field CPFEMs, resulting in the generation of parameter space distributions that could be uniformly sampled. The arbitrary allocation of these parameters to the integration points of elements comprising a domain was then shown to produce stochastic-based predictions as there

was subtle variations in the von Mises stress field of a rerun model of blast-loaded WE43-T6 plate. It is believed that such models could facilitate the transition from the deterministic-based models, typically used in the design of structural components, to those that are probabilistic-based. Furthermore, the parameters allocated to the elements of the domain could also reflect more than one mesostructure realisation type (e.g. collections of grains within a specific portion of a material's bulk may be larger than the rest, orientated differently, or have differing shapes, e.g. columnar, equiaxed, etc.), thus adding macro-zone considerations to the component-level model.

Moreover, if the concurrent spatial multi-scale model detailed in Section 5.3 could be made more computationally efficient and made to add mesostructure resolution (where a new realisation is generated with each run) to specific portions of a component model that require an increased level of detail (based on *ad-hoc* defined conditions) on-the-fly as the simulation progresses, then, through multiple runs, mesostructure characteristics (e.g. badly orientated grains, grain boundaries, etc.) that lead to stress localisation, and thus undesirable behaviour, could be specifically considered. Additionally, crack initiation and its subsequent propagation through each unique polycrystalline realisation could be studied if inter- and trans-granular cracking is implemented. Presented in the following is a summary of an explicit-explicit subcycling algorithm intended to improve the computational efficiency of models exhibiting a wide range of element sizes, thus paving the way to enable such modelling architectures.

6.4.1 Summary of an explicit-explicit subcycling algorithm

At the time this thesis was written, an explicit-explicit subcycling algorithm capable of self-sorting and running numerous parallel time-stepping regimes at arbitrary non-integer time-step ratios was developed in DEST [146], the same environment the crystal plasticity-based user-subroutine was initially developed in. It is expected that such an algorithm would improve the computational efficiency of concurrent spatial multi-scale analyses, thus enabling mesostructural resolution in component-level models. Presented in the following is a brief summary of this algorithm.

The summary of this capability begins with the consideration of a domain $\Omega \subset \mathbb{R}^3$, with boundary $\partial\Omega$, divided into $\mathcal{S}$ non-overlapping subdomains Ω_i having masses $\mathbf{M}_i = \sum_{e=1}^{m=\#elements} \int_{\Phi_i(\Omega_e)} \rho \mathbf{N}_i^a \mathbf{N}_i^b dv$. Each subdomain operates independently, integrates through time at their own rate t_i , and their union forms the entire domain. To explain the algorithm, let's first consider a domain with only two subdomains, a large Ω_L and a small Ω_s . The equations

of motion for these subdomains are defined separately and the continuity of acceleration at their interface Γ is ensured.

A critical aspect of the algorithm is the use of time-step ratios to synchronize the times of the two subdomains. The current and next time-step ratios (t_{ratio}^n and t_{ratio}^{n+1} , respectively, where n is the n^{th} time-step) help determine whether a *pull-back* is needed, ensuring that both time domains can exchange quantities at the same time t . This synchronization mechanism allows the subdomains to maintain accurate communication without a user-set time-step ratio. The degree of *pull-back* is determined using a trial time t_{Ti} and time-step *pull-back* ratio α_i [141, 147], which adjusts the time-step of the subdomain with the smaller ratio to synchronize with the other subdomain. This ensures that both subdomains can proceed through their respective time-steps in a coordinated manner.

Furthermore, the algorithm employs an added-mass technique [148] for nodes at the interface Γ . It calculates the combined mass and internal forces at these nodes and updates the acceleration of the small subdomain based on the large subdomains acceleration after each large time-step.

This completes the two time-subdomain subcycling algorithm. Figure 6.3 presents the procedure through a flowchart which makes evident the minimal amount of communication required between the two subdomains, and thus highlights why it is appropriate to dedicate each subdomain their own thread. A pseudo-code representation of the implementation is also provided in Algorithm 2. Having formulated a two time-subdomain subcycling algorithm, the extension of it to multiple time-subdomains is now presented.

