

Modelling the Effects of Heterogeneity on the Mechanical Response of Solids

BY

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PREFACE

This thesis is submitted for the degree of Doctor of Philosophy at Imperial College London. The research was conducted at the Imperial College London, in the Aeronautical Engineering department during the period August 2012 to December 2016 under the supervision of Dr Vito Tagarielli. The research was funded by the EPSRC.

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DEDICATION

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ABSTRACT

The main objective of the current thesis is to develop and verify a simple technique which is able to introduce heterogeneity in the constitutive models of solids and investigate the mechanical behaviour at low strain rates. By adopting simple constitutive models which are computationally inexpensive the aim is to capture effects of spatial variation of materials properties, geometric variation effects such as void distribution and interaction and thus being able to capture fracture and failure. In addition, important aspects are being able to predict realistic paths for the onset and evolution of damage as well as material size effects. Such techniques will be applied in order to predict experiments in various kind of materials including foams, composites.

The technique developed in the current thesis involves introduction of material heterogeneity at the micro-level using the finite element method. Distribution of material properties and geometric fields are numerically generated based on probability density functions. FE models are generated by manipulating the input file via a FORTRAN program. A Monte Carlo type analysis is performed in ABAQUS where the stochastic volume element (SVE) generated, is solved deterministically using ABAQUS implicit solver. The process is repeated N times in order to obtain the scatter and the mean of the macroscopic response. Mesh convergence studies as well as sensitivity of the size of the number of cells is conducted.

Following this approach numerical modelling of four types of materials are studied; a sintered titanium solid with 0.95 relative density; a polycrystalline elasto-plastic solid; a low porosity elasto-plastic solid with relative densities in the range 0.70-0.99 and a cellular elasto-plastic solid with relative densities in the range 0.37-0.48.

Predictions are compared to previously numerical studies as well as to experiments. For all materials examined, the heterogeneous approach proved to capture the mechanical behavior of materials at no additional computational cost.

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I would like to thank Vito Tagarielli for the great support throughout this project.

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Accurate simulations of the mechanical response of engineering materials are necessary to allow effective design of solid components. Engineering solids have complex microstructures at different length-scales and consequently their constitutive modelling may present several difficulties, reflected in the large body of literature published on this general subject.

The current constitutive modelling approaches can be broadly subdivided in *phenomenological* or *physically-based*, with the former referring to models which describe material response from the sole observation of the macroscopic behaviour, and the latter referring to approaches which explicitly describe mathematically the physical mechanisms taking place during deformation and failure of solids. As in reality materials deform by different mechanisms at different length-scales, often physically-based models need to be of multi-scale type.

Phenomenological approaches, such as reported in [1-16], neglect information on the heterogeneity in materials microstructures and can be effective if appropriately calibrated. On the other hand calibration requires extensive multi-axial testing and the models are not capable to predict localised deformation which is triggered by the material's microstructure.

Multi-scale modelling approaches allow explicit modelling of material heterogeneity at different length scales; for example, Figure 1.1 shows the relevant scale lengths for modelling of a metals and a composite. Two types of multiscale modelling approaches can be defined, *hierarchical* and *concurrent*. In hierarchical multi-scale modelling, the analysis begins at the smallest length-scale and its results inform simulations at immediately larger length-scales, until the largest scale is simulated. This method is often also called the “bottom up” approach. Various authors have adopted this technique [17-25]. In concurrent multi-scale modelling, simulations are conducted at the largest length-scale, but the modelling detail is refined locally down to the immediately lower length-scale where more accurate descriptions of the material are deemed necessary. This method is computationally demanding and has been employed by various authors [26-40].

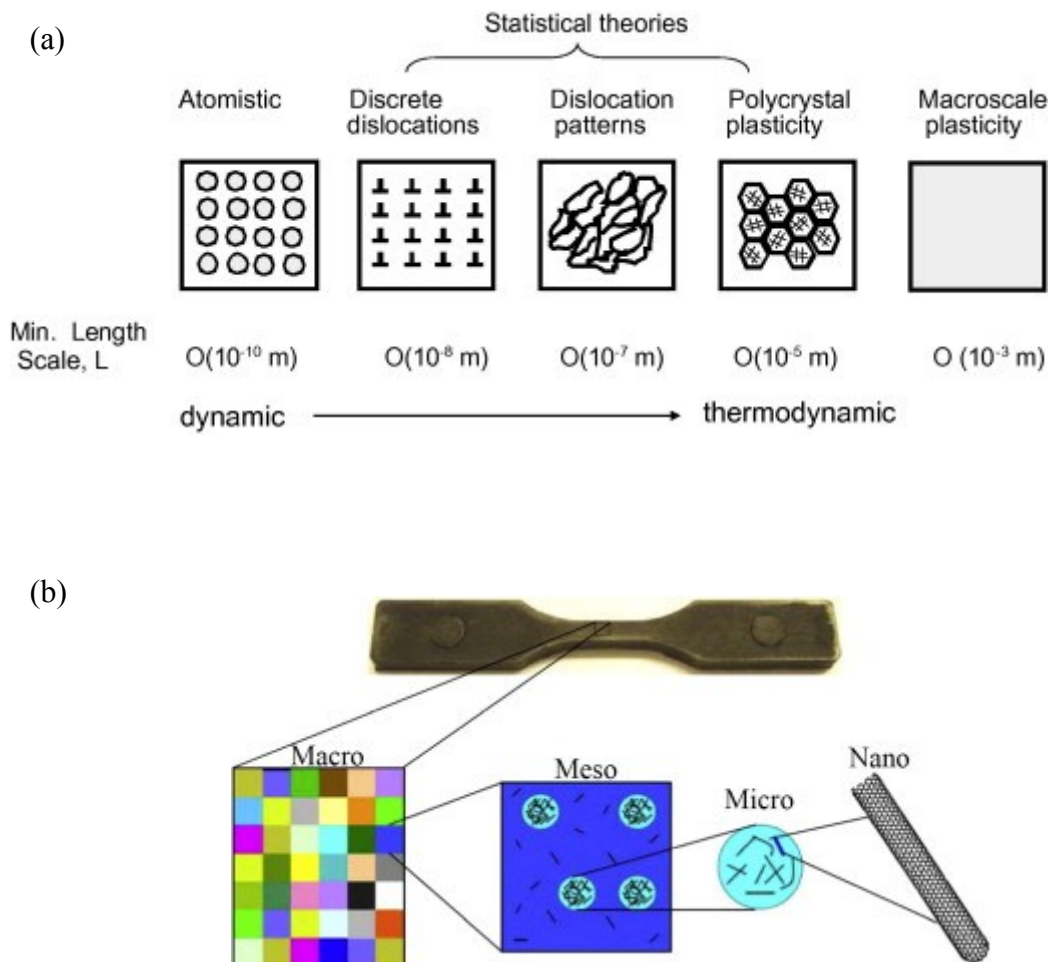


Figure 1.1 Different scales involved in the simulation of (a) polycrystalline material [41] and (b) carbon nanotube polymer composite [17].

A multi-scale modelling approach allows taking into account most physical mechanisms which contribute to the macroscopic material response; it does, however, also require substantial computational power and above all detailed information on the material's microstructure at all length-scales. Such information is often not available and in general difficult and costly to obtain, as recognised by several authors [42-44].

Examples of microstructures of different types of materials are shown in Figure 1.2; a syntactic foam, an iron-copper composite, a metal alloy and a carbon fibre composite.

In this thesis we propose the idea that it may not be necessary to possess full knowledge of the microstructural details, in order to perform predictive simulations of materials response. We also propose that, to perform true predictions of the deformation and fracture response of solid materials it is necessary to account for material heterogeneity. We propose to do this in an approximate way, by adopting simple numerical models whose calibration requires easily measurable quantities and the probability distributions of a number of different physical parameters. We aim at developing effective constitutive models able to capture the macroscopic effects of small-scale heterogeneity.

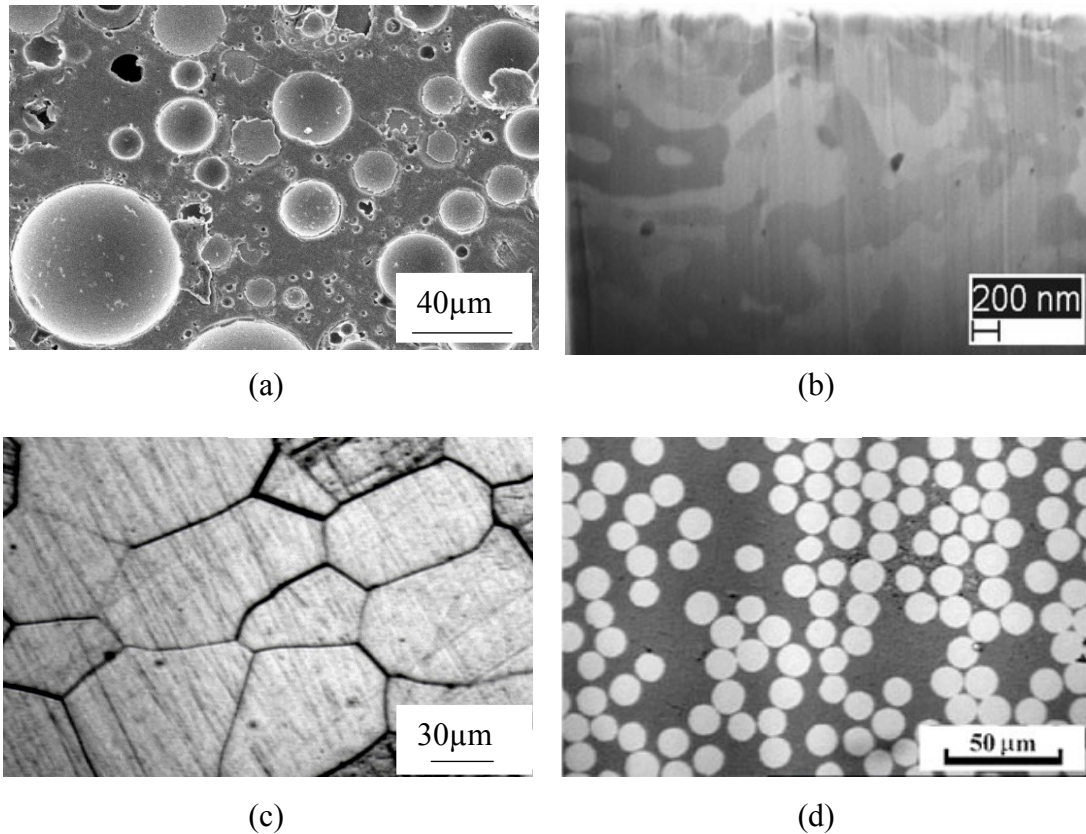


Figure 1.2 SEM image of the microstructure of syntactic polyurethane foam. The composite consists of polyurethane as the matrix with hollow particles [45]. (b) SEM image of iron-copper nano composite. Bright regions represent the iron whereas dark regions represent the copper [46] (c) Optical image of a metal alloy, showing the grain boundaries [47] (d) Optical image of carbon reinforced composite. Matrix is resin (black) and fibres are carbon (white) [48].