The algorithm can be extended to handle multiple subdomains by sorting them according to their time-steps and matching them in pairs. This process ensures that synchronization is maintained across all subdomains. Additionally, subdomains that are not spatially adjacent but have equivalent time-steps can be integrated concurrently. The pseudo-code representation of the multi-time domain procedure is subsequently presented in Algorithm 3, and as such, it is shown that the re-sorting of subdomains after Δt_L^n allows for a time-step ratio, m , that may change as the simulation advances, and that the algorithm even allows for the switching of Ω_s and Ω_L , following a single large time-step. It should be noted, that Algorithm 2 requires slight modification to allow for the transfer of system variables that are spatially adjacent but

Algorithm 2 Two-domain constant acceleration multi-time-step integration algorithm [146]

```

1: while  $t_s$  and  $t_L$  integrate through time do
2:    $k = 0$ ;
3:   if  $t_s$  and  $t_L == 0.0$  then
4:     compute  $\mathbf{f}_s^{int}, \mathbf{f}_s^{ext}$  and  $\mathbf{M}_s$  with Eqs. 3.21; ▷ small force and mass vectors
5:     compute  $\mathbf{f}_L^{int}, \mathbf{f}_L^{ext}$  and  $\mathbf{M}_L$  with Eqs. 3.21; ▷ Large force and mass vectors
6:     for all nodes  $n_i^\Gamma$  do
7:        $\mathbf{M}_\Gamma = \mathbf{M}_{\Gamma L} + \mathbf{M}_{\Gamma s}$ ; ▷ mass exchange
8:        $\mathbf{f}_\Gamma^{int} = \mathbf{f}_{\Gamma L}^{int} + \mathbf{f}_{\Gamma s}^{int}$ ; ▷ internal force summation
9:        $\ddot{\mathbf{u}}_\Gamma^n = (\mathbf{f}_{\Gamma L}^{ext} - \mathbf{f}_{\Gamma s}^{int})/\mathbf{M}_\Gamma$  ▷ Large acceleration
10:    end for
11:    compute  $t_{Ts}^{n+k}, t_{TL}^{n+k+1}, t_{ratio}^{n+k}$  and  $t_{ratio}^{n+k+1}$ ; ▷ time-step ratios
12:  end if
13:  while  $t_{ratio}^{n+k+1} \leq 1$  or  $(t_{ratio}^{n+k} \leq 1 \text{ and } t_{ratio}^{n+k+1} \leq 1 + \text{tol})$  do
14:    let  $\ddot{\mathbf{u}}_{\Gamma s}^n = \ddot{\mathbf{u}}_{\Gamma L}^n$ ; ▷ prescribe Large acceleration
15:    solve subdomain  $\Omega_s$  Eqs. 3.25 for  $\Delta t_s$ 
16:     $t_s = t_s + \Delta t_s, k += 1$ ;
17:    compute  $\mathbf{f}_s^{int}, \mathbf{f}_s^{ext}$  with Eqs. 3.21; ▷ small force vectors
18:    compute  $t_{Ts}, t_{ratio}^{n+k}$  and  $t_{ratio}^{n+k+1}$ ; ▷ time-step ratios
19:  end while
20:  compute  $\alpha_L$  and  $\alpha_s$ ; ▷ Large and small Pullback
21:  if  $\alpha_L \geq \alpha_s$  then
22:     $\Delta t_L = \alpha_L \Delta t_s$ ;
23:  else if  $\alpha_s > \alpha_L$  then
24:     $\Delta t_s = \alpha_s \Delta t_s$ ;
25:    let  $\ddot{\mathbf{u}}_{\Gamma s}^n = \ddot{\mathbf{u}}_{\Gamma L}^n$ ; ▷ prescribe Large acceleration
26:    solve subdomain  $\Omega_s$  Eqs. 3.25 for  $\Delta t_s$ 
27:     $t_s = t_s + \Delta t_s, k += 1$ ;
28:    compute  $\mathbf{f}_s^{int}, \mathbf{f}_s^{ext}$  with Eqs. 3.21; ▷ small force vectors
29:    compute  $t_{Ts}, t_{ratio}^{n+k}$  and  $t_{ratio}^{n+k+1}$ ; ▷ time-step ratios
30:  end if
31:  solve subdomain  $\Omega_L$  Eqs. 3.25 for  $\Delta t_L$ 
32:   $t_L = t_L + \Delta t_L$ ; ▷ increment Large time
33:  for all nodes  $n_i^\Gamma$  do
34:    compute  $\mathbf{f}_L^{int}, \mathbf{f}_L^{ext}$  with Eqs. 3.21; ▷ Large force vectors
35:     $\mathbf{f}_\Gamma^{int} = \mathbf{f}_{\Gamma L}^{int} + \mathbf{f}_{\Gamma s}^{int}$ ; ▷ internal force summation
36:     $\ddot{\mathbf{u}}_\Gamma^n = (\mathbf{f}_{\Gamma L}^{ext} - \mathbf{f}_{\Gamma s}^{int})/\mathbf{M}_\Gamma$  ▷ Large acceleration
37:  end for
38:  compute  $t_{TL}, t_{ratio}^{n+k}$  and  $t_{ratio}^{n+k+1}$ ; ▷ time-step ratios
39: end while