Several authors have examined the effect of material property variation on the overall response of the quasi-brittle materials such as reported in [49-53]. For example in [49], the response of a composite beam (Figure 1.3) in three-point bending is analysed by assigning random material properties to each finite element. The heterogeneity is introduced by spatially varying certain material properties according to measured probability density functions. The macroscopic response is then examined by performing Monte Carlo finite element simulations.

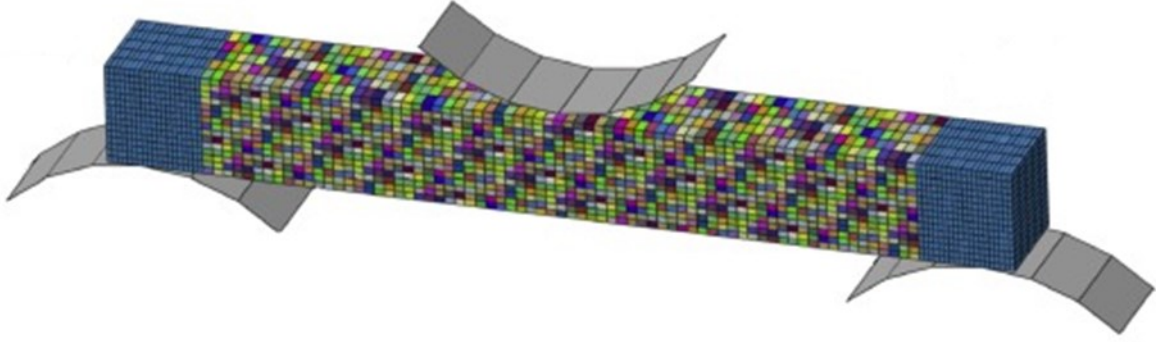


Figure 1.3 Example of a three-point bending FE model with random material properties [49].

Other authors have focused on the generation and analysis of virtual microstructures representing different materials at a certain length-scale. A large amount of work exists [54-77] for porous solids or reinforced matrix composites, such as those sketched in Figure 1.4. In this work we will pursue simplified approaches to modelling of the microstructure of porous solids with a wide range of porosity.

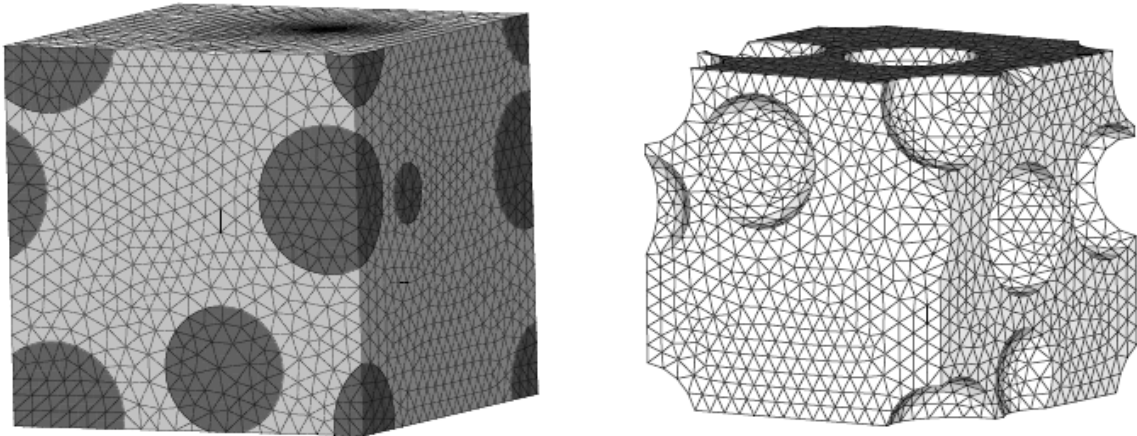


Figure 1.4 Example of an FE model with randomly distributed equal in size spherical particles (left) and voids (right) for a volume fraction, $f = 0.2$ [57].

1.1.1 Methodology

The technique developed in the current thesis involves introduction of material heterogeneity at the micro-level using the finite element method. Distribution of material properties and geometric fields are numerically generated based on probability density functions. FE models are generated by manipulating the input file via a FORTRAN program or via a user-material subroutine.

1. Generation of random sample for material properties and/or geometric fields
2. Assignment of material properties or geometric fields to all elements
3. Run the input file generated deterministically and solve using ABAQUS/ explicit solver

Repetition of the three steps above for an adequate large number of random samples, as required by the Monte Carlo Simulation method, and conduct statistical analysis for the global response. Details of the algorithms used to reproduce the microstructure of each type of material is given in every chapter individually.

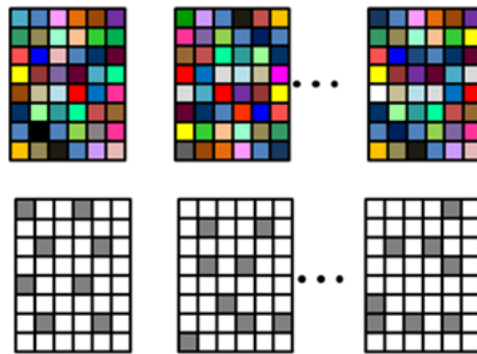


Figure 1.5 2D Random geometric field representing a two phase material (bottom), random material properties (top) representing a polycrystalline material using the finite element method.

1.1.2 Boundary Conditions

There is general consensus that periodic boundary conditions should be used in the FE analysis of periodic stochastic volume elements (SVEs) and representative volume elements (RVEs). Several authors in [44], [61], [78], [79] have used periodic boundary conditions to predict the response of RVE's. Since this method requires geometrical periodicity, we cannot use this type of analysis due to the current microstructures not exhibiting these conditions. [80] and [81] have shown that as the SVEs or RVEs get progressively larger in size, predictions obtained by imposing uniform displacement boundary conditions approach those made using periodic boundary conditions. Preliminary simulations confirmed this for the case of the SVEs employed in the thesis. In our simulations, conducted on non-periodic microstructures, uniform boundary conditions were imposed, forcing the faces of the cubic SVEs to remain planar as deformation proceeds. This approach has been adopted by recent papers such as in [54], [67], [72]. The specific boundary conditions employed in the thesis are discussed in each chapter individually.

1.2 Thesis Objectives

The broad objective of the thesis is to investigate the effect of heterogeneity at small length-scales on the non-linear mechanical response at larger scales. As the subject is very vast, the attention is focused on the following specific problems:

1. Elasto-plastic response of a fully-dense, heterogeneous elasto-plastic solid;
2. Elasto-plastic response of a random low porosity solid;
3. Elasto-plastic response of a random metallic foam;
4. Ductile fracture response of a heterogeneous material.

These four problems are the subjects of the following four chapters. As the problems under investigation are very different, the relevant literature is discussed in the individual chapters.

For each of the problems 1-3, we aim at developing modelling approaches that:

- are computational inexpensive;
- can be calibrated by direct measurements;
- include the effects of heterogeneity on the macroscopic material response.

For problem 4, we focus on stochastic predictions of strain localisation and failure of a metallic material.

1.3 Outline Of The Thesis

The following four chapters will examine the four problems listed above; conclusions and suggestions for future work are summarised in the last chapter, as detailed below.

Chapter 2 Simulation of the elasto-plastic response of heterogeneous ductile solids

In this chapter a numerical method is developed to investigate the macroscopic elasto-plastic response of heterogeneous solids featuring microscopic spatial variations of Young's modulus, yield stress and hardening modulus. Monte Carlo analyses of the response of stochastic volume elements (SVEs) are conducted in ABAQUS/standard; the material behaviour at the microscopic level is assumed to be isotropic and plastically incompressible. Simulations are conducted at different stress triaxialities and allow generating the yield surface of the

heterogeneous solids. The predicted responses of heterogeneous solids are compared to those of homogeneous solids and to simple analytical bounds.

Chapter 3 Predictions of the elasto-plastic response of low-porosity solids

In this chapter a novel numerical method is developed to model the macroscopic quasi-static mechanical response of solids with porosity in the range 0.01-0.3. A virtual microstructure was generated, consisting of two phases, the parent material and voids. The parent material exhibits an incompressible elasto-plastic behaviour while the voids are taken as plastically compressible solid displaying densification response at large strain. Statistical and mesh convergence studies are conducted to determine the minimum size of the representative volume element (RVE). Monte Carlo Finite Element (FE) simulations are performed to determine the overall behaviour. The predictions are compared with previously published numerical studies.

Chapter 4 Modelling the mechanical response of cellular solids made from sintered titanium powders

In this chapter two new algorithms are developed to generate virtual microstructures of Titanium foams with relative density in the range 0.37-0.48. Foams are modelled as two-phase composites consisting of solid Titanium and voids; Monte Carlo Finite Element (FE) simulations are conducted to predict the measured macroscopic material response in uniaxial tension and compression, as well as in pure shear. The elasto-plastic and damage response of the parent material is deduced from its measured mechanical responses in tension and compression, while the material occupying the voids is assigned a plastically compressible constitutive response to mimic the effects of pore collapse and subsequent self-contact. A statistical and mesh convergence studies are performed to determine the minimum size of the representative volume element (RVE). The simulations are compared to experiments.

Chapter 5 Predictive modelling of the fracture toughness of a sintered titanium alloy

Experiments are conducted on the fracture response of sintered Titanium. A stochastic analytical model is constructed and validated by experiments and stochastic finite element simulations. The analytical model is used in conjunction with experiments to determine the

stochastic material properties of the solid, used to calibrate the stochastic FE simulations. These are then successfully employed to make predictions of the fracture toughness of the material, using as input only the results of repeated uniaxial tensile and compressive tests.

Chapter 6 Conclusions and future work

This chapter integrates the main conclusions of the thesis in addition to describing possible future work.

1.4 Published work

The following publications were produced during this PhD project:

1. ZACHAROPOULOS, P., SCHIFFER, A., & TAGARIELLI, V. L. 2016. Simulation of the elasto-plastic response of heterogeneous ductile solids. *Submitted to International Journal of Engineering Science*.
(See Chapter 2)
2. ZACHAROPOULOS, P., SCHIFFER, A., & TAGARIELLI, V. L. 2016. Predictions of the elasto-plastic response of low-porosity solids. *Submitted to International Journal of Engineering Science*.
(See Chapter 3)
3. ZACHAROPOULOS, P. & TAGARIELLI, V. L. 2016. Numerical modelling of the mechanical response of a sintered Titanium foam. *Accepted to International Journal of Solids and Structures*.
(See Chapter 4)
4. ZACHAROPOULOS, P. & TAGARIELLI, V. L. 2016. Stochastic predictive modelling of the fracture toughness of a sintered Titanium alloy. *In preparation*
(See Chapter 5)

CHAPTER 2

SIMULATION OF THE ELASTO-PLASTIC RESPONSE OF HETEROGENEOUS DUCTILE SOLIDS

ABSTRACT

We present a numerical investigation of the macroscopic elasto-plastic response of heterogeneous solids featuring microscopic spatial variations of Young's modulus, yield stress and hardening modulus. Monte Carlo analyses of the response of stochastic volume elements (SVEs) are conducted in ABAQUS/standard; the material behaviour at the microscopic level is assumed to be isotropic and plastically incompressible. Simulations are conducted at different stress triaxiality and allow generating the yield surface of the heterogeneous solids. The stochastic predictions for heterogeneous solids are compared to deterministic predictions for homogeneous solids and to simple bounds derived analytically. It is shown that introducing microscopic variations of the material properties allows, at no added computational cost, predictions of a number of realistic phenomena such as strain localisation, necking instability, tension/compression asymmetry, size effects and plastic compressibility.

2.1 Introduction

Numerical simulations of the response of solid materials are typically conducted assuming uniform mechanical properties, of values determined via mechanical testing. While this approach is effective to determine the elasto-plastic response of sufficiently large engineering components, it cannot capture the heterogeneous nature of solids, which always causes strain localisation and deeply affects the initiation and evolution of fracture mechanisms.

Extensive phenomenological modelling work exists in the literature, attempting to describe the macroscopic material response of ductile solids via appropriately calibrated constitutive models. Some of these models focus on the response of metals, considering the heterogeneity due to their polycrystalline nature, and using crystal plasticity for the response of each grain, i.e. assuming yield occurs on the slip systems when these are loaded by the critical resolved shear stress [1-3, 82-85]. These approaches are physically based but require extensive testing and calibration of the material at both macroscopic and microscopic scale.

A different approach to capturing the effects of geometric and material inhomogeneity upon the macroscopic response is to conduct multi-scale modelling [41, 86, 87]. By this approach the material microstructure is explicitly described in the simulations, at multiple length scales. Analyses at a certain length scale allow determining mechanical properties to be used in coarser descriptions at larger length scales. Several models for example predict the evolution of dislocation density and use this information to calculate the local flow stress in the material [38, 88-95].

Several authors explored the elasto-plastic behavior of polycrystalline materials using anisotropic elasticity and isotropic or crystal plasticity [96-98]. Other authors have focused on brittle polycrystalline solids, modelled explicitly their microstructure using Voronoi tessellations, and performed finite element simulations to examine effective elastic properties and strength [99-102].

Multiscale modelling approaches have the drawback of the extremely high computational cost. In addition, their calibration at multiple length scales requires extensive testing; at sufficiently small scales such tests cannot be performed and mechanical properties need to be guessed or calculated via reverse engineering. This often prevents multiscale models from yielding true predictions of the material response.

While the multi-scale spatial distribution of mechanical properties cannot be completely known deterministically, often it can be described probabilistically, as recognised by several authors [42-44, 103]. Such knowledge may be incorporated in simulations of material response and several authors have described the behaviour of quasi-brittle solids by this stochastic approach, employing spatial distributions of the material properties determined from measured probability density functions [49-53] and were able to capture different phenomena observed in reality such as strain localisation, statistical toughening and size effects. This approach is discussed in [104-106].

Only few stochastic plasticity models have appeared to date, seen in [107, 108], who focused on designing efficient numerical methods to solve nonlinear stochastic problems and applied such methods to simple 2D problems such as Hertzian contacts. Much of the existing work is limited to the case of small deformation and to the response to uniaxial loading. In this chapter we propose a systematic analysis of the effects of material inhomogeneity on the elasto-plastic macroscopic response up to large strains, using Monte Carlo analysis and the FE method. Cuboidal SVEs are considered and a regular tessellation is employed to create a statistical mesh, such that each element of this statistical mesh possesses different mechanical properties; a FE mesh (not necessarily coincident with the statistical mesh) is then superimposed to conduct the simulations. The microscopic material response is assumed to be isotropic linear elastic, followed by incompressible plasticity with linear isotropic strain hardening. Spatial variations of Young's modulus, yield stress and hardening modulus are introduced at the micro-level according to a uniform random probability distribution; the SVEs are then subject to loading at different triaxiality to determine their macroscopic response.

The structure of the chapter is as follows; in Section 2.2 we develop simple mathematical bounds for the uniaxial response of heterogeneous elasto-plastic solids. In Section 2.3 we present the numerical method and the simulation technique. Results are discussed in Section 2.4. The main conclusions are summarised in Section 2.5.

2.2 Bounds to the uniaxial response of heterogeneous solids

We derive analytical bounds to the macroscopic uniaxial stress-strain response of elasto-plastic solids with microscopic variations of either the Young's modulus E , the yield strength σ_y or the hardening modulus H ; the material Poisson's ratio ν is taken as uniform and equal to 0.3. We assume that the material consists of a cuboidal array of N elasto-plastic homogeneous cells with linear strain hardening; the relevant microscopic material properties are assumed to follow a uniform random distribution as follows

$$E_i(r_i) = E_{\min} + r_i(E_{\max} - E_{\min}) = E_{\min} + r_i\Delta E \quad (2.1)$$

$$\sigma_{yi}(r_i) = \sigma_y^{\min} + r_i(\sigma_y^{\max} - \sigma_y^{\min}) = \sigma_y^{\min} + r_i\Delta\sigma_y, \quad (2.2)$$

$$H_i(r_i) = H_{\min} + r_i(H_{\max} - H_{\min}) = H_{\min} + r_i\Delta H, \quad (2.3)$$

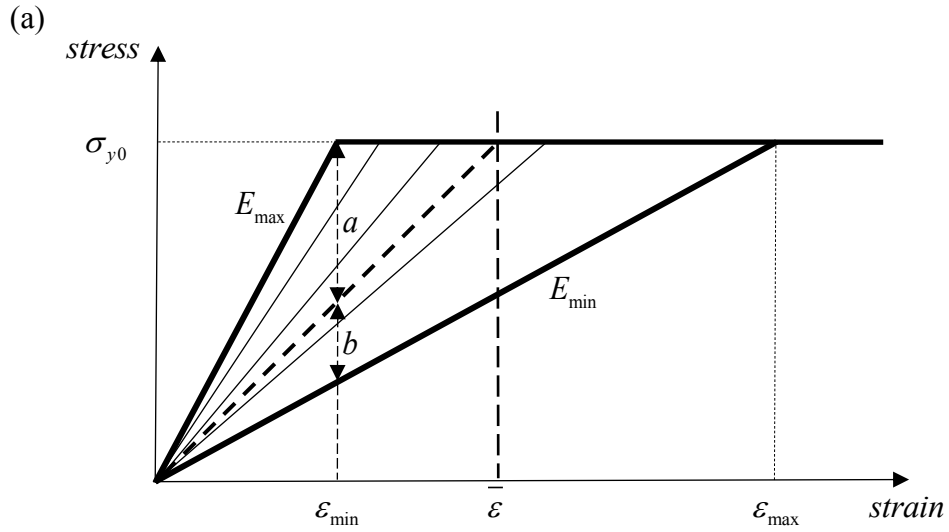
with $i = 1 \dots N$. Here $E_{\max}$, $E_{\min}$, $\sigma_y^{\min}$, $\sigma_y^{\max}$, $H_{\max}$ and $H_{\min}$, are the extrema of the ranges of variation of the mechanical properties and r_i denotes a uniformly distributed, uncorrelated random number in the interval $[0,1]$. The average values of the mechanical properties are E_0 , σ_{y0} and H_0 . An upper bound for the macroscopic response of the heterogeneous solid can be obtained assuming equal strain in all cells (Voigt upper bound) while a lower bound can be calculated assuming equal stress in all cells (Reuss lower bound).

2.2.1 Stochastic variations of Young's modulus

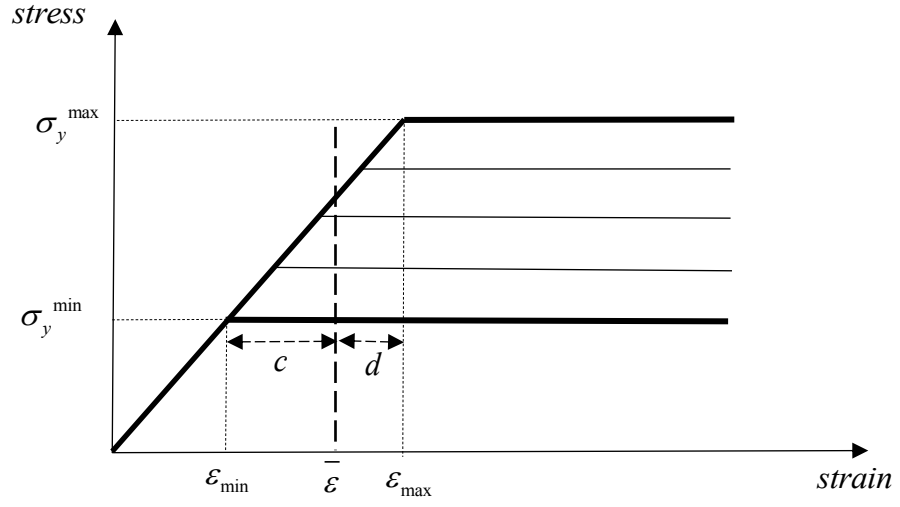
First we consider the case where the Young's modulus E varies randomly across the solid according to Eq. (2.1) while yield strength and hardening modulus σ_{y0} and H_0 remain uniform. We also assume $H_0 = 0$, i.e. all cells are perfectly plastic.

Upper bound

The stress-strain curves of each cell of the statistical mesh are sketched in Figure 2.1(a); it is assumed that all cells undergo the same microscopic strain, equal to the current macroscopic strain $\bar{\epsilon}$. For $\bar{\epsilon} < \epsilon_{\min}$, where $\epsilon_{\min} = \sigma_{y0}/E_{\max}$, all cells behave elastically; if $\epsilon_{\min} \leq \bar{\epsilon} \leq \epsilon_{\max}$, where $\epsilon_{\max} = \sigma_{y0}/E_{\min}$, some of the cells behave elastically while others undergo plasticity; all cells deform plastically if $\bar{\epsilon} > \epsilon_{\max}$.