```

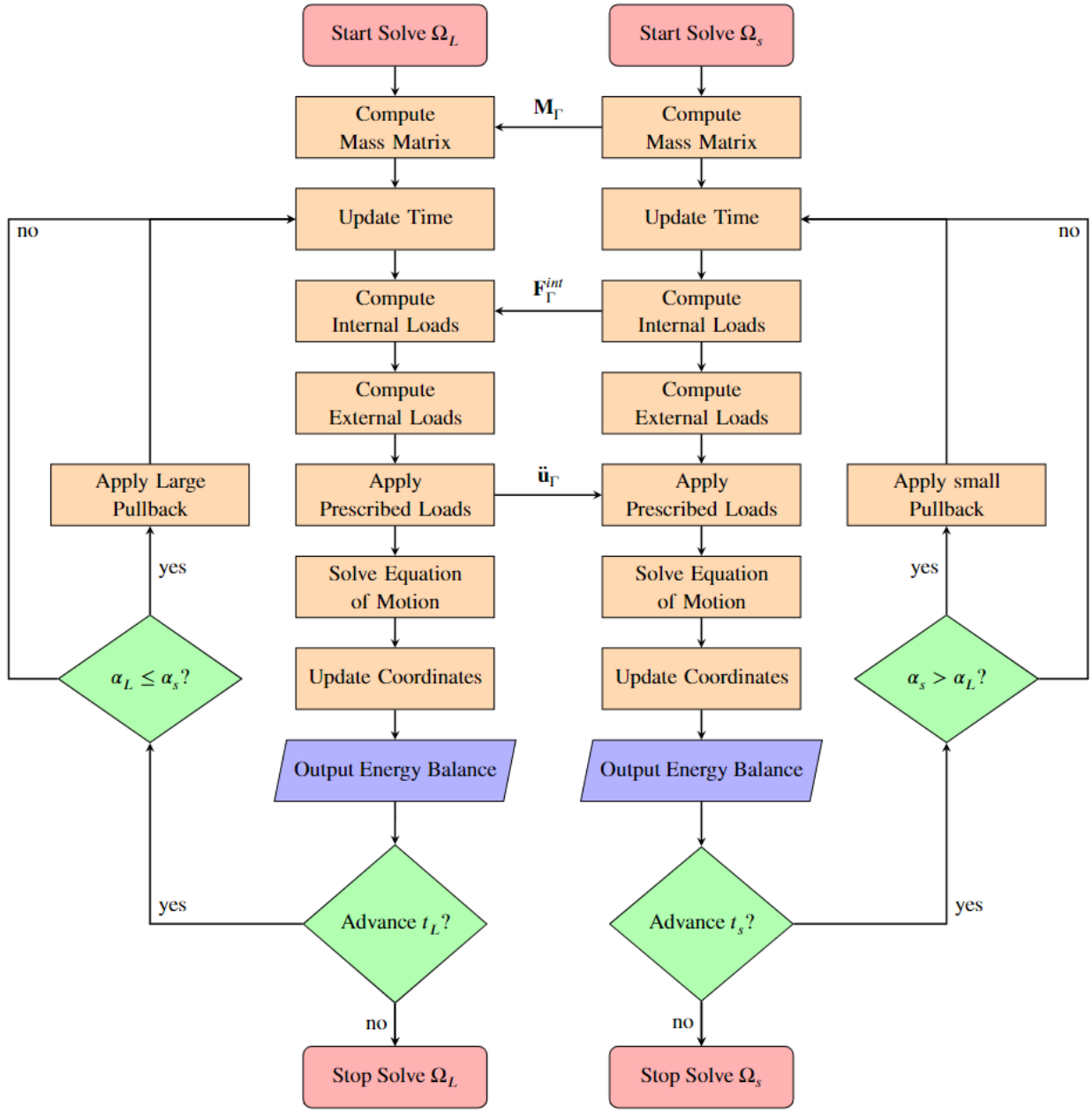


Figure 6.3: Flowchart of two time-subdomain subcycling algorithm with transfer of variables.

not temporally. As such, the following modification was made,

$$\mathbf{M}_\Gamma = \mathbf{M}_{\Gamma\tilde{L}} + \mathbf{M}_{\Gamma s}; \quad \mathbf{f}_\Gamma^{int} = \mathbf{f}_{\Gamma\tilde{L}}^{int} + \mathbf{f}_{\Gamma s}^{int}; \quad \ddot{\mathbf{u}}_{\Gamma s} = \ddot{\mathbf{u}}_{\Gamma\tilde{L}}, \quad (6.1)$$

where $\tilde{L}$ denotes the spatially adjacent large subdomain.

With this capability, a model similar to that detailed in Section 5.3.2 could be run to assess the potential gains in computational efficiency. Moving on, the following section discusses the effort that went into making the capabilities developed in this thesis user-friendly.

Algorithm 3 Multi-domain constant acceleration multi-time-step integration algorithm

```

1: while subdomains integrate through time do
2:   if  $t_i = 0.0$  then
3:     for all subdomains  $\Omega_i$  do
4:       compute  $t_{Ti}$ ; ▷ subdomains' trial times
5:     end for
6:     sort subdomains  $\Omega_i$  from  $\min\{\Delta t_i\}$  to  $\max\{\Delta t_i\}$ ; ▷ sort subdomains in order
7:     let  $\Omega_s = \min\{\Omega_i\}$  and  $\Omega_L = \Omega_{s+1}$ ; ▷ smallest time-step domain is  $s$  and next up is  $L$ 
8:   end if
9:   while ( $t_s < \text{simulation run time}$ ) and  $\Omega_L$  exists do
10:    two-domain-algorithm ( $\Omega_s, \Omega_L$ ) ▷ using Algorithm 2
11:    sort subdomains  $\Omega_i$  from  $\min\{\Delta t_i\}$  to  $\max\{\Delta t_i\}$ ;
12:    if  $\Omega_{L+1}$  exists then ▷ check for more subdomains to integrate
13:      if  $t_{Ts} < t_{TL+1}$  then
14:        continue; ▷ iterate current small-large pair again
15:      else
16:        let subdomains  $\Omega_s = \Omega_L$  then  $\Omega_L = \Omega_{s+1}$ ; ▷ move to next pair up
17:      end if
18:    else
19:      break; ▷ all subdomains are synchronised in time
20:    end if
21:  end while
22: end while

```

6.5 Encouraging a user-base

In addition to incorporating the developed plasticity models into the commercially available FEA tool, LS-Dyna, the homogenisation approach was also implemented into the object-orientated polycrystalline generating programme, VorTeX. While this thesis was being written, VorTeX was given a GUI (see Figure 6.4) which the author hopes various single-click capabilities will be integrated to. Examples of such capabilities include the generation of statistically representative tessellations that reflect experimentally measured micrographs, and one that produces an executable that could be run on ARC to size CPFEMs into RVEs and subsequently create the parameter space distributions to be used by stochastic-based component-level plasticity models. Furthermore, VorTeX could also be used for product data management purposes to store experimental and digitally-based information. On top of technical capabilities, a number of publications in academic journals is expected from the work presented in this thesis, and, as such, are discussed next.