(b)



(c)

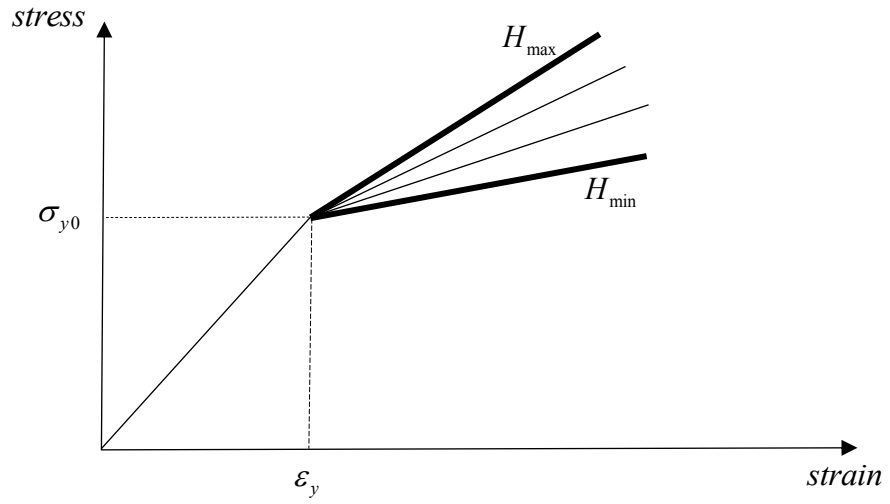


Figure 2.1 Schematic stress versus strain response of the microscopic cells, for the cases of variation of (a) Young's modulus, (b) yield stress and (c) hardening modulus.

For a given applied strain $\bar{\epsilon}$, a number N_p of cells is in the plastic regime; we define the fraction of plastic elements as

$$P_p = N_p / N. \quad (2.4)$$

The fraction of elements being in the elastic regime is thus given by

$$P_e = N_e / N = 1 - P_p \quad (2.5)$$

where N_e is the number of elastically deforming cells.

If $\bar{\varepsilon} < \varepsilon_{\min}$, all cells undergo a purely elastic response, $P_p = 0$. If $\bar{\varepsilon} > \varepsilon_{\max}$, $P_p = 1$. In the transition region, $\varepsilon_{\min} \leq \bar{\varepsilon} \leq \varepsilon_{\max}$, with reference to Figure 2.1(a), the fraction of plastic elements is given by

$$P_p = \frac{a}{a+b} = \left(1 - \frac{\varepsilon_{\min}}{\bar{\varepsilon}}\right) / \left(1 - \frac{\varepsilon_{\min}}{\varepsilon_{\max}}\right) \quad (2.6)$$

where the variables a and b represent the length of the two segments sketched in Figure 2.1(a). In this region, plastic and elastic regions coexist. The homogenized stress $\bar{\sigma}$ is obtained by averaging the stresses in all cells, as follows

$$\bar{\sigma}(\bar{\varepsilon}) = \frac{1}{N} \left(N_p \sigma_{y0} + \sum_{i=1}^{N_e} E_i(r_i) \bar{\varepsilon} \right). \quad (2.7)$$

Combining Eqs. (2.4) - (2.7), the expected value of the induced homogenized stress is obtained as

$$\bar{\sigma} = \frac{1}{E_{\max} - E_{\min}} \left(E_{\max} \sigma_{y0} - \frac{E_{\min}^2 \bar{\varepsilon}}{2} - \frac{\sigma_{y0}^2}{2\bar{\varepsilon}} \right). \quad (2.8)$$

For $\bar{\varepsilon} < \varepsilon_{\min}$ all cells respond elastically and

$$\bar{\sigma} = \left(\frac{E_{\min} + E_{\max}}{2} \right) \bar{\varepsilon} = E_0 \bar{\varepsilon}. \quad (2.9)$$

For $\bar{\varepsilon} > \varepsilon_{\max}$, $P_p = 1$ and $\bar{\sigma} = \sigma_{y0}$.

Lower bound

Now assume that all cells are connected in series and are experiencing an increasing uniform macroscopic stress $\bar{\sigma}$. If $\bar{\sigma} < \sigma_{y0}$, the homogenized engineering strain $\bar{\varepsilon}$ is given, assuming small deformations, by

$$\bar{\varepsilon}(\bar{\sigma}) = \frac{1}{N} \sum_{i=1}^N \frac{\bar{\sigma}}{E_i} = \frac{1}{N} \sum_{i=1}^N \frac{\bar{\sigma}}{E_{\min} + r_i(E_{\max} - E_{\min})}. \quad (2.10)$$

The expected value of this quantity can be easily calculated, considering that r_i are uniform random variables, and such calculation leads to

$$\bar{\sigma} = \frac{\Delta E \bar{\varepsilon}}{\ln(E_{\max} / E_{\min})}. \quad (2.11)$$

The response is linear elastic for $\bar{\sigma} < \sigma_{y0}$; when the applied stress is equal to the yield stress, the strain is undetermined (for this perfectly plastic material) and $\bar{\sigma} = \sigma_{y0}$.

2.2.2 Stochastic variations of yield stress

Next, we consider the case of the microscopic yield stress σ_y varying randomly across the material domain according to Eq. (2.2), while Young's modulus and hardening modulus E_0 and $H_0 = 0$ remain uniform.

Upper bound

The stress-strain curves assumed for the different cells are sketched in Figure 2.1(b). We assume that all cells are subject to the uniform macroscopic applied strain $\bar{\varepsilon}$. Again, three regions of the response can be identified; for $\bar{\varepsilon} < \varepsilon_{\min}$, where in this case we take $\varepsilon_{\min} = \sigma_y^{\min} / E_0$, all cells respond elastically; a transition region exists for $\varepsilon_{\min} \leq \bar{\varepsilon} \leq \varepsilon_{\max}$, where $\varepsilon_{\max} = \sigma_y^{\max} / E_0$, in which a fraction of the cells undergoes plasticity; for $\bar{\varepsilon} > \varepsilon_{\max}$ all cells deform plastically. In the transition region, the fraction of plastic cells P_p can be computed, with reference reference to Figure 2.1(b), as

$$P_p = \frac{c}{c+d} = \frac{E_0 \bar{\varepsilon} - \sigma_y^{\min}}{\sigma_y^{\max} - \sigma_y^{\min}} \quad (2.12)$$

where c and d denote the length of the two segments shown in Figure 2.1(b). The homogenized stress $\bar{\sigma}$ is the average of the stresses in all cells

$$\bar{\sigma}(\bar{\varepsilon}) = \frac{1}{N} \left(N_e E_0 \bar{\varepsilon} + \sum_{i=1}^{N_p} \sigma_{yi}(r_i) \right). \quad (2.13)$$

The quantity $\sigma_{yi}(r_i)$ in the latter equation is a uniformly distributed variable on the interval $[\sigma_y^{\min}, E_0 \bar{\varepsilon}]$.

The expected value of the expression in Eq. (2.13) can be calculated as

$$\bar{\sigma} = E_0 \bar{\varepsilon} - \frac{(E_0 \bar{\varepsilon} - \sigma_y^{\min})^2}{2(\sigma_y^{\max} - \sigma_y^{\min})}. \quad (2.14)$$

For $\bar{\varepsilon} < \varepsilon_{\min}$ it is simply $\bar{\sigma} = E_0 \bar{\varepsilon}$, while for $\bar{\varepsilon} > \varepsilon_{\max}$ the material collapses at constant stress

$$\bar{\sigma} = (\sigma_y^{\max} + \sigma_y^{\min}) / 2 = \sigma_{y0}.$$

Lower bound

Now assume that all cells are connected in series and subject to a uniform stress $\bar{\sigma}$. The material's initial response is linear elastic, $\bar{\sigma} = E_0 \bar{\varepsilon}$. As the applied stress attains the value $\bar{\sigma} = \sigma_y^{\min}$, the material collapses at constant stress and the macroscopic strain is undefined.

2.2.3 Stochastic variations of hardening modulus

Finally, we consider spatial variations of the hardening modulus H across the material domain according to Eq. (2.3), while Young's modulus E_0 and yield stress σ_{y0} are taken as uniform. All cells, in this case, will yield at the same strain $\varepsilon_y = \sigma_{y0} / E_0$, as sketched in Figure 2.1(c).

Upper bound

All cells are imposed a uniform applied strain, $\bar{\varepsilon}$. In the elastic region ($\bar{\varepsilon} \leq \varepsilon_y$) the macroscopic stress is given by $\bar{\sigma} = E_0 \bar{\varepsilon}$, while for $\bar{\varepsilon} > \varepsilon_y$, the homogenized stress $\bar{\sigma}$ is the average of the stresses in all cells and given by

$$\bar{\sigma}(\bar{\varepsilon}) = \frac{1}{N} \sum_{i=1}^N \left(\sigma_{y0} + (\bar{\varepsilon} - \varepsilon_y) H_i(r_i) \right). \quad (2.15)$$

The expected value of the expression in Eq. (2.15) is given by

$$\bar{\sigma} = E \left[\bar{\sigma}(r_i) \right] = \sigma_{y0} + H_0 \left(\bar{\varepsilon} - \frac{\sigma_{y0}}{E_0} \right). \quad (2.16)$$

Lower bound

Now assume that all cells are connected in series and experience the same stress $\bar{\sigma}$. For $\bar{\sigma} < \sigma_{y0}$ the response is elastic; for $\bar{\sigma} \geq \sigma_{y0}$, the global strain is given by the average of the strains in the cells:

$$\bar{\varepsilon}(\bar{\sigma}) = \varepsilon_y + \frac{\bar{\sigma} - \sigma_{y0}}{N} \sum_{i=1}^N \frac{1}{H_{\min} + r_i \Delta H}. \quad (2.17)$$

Similar to the analysis presented in Section 2.2.1, the expected value of Eq. (2.17) can be calculated and the homogenised stress-strain response may be written as

$$\bar{\sigma} = \sigma_{y0} + \frac{(\bar{\varepsilon} - \varepsilon_y) \Delta H}{\ln(H_{\max} / H_{\min})}. \quad (2.18)$$

2.3 Numerical scheme

The Monte Carlo Simulation (MCS) method was used to examine the response of elasto-plastic materials with random spatial variations of material properties under different loading conditions. The simulations were carried out in ABAQUS/Standard, conducting repeated FE simulations on 10 realisations of random stochastic volume elements (SVEs) and analyzing the mean and spread of the population of outputs. The details of the numerical implementation are described below. Details of how the microstructures were produced can be found in APPENDIX A in Section 2.6.