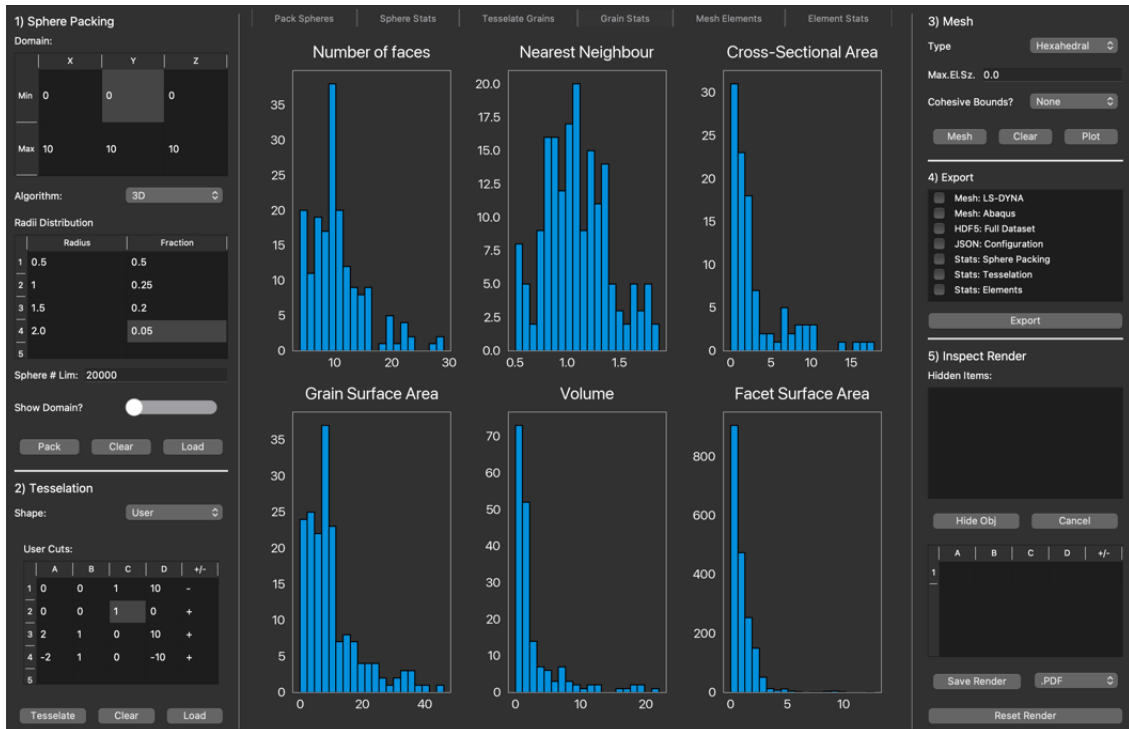
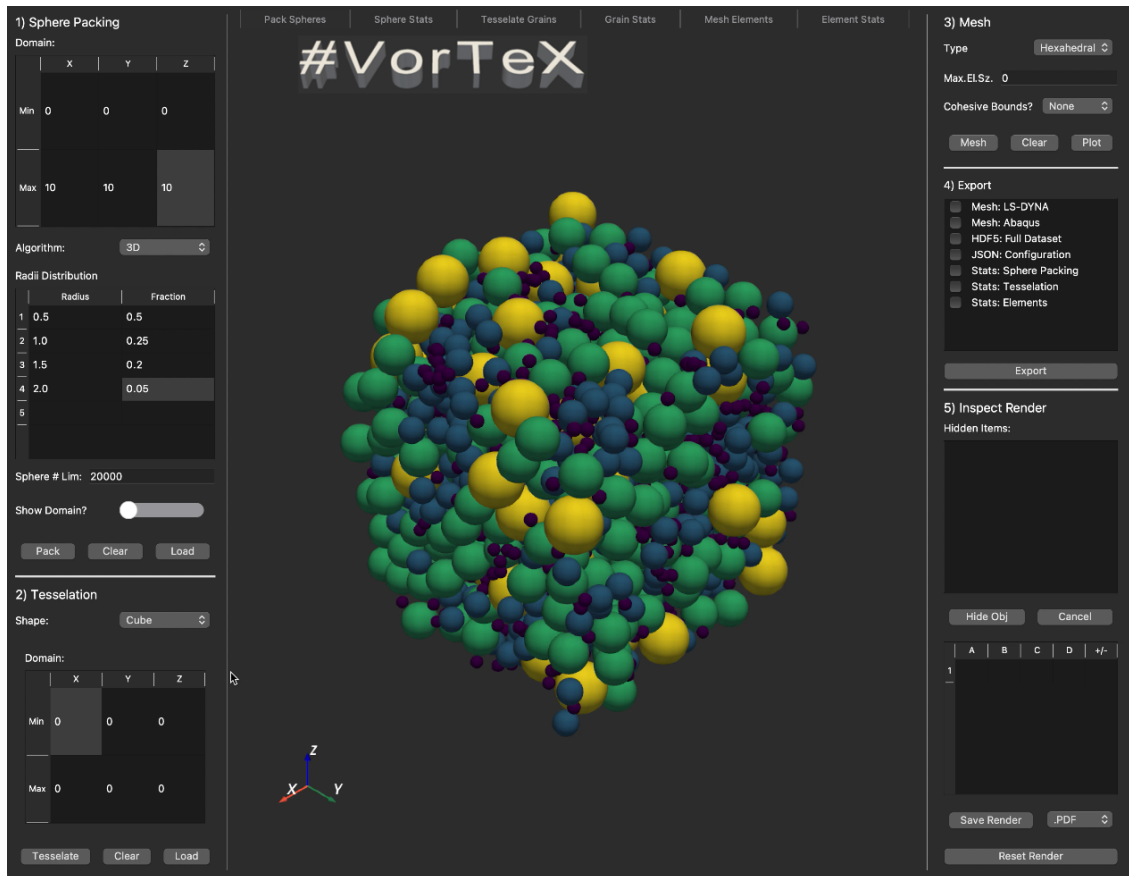


Figure 6.4: Screenshots of VorTeX GUI.

6.6 Publications

Anticipated publications resulting from the work presented in this thesis include:

- Proposed title: A Virtual Test Environment for Study of Aleatoric Mesostructure Effects on Constitutive Laws for Magnesium Alloys.
 - Aim: Proposition of full-field homogenisation approach that allows study of the effects aleatoric mesostructure features have on bulk-level characterisation.
 - Status: Rejected, September 2022.
 - Reason: At the time this paper was submitted the homogenised-twin implementation was not working, therefore, the developed explicitly-run crystal plasticity-based user-subroutine only considered slip. The main reason for the reviewers rejection was this, since twinning is so prominent in magnesium alloys. However, as presented, twinning has now been incorporated quite successfully. Therefore this paper needs redrafted to reflect this, and as such will be resubmitted.
- Proposed title: Optimisation of component's micro-structure to improve performance for a specific application.
 - Aim: Put forward a top-down strategy that enables use of homogenisation approach to aid with material system design to improve component performance. Such a strategy would see micro- or meso-structure characteristics designed by means of an optimisation.
 - Status: Proposed.
- Proposed title: A multi-time stepping algorithm for the modelling of heterogeneous structures with explicit time integration
 - Aim: Named author on this paper. Paper details formulation presented in this thesis alongside its use in analytical and computational models.
 - Status: Submitted: December 2023.
- Proposed title: Investigation of mesostructure topology, texture, and plasticity on intergranular cracking.

- Aim: A study that makes use of the homogenisation approach and intergranular cracking methodology. This study will look to allude whether mesostructure features have bearing on the extent of fracture observed.
- Status: Proposed.
- Proposed title: Concurrent multi-scale spatial coupling of conforming meshes.
 - Aim: To run the spatial multi-scale FEM detailed in Section 5.3.2 with the multi-time stepping algorithm formulated in Section 6.4.1. This paper will include a study that will investigate the effect of rouge grains in stress raising areas of component-level models, potentially with the added consideration of intergranular cracking.
 - Status: Proposed.

Furthermore, the work presented in this thesis was well received at the following conferences:

- DSTL DMF conference, seminar, May 2021.
- Rolls-Royce Cornerstone conference, seminar, June 2021.
- Rolls-Royce Cornerstone conference, poster presentation, June 2022.
- DSTG crystal plasticity modelling workshop, August 2022.
- Multiscale Materials Modeling conference, October 2022.
- DSTL crystal plasticity modelling workshop, January 2023.

Having given an account of when the presented work had or will be reviewed by the community, the following chapter brings the thesis to a close with concluding remarks.

7

Conclusions

The objective of the work presented in this thesis was to devise a multi-scale approach to the development of high-rate-based microstructure-aware constitutive models for magnesium alloys. To aid with presenting this, the following questions were initially posed in the Introduction,

- Can constitutive models that correctly predict the flow stresses of WE43-T6 plate and AZ31B-O sheet be developed to enable their consideration in the design of components (such models are currently not available in commercial code)?
- Is it possible to generate approximations of the full-field stress heterogeneity that develops at the mesoscale from bulk mechanical characterisations of a material using CPFEMs?
- Could a hierarchical link between these CPFEMs and component-level constitutive models be established where the effect of altering micro- and meso-scale features (such as solutes and precipitates, texture, grain size distribution, etc.) influences the scale above?
- Subsequently, would it be possible to design these micro- and meso-scale features to improve the performance of a component for its specific application?

- Finally, could the datasets generated through the homogenisation and characterisation of CPFEMs be leveraged to facilitate novel, data-rich modelling strategies?

Answers to the above questions were provided by first conducting an analysis that assessed the blast resisting properties of a hard steel plate using the commercially available FEA software package, LS-Dyna; this analysis was typical of one completed in industry. As magnesium alloys are significantly lighter than steel alloys, there existed the opportunity to use a thicker section for the same mass penalty, potentially improving blast resisting characteristics. It was shown that the hard steel plate exhibited penetrative fracture at an earlier time compared to the WE43-T6 plate, with the shock severity also being less severe for the magnesium alloy-based plate. It was however recognised that the predicted performance of the WE43-T6 plate might not be entirely accurate due to the fact that an isotropic constitutive model was used to model a material with anisotropic mechanical properties, and also that the criteria for fracture may not have been representative.

This study highlighted the fact that it was difficult to design structural components destined for high-rate applications from rolled or extruded magnesium alloys due to the lack of constitutive models available that could predict their inherent anisotropic mechanical properties. These properties were shown to arise from the HCP unit cell coupling with composition and processing route of the material. Therefore, component-level constitutive models that could predict the experimentally measured orientation-dependent flow stress behaviour of WE43-T6 plate and AZ31B-O sheet were first developed. The WE43-T6 plate analysis was subsequently rerun and showed that the consideration of out-of-plane flow stress behaviour was found to be inconsequential. An analysis investigating the use of AZ31B-O sheet was also ran for investigative purposes due to the strong orientation-dependent behaviour this material exhibited (stemming from its microstructure) making it an ideal model material to showcase the developments presented in this thesis.