2.3.1 FE scheme

Cuboidal SVEs of volume V were generated in ABAQUS/CAE via Python scripts and meshed by fully-integrated 8-noded brick elements of cuboidal shape and volume V_e (number of elements $N_{FE} = V / V_e$). A regular tessellation was superimposed to the FE mesh to subdivide the domain in a number N_{CELL} of cuboidal cells ($N_{CELL} \leq N_{FE}$); each cell was assigned different material properties to introduce inhomogeneity. The statistical tessellation was such that each cell included an integer number of finite elements.

The elasto-plastic microscopic response of the material in each cell was modelled using linear isotropic elasticity (Young's modulus E , Poisson's ratio ν) and incompressible J_2 plasticity with linear strain hardening (yield strength σ_y , hardening modulus H) and isotropic hardening. A pseudo-random number generator in Python was used to generate the values of the microscopic material properties, in accordance with Eq. (2.1)-(2.3).

2.3.2 Boundary conditions and load cases

In the analysis of periodic SVEs and representative volume elements (RVEs), periodic boundary conditions are typically used. The chosen set of boundary conditions affects the predicted mechanical response of the material, as shown in [44, 61, 78, 79]. Other authors however for example in [80, 81] have shown that as larger SVEs or RVEs are used, predictions obtained by imposing uniform displacement boundary conditions approach those made using periodic boundary conditions. Preliminary simulations confirmed this for the case of the SVEs analysed here and in our simulations, conducted on non-periodic microstructures, we impose uniform boundary conditions, forcing the faces of the SVEs to remain planar as deformation proceeds as in [54, 67, 72, 75].

In uniaxial tension and compression, one of the faces of the SVE had normal displacements constrained while the opposite face was subject to normal displacements linearly increasing with simulation time, such to induce macroscopic tensile or compressive strain. The lateral faces were constrained to remain planar and the normal displacements of opposite lateral faces were forced to be equal and opposite; these constraints are imposed via the constraint equation tool of ABAQUS, making use of appropriate dummy nodes.

We also simulated multi-axial loading conditions, by imposing different values of stress triaxiality in the elastic phase of loading. This was done by subjecting the SVE to normal macroscopic strains in the principal directions (denoted by 1,2,3) given by

$$\begin{aligned}\varepsilon_1(t) &= \dot{\varepsilon} t \\ \varepsilon_2(t) &= \dot{\varepsilon} t \beta \\ \varepsilon_3(t) &= \dot{\varepsilon} t\end{aligned}\tag{2.19}$$

where t represents the simulation time and $\dot{\varepsilon}$ denotes the strain rate which was set to $\dot{\varepsilon} = 5 \text{ s}^{-1}$ in all simulations.

Nine pairs of parameters (α, β) were chosen, identical to those used in [61] and summarised in Table 1, to give 18 different values of stress triaxiality, of which 9 positive (loading cases 1-9) and 9 negative (loading cases 10-18).

Loading case	1	2	3	4	5	6	7	8	9
α	1	1	1	1	1	1	1	0.5	0
β	0	0.05	0.1	0.15	0.25	0.5	1	1	1

Table 1 Loading parameters corresponding to Eq. (2.19).

Histories of macroscopic principal stresses and strains were extracted from each simulation and allowed determining the corresponding histories of hydrostatic stress and equivalent von Mises stress, as well as the volumetric and equivalent von Mises strains, as

$$\sigma_H = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3} \quad (2.20)$$

$$\sigma_{VM} = \left[\frac{(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_3 - \sigma_2)^2}{2} \right]^{1/2} \quad (2.21)$$

$$\varepsilon_V \cong \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \quad (2.22)$$

$$\varepsilon_{VM} = \frac{\sqrt{2}}{3} \left[(\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_1 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_2)^2 \right]^{1/2} \quad (2.23)$$

2.3.3 Sensitivity of the uniaxial response to N_{CELL} and N_{FE}

The predictions are affected by the density of the statistical and FE meshes used, representing, respectively, a material length scale and the accuracy of the FE discretisation. In the following we determine the sensitivity of the predictions to these parameters, with the secondary

objective of determining the minimum values of N_{FE} and N_{CELL} which made the predictions insensitive to such parameters.

First, we examine the sensitivity of the predictions to N_{CELL} , in the case $N_{FE} = N_{CELL}$ (each statistical cell is meshed by a single constant-stress finite element). Figure 2.2(a) shows examples of SVEs with N_{CELL} varying in the range 832-187500. For each choice of N_{CELL} , MCS were performed on two sets of realisations of the microstructure.

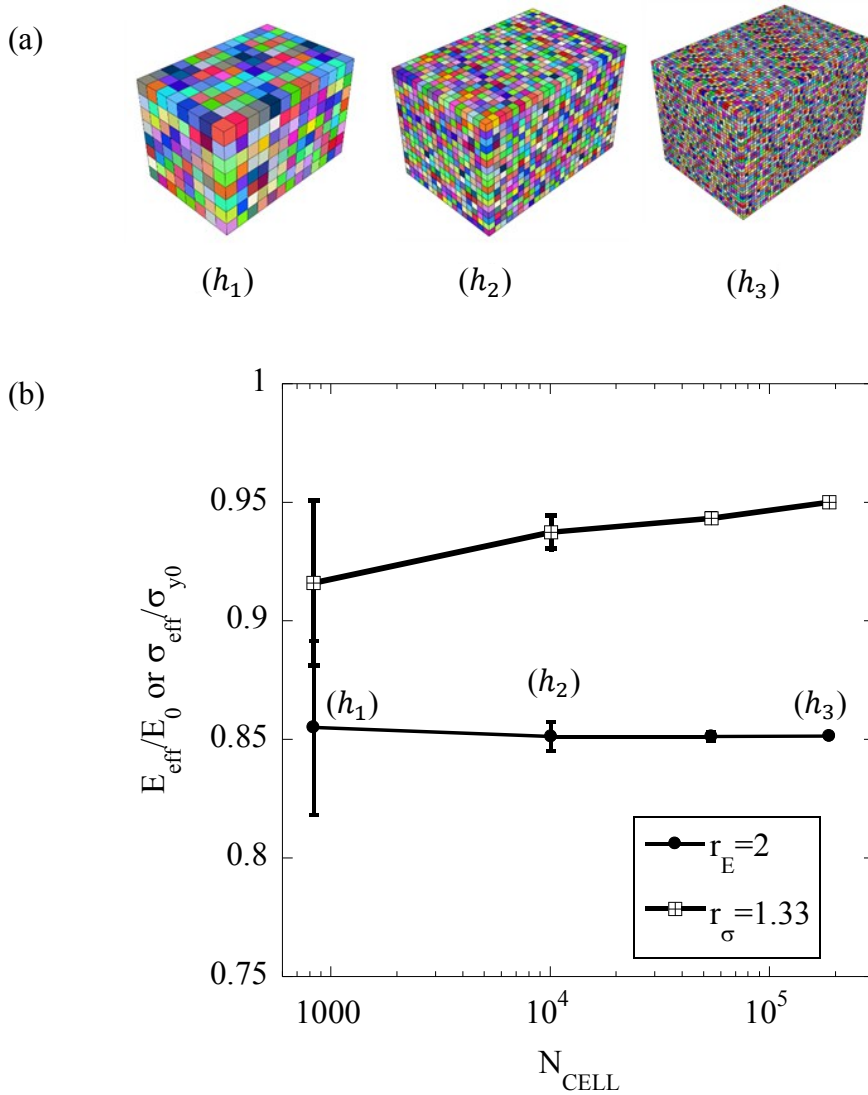


Figure 2.2 (a) Examples of SVEs at increasing N_{CELL} ; (b) Sensitivity of the normalised effective modulus E_{eff}/E_0 , (Set I) and normalised effective strength, σ_{eff}/σ_{y0} (Set II) to N_{CELL} .

Set I was generated by implementing spatial variations of the Young's modulus according to Eq. (2.1), while keeping yield strength σ_{y0} and hardening modulus $H_0 = 0$ uniform. For Set II, random variations of the yield stress were considered, according to Eq. (2.2), keeping elastic modulus and hardening modulus $H_0 = 0$ uniform. We define, for Set I, a non-dimensional measure of the modulus variability r_E , as

$$r_E = \frac{\Delta E}{(E_{\max} + E_{\min}) / 2} . \quad (2.24)$$

Such parameter was set to 2 in the simulations, $r_E = 2$. Similarly, for Set II we define a non-dimensional measure of the variability of the microscopic yield stress as

$$r_\sigma = \frac{\Delta \sigma_y}{(\sigma_y^{\max} + \sigma_y^{\min}) / 2} . \quad (2.25)$$

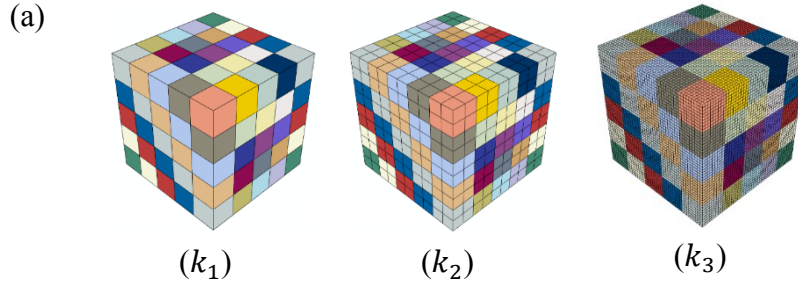
A value $r_\sigma = 1.33$ was chosen in the simulations. The SVEs were subject to loading in uniaxial tension and loading was interrupted at a total tensile strain of 5%; the effective macroscopic modulus E_{eff} and the peak true tensile stress σ_{eff} were extracted from the macroscopic true stress-strain histories, for Set I and Set II, respectively.

In Figure 2.2(b) we summarize the results of these calculations, showing predictions of the normalised effective modulus E_{eff} / E_0 for Set I, and the normalized effective strength $\sigma_{\text{eff}} / \sigma_{y0}$ for Set II, for each choice of N_{CELL} . The error bars included in Figure 2.2(b) represent the ranges of each output population (the distributions of outputs were approximately Gaussian).