The component-level constitutive model developed for AZ31B-O, however, possessed a flaw which saw different portions of the yield surface in principle space, reflecting different loading scenarios, evolve at differing rates with plastic strain. This was due to a simplified approach being opted for to implement the tension-compression asymmetry seen in AZ31B-O sheet. As such, yielding in one portion might evolve another portion of the yield surface without the necessary mechanisms activating to merit it. To overcome this shortcoming, it was recommended that physically-based considerations be incorporated through the use of

lower length-scale models. Nevertheless, the developed component-level constitutive model was still considered satisfactory to answer the first question.

Lower length-scale considerations could have been implemented via hierarchical or concurrent means. A hierarchical approach was opted for as it was believed that these should be established prior to any concurrent-based developments, and because the required top-level constitutive models were already made available. As the mechanisms driving plasticity are found interior to a grain, but the orientation of a collection of grains was found to dictate anisotropic bulk-level mechanical behaviour, crystal plasticity-considered approaches were preferred. These can be classified into two branches, mean-field (analytical averaging) or full-field (explicit modelling of mesostructure). Full-field approaches were chosen over mean-field ones as they enable the direct consideration of mesostructure and because they generate the heterogeneous stress field underpinning bulk-level properties, enabling the further study of even more localised mechanisms.

To facilitate this, polycrystalline-based FEMs statistically representative of the material system being studied required generated. An explicitly-run crystal plasticity-based user-subroutine was subsequently developed and allocated to these polycrystalline models. The decision to implement the user-subroutine into an explicit-based solver was made due to the rate-dependent nature of the capability being devised. The user-subroutine calculated plastic deformation through the thermally activated mechanisms, dislocation glide and twinning. Twinning could have been implemented discretely or by homogenising their contribution, with the latter being opted for due to computational efficiency.

The ability to predict the deformation of the polycrystalline structures through the relative activity of the various available crystal plasticity-based deformation mechanisms now existed. However, to enable this, the polycrystalline structures needed to be sized into RVEs to allow length-scale transitioning. This was because an optimisation algorithm that sought parameters for the crystal plasticity-based model to yield experimentally measured bulk-level characterisations of a material, through a least squares error minimisation, was used. It was noted that parameters not uniquely defined and determined in this manner were shown to incorrectly predict the stress in individual grains, but, regardless of this, it was still believed to give a good approximation. The second question was considered answered with this capability described thus far. The issue regarding the potential to converge on a local minima during the optimisation, and thus incorrectly predict the stress heterogeneity, is discussed in the following.

Through the application of the above-mentioned to generate CPFEMs that reproduced the bulk-level mechanical behaviour of magnesium alloys WE43-T6 plate and AZ31B-O sheet, the effect of altering micro- and meso-scale features was shown. This was because both of these were modelled using the same method but yielded (as shown) entirely different bulk-level mechanical behaviour owing to varying micro- and meso-scale features. Subsequently, the third question was considered answered. The possibility to design these features to improve the performance of a component for its specific application is discussed next.

The developed hierarchical framework could be used to design the micro- and meso-scale features of a material system to improve its performance for a component's specific application, as the developed CPFEMs, which capture such details, can be homogenised and characterised to enable parameterisation of the developed component-level constitutive models (i.e. the parameters of the component-level constitutive model are now based on lower length-scale models). This, however, came with a caveat. As it was unknown whether the converged upon parameters reflected what was occurring physically (resulting in the incorrect prediction of the stress heterogeneity), the ability to accurately realise changes in the microstructure through the crystal plasticity parameters could not be guaranteed as their sensitivities were unknown. This could however be addressed by replacing the phenomenological strain-based hardening law with one physically-based, and conducting specifically tailored experiments (or running even further lower length-scale models) to parameterise it. Conversely, the ability to design texture was believed to exist due to how the stresses induced in the grains averaged and coupled with texture to yield the desired homogenised mechanical behaviour; this could be achieved through the use of an optimisation algorithm, thus facilitating top-down scale-bridging. Designing grain size distributions was, however, not believed possible as the invoked Hall-Petch hardening rule directly related to grain size, and as a result, the parameter controlling this behaviour suffered from the same uncertainty, regarding sensitivity, as the phenomenological strain-based hardening law. With this, question four was deemed answered. A capability that existed due to fully realising mesostructural stress fields was the ability to generate datasets quantifying the uncertainty on bulk-level mechanical behaviour arising from the aleatoric nature of the mesostructure. This dataset in-turn could then serve as the basis for stochastic-based modelling. This, in addition to other capabilities that could leverage the data made available through the CPFEMs, are discussed next, thus providing an answer to the final question.

To quantify the aleatoric nature of mesostructure, a sufficiently large population first required generating. As each mesostructural realisation of a particular alloy composition has a unique stress field deriving from its specific topology and texture, the homogenised mechanical behaviour of their CPFEMs sized into RVEs subtly varies when compared to others. To quantify the extent of this variation, a Monte-Carlo study was conducted which saw numerous sets of RVE realisations generated and subjected to a defined loading analysis until convergence in measures quantifying uncertainty were achieved. These measures were assessed by fitting the flow stresses predicted by RVE-sized CPFEMs (through a least square regression) to a hardening law that captured the characteristics of the observed behaviour. This in-turn enabled the variation in constitutive behaviour observed across the RVEs for each load case to manifest through the available parameters. The sufficiency of the population size to quantify uncertainty was then assessed by plotting the coefficient of variation against the number of realisations for each parameter space. Plateauing indicated convergence in measures of second order statistics, and that the population size was sufficient for it to be constituted as a distribution. This was completed for both studied magnesium alloy compositions, WE43-T6 and AZ31B-O.

Stochastic-based modelling was made possible through the continuous sampling of the aforementioned parameter space distributions and the arbitrary allocation of these to elements running the developed component-level constitutive model and comprising the domain. To first verify the hierarchical parameterisation, a test coupon verification study was conducted whose results were compared to the experimentally measured true stress-strain data used as part of the optimisation to determine the parameters of the crystal plasticity-based model. The model was able to reproduce the behaviour of WE43-T6 with only slight divergences being observed in the elastic and early onset of yielding regimes for normal direction loading (believed to be due to non-representative values of the Youngs modulus being used, and the CPFEM parameters of the 2nd optimisation not being used). Highly plausible predictions of behaviour with loading orientation were also observed. The hard-coded stochastic capability was then investigated through the re-running of the test coupon FEM numerous times (each run resulted in a unique realisation of parameter allocations). No variability was predicted, which was believed to be due to the parameters being sufficiently averaged over the domain. Consequently, it was thought that in order for this stochastic-seeding approach to yield variability, models that localised stress would be required. Subsequently, the blast-loaded plate analyses were

re-run, but this time with the parameters reflecting the homogenisation and characterisation of the CPFEMs. These models yielded subtle variations in the von Mises stress field, thus highlighting that stochastic-based predictions were made to an extent. Other capabilities offered by fully realising mesostructural stress fields include the ability to incorporate additional mechanisms dependent on stress localisation, such as inter- and trans-granular cracking, whose implementation is discussed in the following.

Intergranular cracking was implemented into the CPFEMs first, as this fracture mechanism was found to be most prevalent in experimentally tested AZ31B-O specimens. This was achieved through the use of cohesive elements and a user-subroutine that assessed forces against failure criteria. As there was a lack of experimental data for its calibration, values were selected that enabled the showcasing of this capability. Intergranular cracking was shown after a degree of plasticity, however, to get the CPFEM to fully fracture, the time-step needed to be significantly reduced over the time domain element deletion occurred. This time-step control needed to be determined *a priori* through numerous runs, making the user-effort extensively large which made it prohibitively difficult to work with the developed CPFEM homogenisation methodology. As such, subcycling algorithms were pursued as a potential solution to this issue.

Before even considering running the the subcycling algorithm with intergranular cracking-implemented CPFEMs, its use to improve the computational efficiency of a spatial multi-scale FEM, that concurrently ran the modified ISML and crystal plasticity-based constitutive models with a conforming mesh, was first investigated. This was because these algorithms tend to determine the time-stepping regimes each element belongs to through their characteristic length, which were noted to be similar for the intergranular cracking-implemented CPFEM, but to vary substantially more for the spatial multi-scale model. This model was able to make predictions of homogenised behaviour typically seen at the component-level model, the heterogeneity arising at the mesoscale, and to at least start to increase the element size from that required by the crystal plasticity-allocated elements to those typically used at the component-level. The expected speed-up in runtime when the model was run with the subcycling algorithm was however minimal. Nevertheless, the study helped identify that a better suited, more efficient algorithm should self-sort and run numerous parallel time-stepping regimes at arbitrary non-integer time-step ratios.

A shortcoming of the developed component-level constitutive model was that it could not reproduce the full orientation-dependent mechanical behaviour of AZ31B-O sheet under

compression due to limitations with the expression describing yielding. As such, ANNs were considered as a potential workaround as they eliminate the need to for material specific functional relations. However, their use was not pursued further. Nonetheless, it should be noted that ANNs also offer exciting new avenues for material design as they have the ability to make predictions on the effect micro- and meso- structure have on bulk-level mechanical behaviour. With this, the questions initially posed have been answered, and as detailed in the Future work chapter, their are still activities that require completed to fully realise the rate-dependence and thermal softening capabilities of the developed crystal plasticity-based user-subroutine. Nevertheless, it is believed that a compelling case has been made for the proposed methodology in constructing high-rate-based microstructure-aware constitutive models for magnesium alloys.

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