The analysis of Figure 2.2(b) shows that E_{eff} / E_0 is scarcely sensitive to N_{CELL} , but lower than the value of 1 expected in a deterministic simulation and dictated by the upper bound. The spread of such quantity decreases very rapidly with N_{CELL} . For Set II, the quantity $\sigma_{\text{eff}} / \sigma_{y0}$

initially increases with N_{CELL} but for $N_{CELL} > 10000$ its dependence on N_{CELL} is mild. Again, the scatter in this normalised measure of strength is very low in the range of N_{CELL} considered. The simulations suggest a size dependence of the tensile response for Set II, such that larger samples are stronger than smaller ones. This was reported in [109-113].

Next, we examine the sensitivity of the FE predictions to N_{FE} , with N_{CELL} and the SVE volume held constant. FE simulations were performed on a single SVE realisation with $N_{CELL} = 125$ and the FE mesh was progressively refined, as illustrated in Figure 2.3(a). Again, two sets of simulations were performed, one with $r_E = 2$ (Set I) and the other with $r_\sigma = 1.33$ (Set II). Each SVE was again subjected to uniaxial tension and the simulations were interrupted when a total tensile strain of 5% was reached.



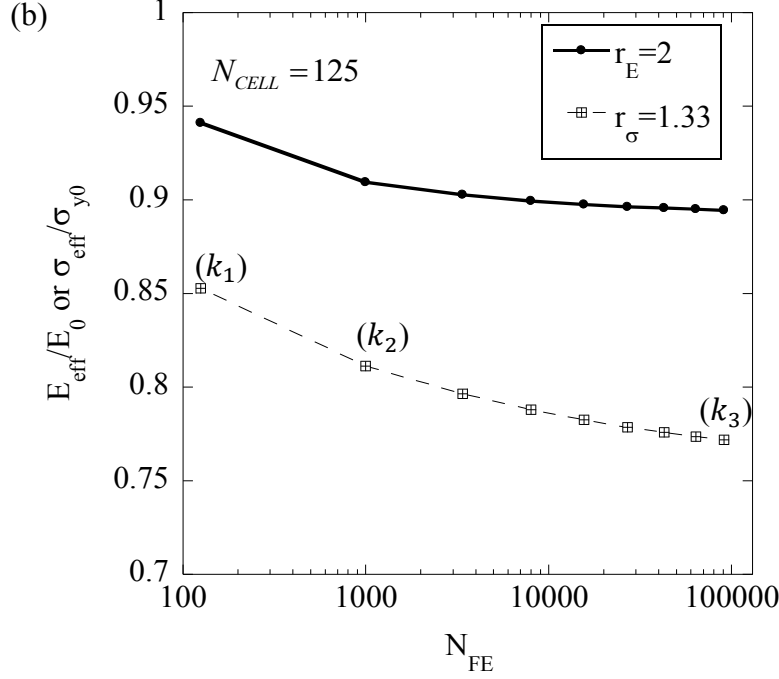


Figure 2.3 (a) Examples of SVEs at increasing N_{FE} ; (b) Sensitivity of the normalised effective modulus, E_{eff}/E_0 (Set I) and normalised effective strength, σ_{eff}/σ_{y0} (Set II) to N_{FE} .

Figure 2.3(b) presents plots of the normalised effective modulus E_{eff}/E_0 for Set I ($r_E = 2$) and the normalized effective strength σ_{eff}/σ_{y0} for Set II ($r_\sigma = 1.33$), for each choice of N_{FE} . It can be seen that both E_{eff}/E_0 and σ_{eff}/σ_{y0} decrease monotonically with increasing mesh density; both these effects are a consequence of the fact that by progressively refining the FE mesh, the simulations better capture the stress concentrations induced by the microscopic variations of mechanical properties. The mesh sensitivity study was repeated for higher values of the statistical mesh density, namely $N_{CELL} = 1000$ and $N_{CELL} = 8000$, for both Set I and Set II. The results are presented in Figure 2.4; Figure 2.4(a) shows the predicted normalised effective modulus as a function of the ratio N_{FE}/N_{CELL} for Set I ($r_E = 2$); Figure 2.4(b) shows the predicted normalised strength as function of the same parameter (Set II, $r_\sigma = 1.33$); Clearly the choice of N_{CELL} does not affect substantially the sensitivity of the predictions to N_{FE}/N_{CELL} ; predictions are scarcely sensitive to the FE mesh if a minimum of 27 finite elements is used to mesh each statistical cell, irrespective of the chosen N_{CELL} .

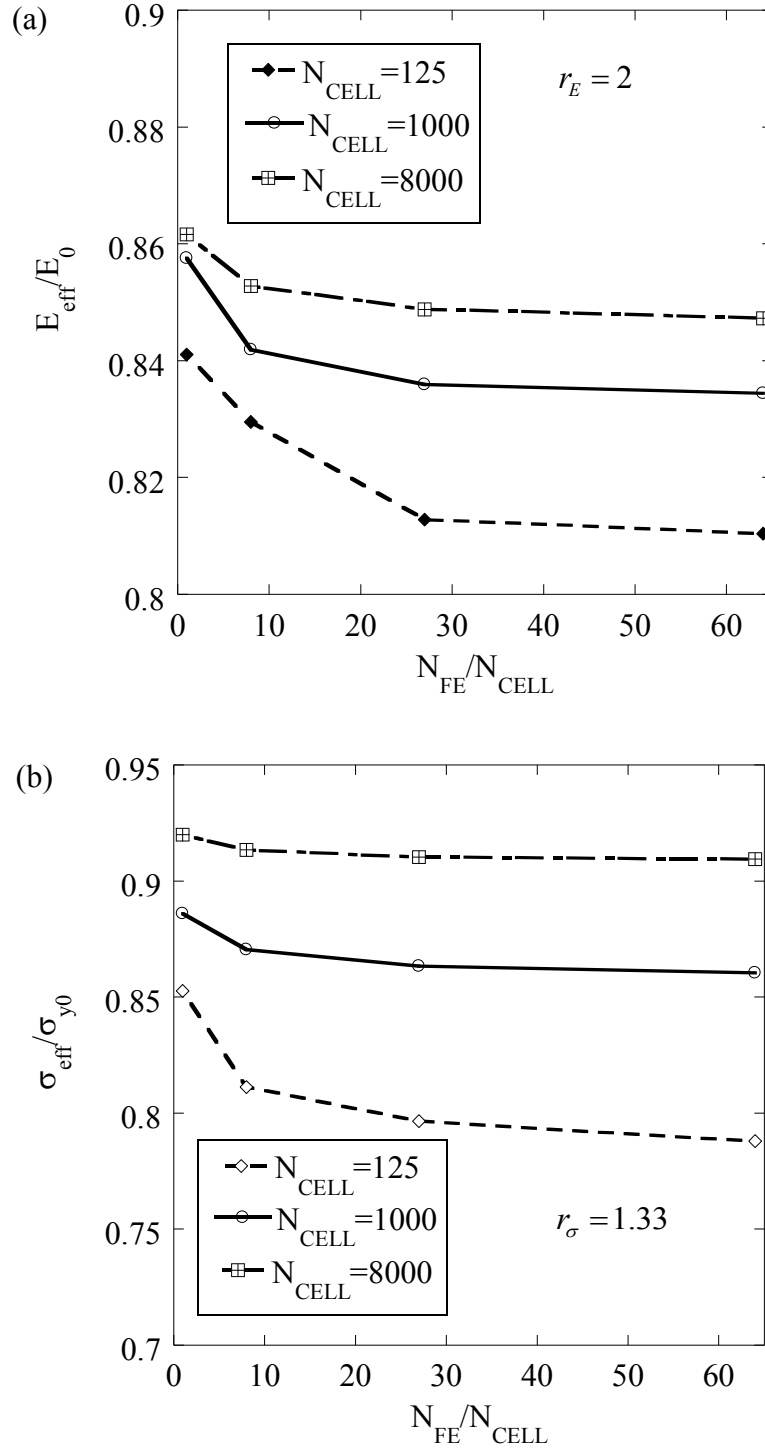


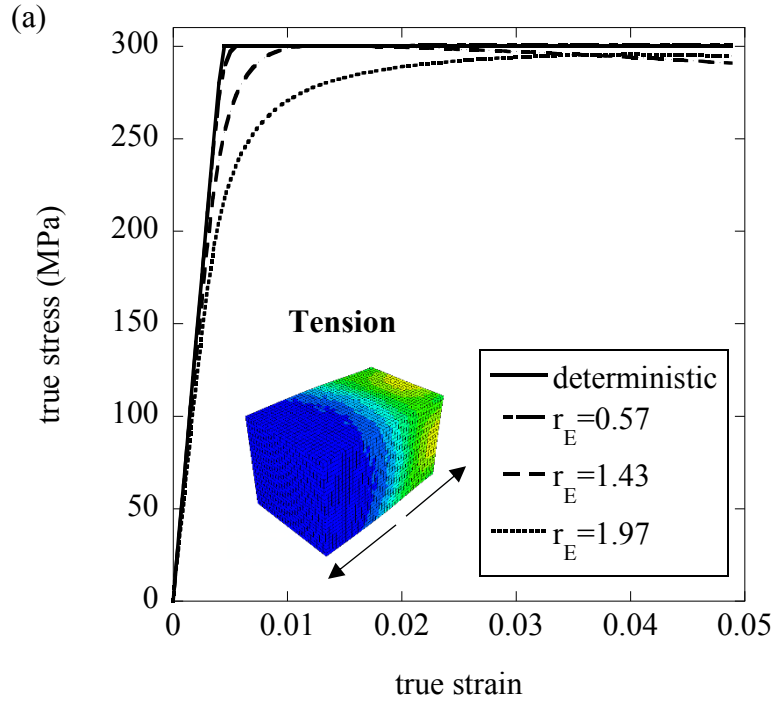
Figure 2.4 (a) Sensitivity of the normalised effective modulus, E_{eff}/E_0 to the number of finite elements per cell, N_{FE}/N_{CELL} , for Set I. (b) Sensitivity of the normalised effective strength, σ_{eff}/σ_{y0} to the number of finite elements per cell, N_{FE}/N_{CELL} , for Set II.

2.4 Results and discussion

In this section we proceed to analyse the numerical predictions in detail and to compare them to the bounds derived in Section 2.2. In all simulations showed below the parameters N_{CELL} and N_{FE} were chosen as ($N_{FE} = N_{CELL} = 23750$). The scatter was less than 1% at this mesh density, as shown in Figure 2.2(b).

2.4.1 Effect of variation of Young's Modulus

In this section we present the results of simulations in which a stochastic spatial variation of Young's modulus was imposed, with uniform yield strength and uniform (vanishing) hardening modulus. The macroscopic uniaxial average stress versus strain histories are presented in Figure 2.5(a) for the case of tension and in Figure 2.5(b) for the case of compression. Simulations were conducted at three different values of r_E as indicated; the inserts show contours of maximum principal strain at a 5% total macroscopic axial strain. A deterministic simulation, in which all material properties were taken as uniform and equal to the average values ($E_0 = 70$ GPa; $\sigma_{y0} = 300$ MPa; $H = 0$), is included in the figures for comparison.



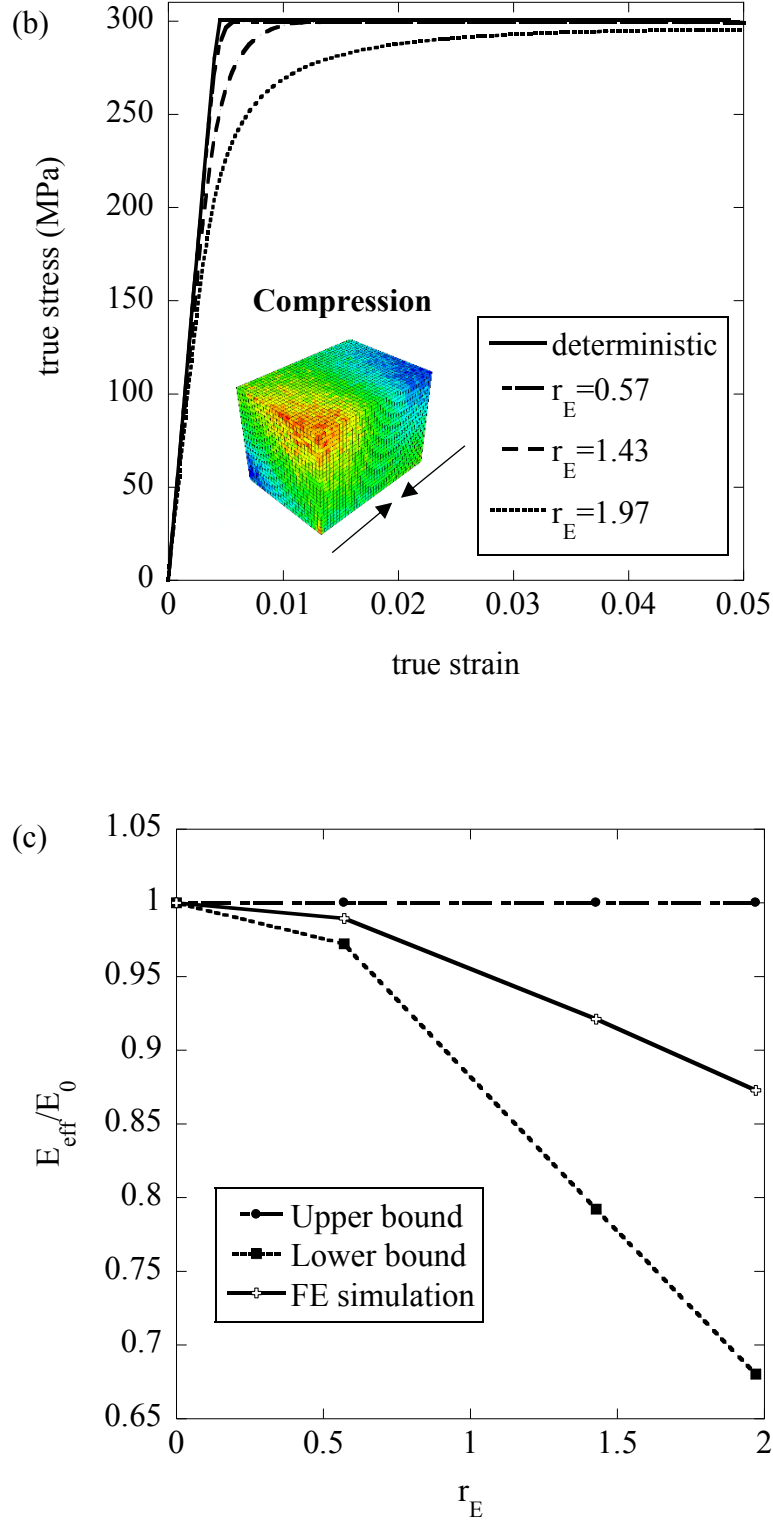


Figure 2.5 Effect of the variation of modulus upon the macroscopic tensile (a) and compressive (b) stress-strain response; (c) Normalised effective modulus, E_{eff} / E_0 as a function of the degree of heterogeneity r_E .

In both tension and compression, the initial yield of the material occurs well below the imposed microscopic yield stress of 300 MPa, as a consequence of the stress concentrations induced by the variations of Young's modulus; the stress at the onset of plasticity decreases with increasing r_E . At higher stresses the material displays a non-linear macroscopic response which reminds of material strain-hardening, but is rather a consequence of the progressive yield of more and more cells, similar to what described by Eq. (2.8) (we recall that the microscopic material response is perfectly plastic). The peak true stress is scarcely sensitive to the imposed variation of Young's modulus in the ranges investigated, and is always close to the imposed microscopic yield stress of 300 MPa.

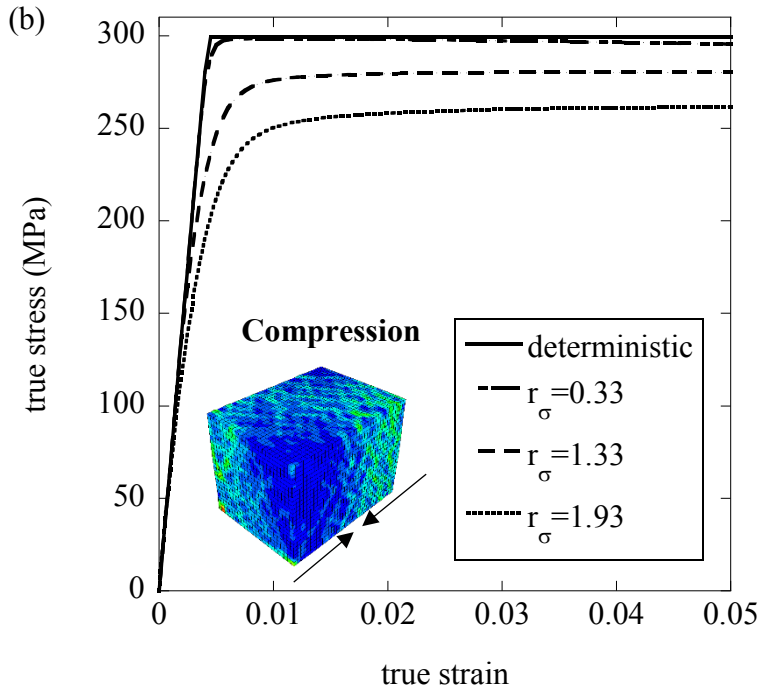
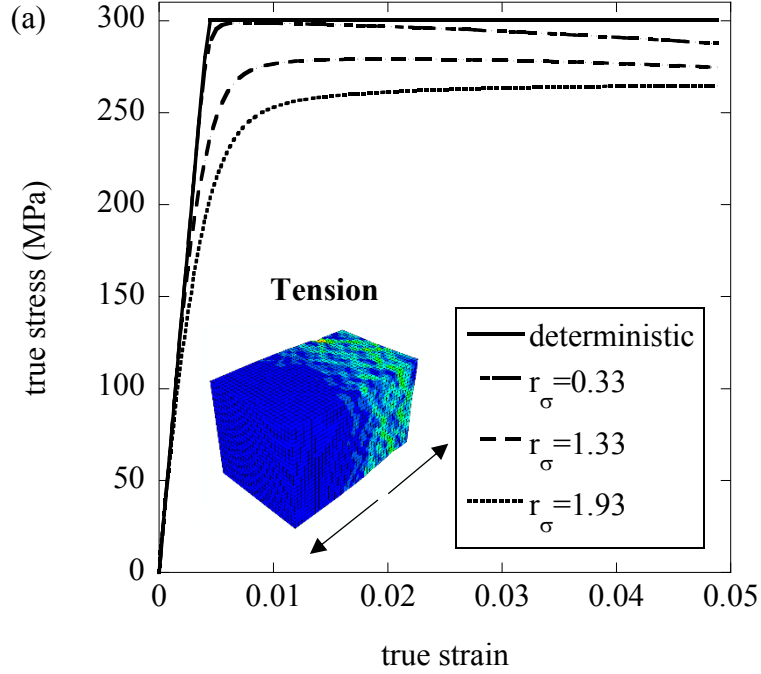
At large strains the mechanisms of deformation are different in tension and compression. In tension the elastic deformation, initially uniform, localises forming necking of the specimen at a random location; correspondingly, the macroscopic response displays a stress peak followed by geometric softening. The macroscopic strain at which a peak in tensile stress is attained is also very sensitive to r_E ; the higher r_E , the higher the strain at peak stress; this suggests that the ductility of a heterogeneous material must increase with the degree of heterogeneity, as quantified in this case by the parameter r_E . In compression the necking mechanism is absent and the macroscopic response progressively evolves towards a plateau response at stress 300 MPa. In the hardening phase of both the tensile and compressive responses the flow stress at a given macroscopic strain decreases with increasing r_E .

Figure 2.5(c) presents a comparison of the numerically predicted normalised effective modulus to the analytical bounds developed above. We note here that $0 \leq r_E \leq 2$ (since $r_E \geq 2$ implies zero or negative Young moduli); in the range investigated the numerical predictions lie approximately mid-way between the Voigt and Reuss bounds.

2.4.2 Effect of variation of yield stress

In Figure 2.6(a) and Figure 2.6(b) we present average macroscopic stress versus strain histories obtained from simulations in which the yield stress varies spatially across the material, while the Young modulus and hardening modulus are kept uniform

($E_0 = 70$ GPa; $\sigma_{y0} = 300$ MPa; $H = 0$). Simulations are repeated at three different levels of variation of the yield stress around the average value σ_{y0} , giving the values of r_σ indicated. Inserts show contours of maximum principal strain at 5% total macroscopic axial strain.



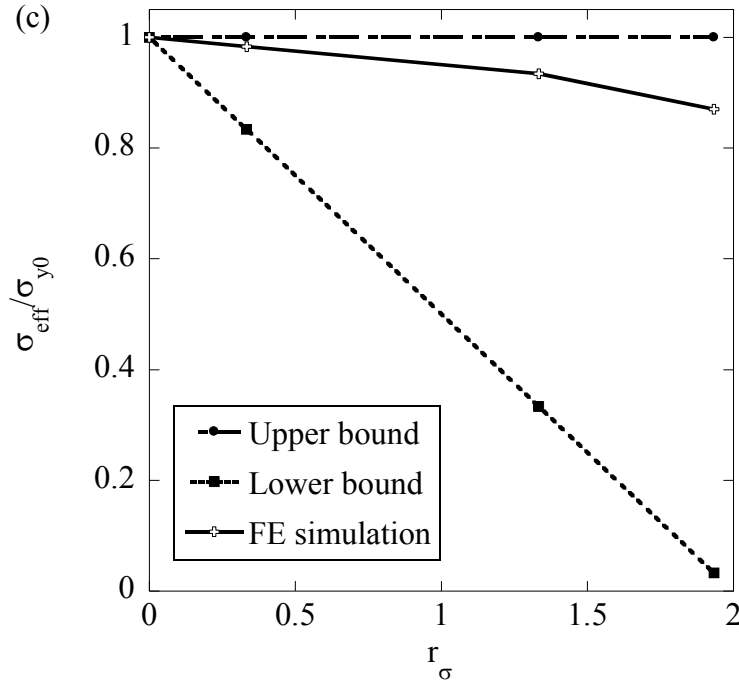


Figure 2.6 Effect of the variation of yield strength upon the macroscopic tensile (a) and compressive (b) stress-strain response; (c) Normalised effective strength, $\sigma_{eff} / \sigma_{y0}$, as a function of the degree of heterogeneity r_{σ} .

The effects of a microscopic variation of yield stress are somewhat different from those observed for variations in Young's modulus; in both tension and compression, compared to the deterministic simulation, the macroscopic response of the heterogeneous material features an onset of plasticity associated to relatively lower stress and a non-linear, apparent strain hardening phase consequence of the progressive yielding of the sample. Again, a higher degree of heterogeneity r_{σ} results in lower flow stress at any applied macroscopic strain. In tension and compression deformation localises along shear bands at $\pm 45^{\circ}$ on the loading axis; in tension these bands evolve into a macroscopic necking mechanism and corresponding strain softening, while in compression these spread to the whole sample, which displays a plateau response at large strains. The microscopic strain at tensile necking increases with r_{σ} , reinforcing the notion that material heterogeneity must affect macroscopic ductility.

In Figure 2.6(c) numerical predictions of the true peak tensile stress are compared to the bounds developed in Section 2.2; predictions appear much closer to the upper bound than to the lower bound; more accurate upper bounds for the macroscopic response may be obtained by making

use of the upper bound theorem of plasticity and assuming a shear banding mechanism; this is omitted here for the sake of brevity.

2.4.3 Effect of variation of hardening modulus

A separate set of simulations was conducted by imposing a spatial variation of the material hardening modulus, with elastic modulus and yield stress kept constant. The degree of variation was chosen as

$$r_H = \frac{\Delta H}{(H_{\max} + H_{\min})/2} = 2. \quad (2.26)$$

The consequent macroscopic response, not shown for the sake of brevity, comprised a linear elastic part followed by a linear strain-hardening phase. The effective hardening modulus, for the (relatively high) degree of variation r_H considered, was much closer to that predicted by the upper bound developed (Eq. (2.16)) than to the corresponding lower bound (Eq. (2.18)). A spatial variation of the hardening modulus alone does not have substantial effects on the macroscopic response, with the exception of resulting in a macroscopic hardening modulus smaller than the average microscopic value (predicted by the upper bound, Eq. (2.16)).

2.4.4 Size dependence of the response

Introducing a spatial variation of material properties in the numerical models effectively introduces a length scale in the problem, namely the dimension of the statistical cell used. Dimensional analysis dictates that the problem must depend on a non-dimensional parameter involving this cell dimension, for example the ratio between size of the SVE and size of the statistical cells, which increases monotonically with N_{CELL} . The parameter N_{CELL} therefore is representative of physical size of the material specimen. The dependence of the macroscopic response upon N_{CELL} has been already highlighted in Figure 2.2(a) and Figure 2.4. We now examine in detail how the macroscopic stress-strain response changes as a function of N_{CELL} .

First, consider the case of a non-uniform elastic modulus and uniform yield stress and hardening modulus ($r_E = 1.43$, $r_\sigma = r_H = 0$). Figure 2.7(a) and Figure 2.7(b) present respectively the tensile and compressive stress-strain curves for a heterogeneous material, compared to the deterministic (homogeneous) case. Each figure includes three curves corresponding to different values of N_{CELL} ; clearly the response is insensitive to this parameter in the range considered, confirming the trends shown in Figure 2.2.

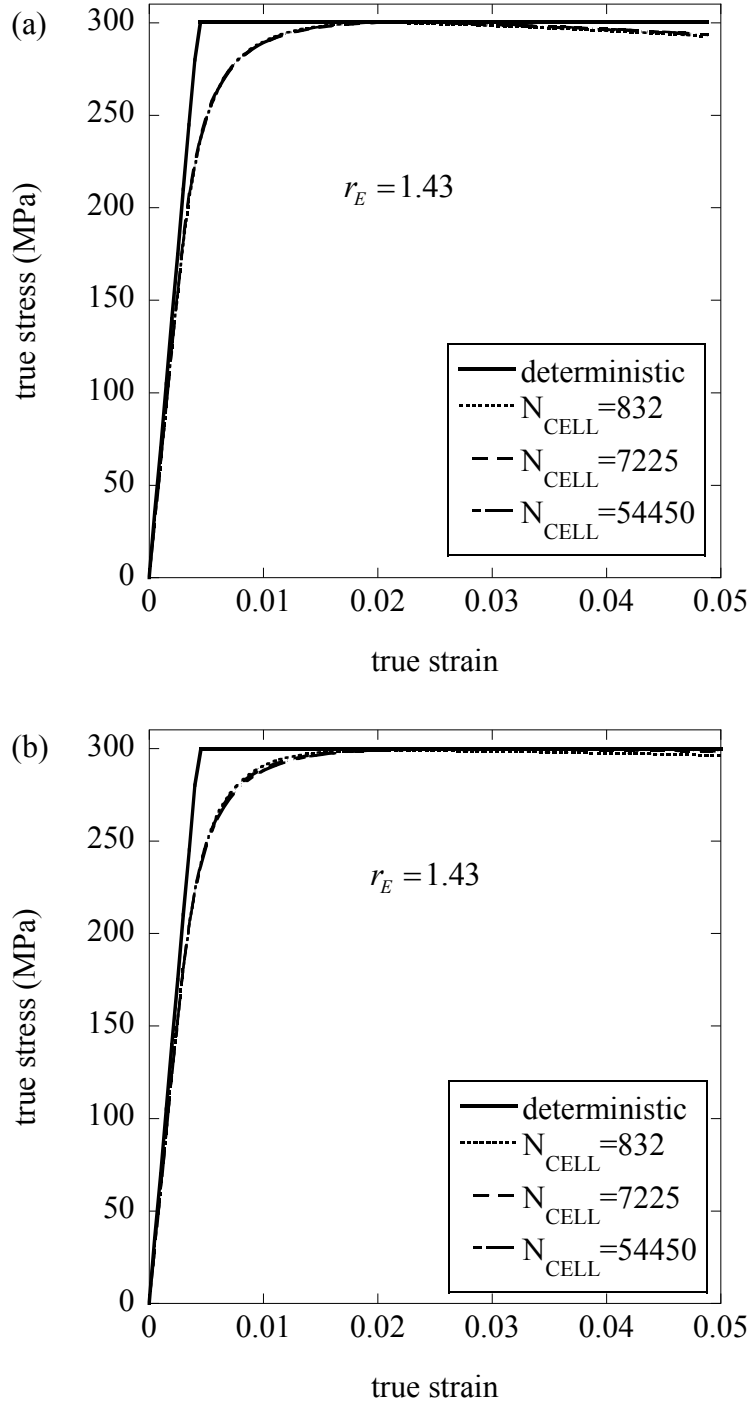
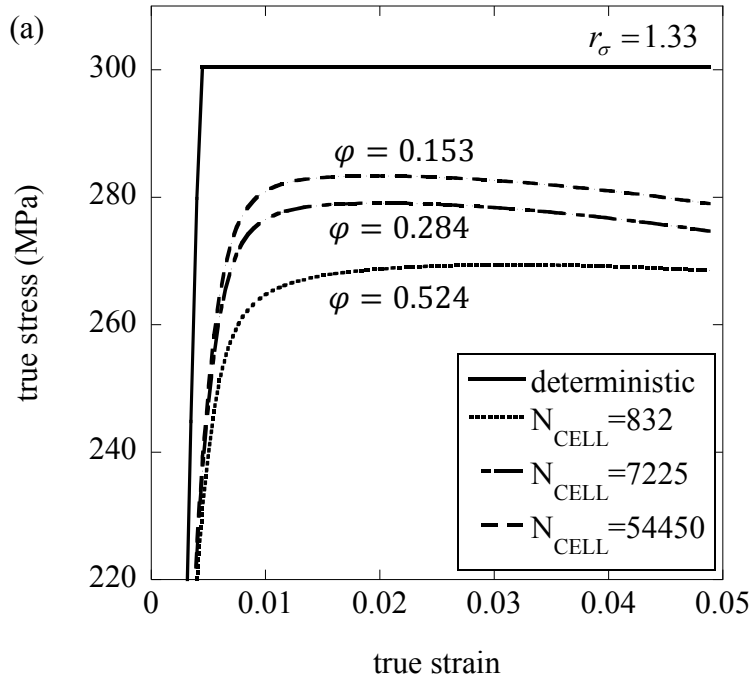


Figure 2.7 Effect of N_{CELL} on the macroscopic tensile (a) and compressive (b) response, for a given degree of elastic heterogeneity, $r_E = 1.43$.

Figure 2.8(a) and Figure 2.8(b) present similar information for the case of spatial variation of yield stress ($r_\sigma = 1.33$, $r_E = r_H = 0$). In this case the material displays a pronounced size effect in both tension and compression, with larger specimens (or equivalently, SVEs with larger values of N_{CELL}) displaying a stronger material response. This has been reported by other

studies on size effects in the response of ductile elasto-plastic solids [111, 112] and justified in terms of the different stress states of material domains lying on the surface of the solids and those contained within this surface. In fact, material cells lying with at least one side on the external SVE surface are less constrained, having at least one vanishing principal stress, and tend to yield earlier than material cells within the volume of the SVE. The ratio φ between the number of material cells lying on the surface and within the specimens depends on N_{CELL} through a simple geometric relation, involving also the aspect ratios of the SVE. Figure 2.8 includes values of φ for SVEs of different size (N_{CELL}); clearly, elements with a higher value of φ display a weaker response in both tension and compression.



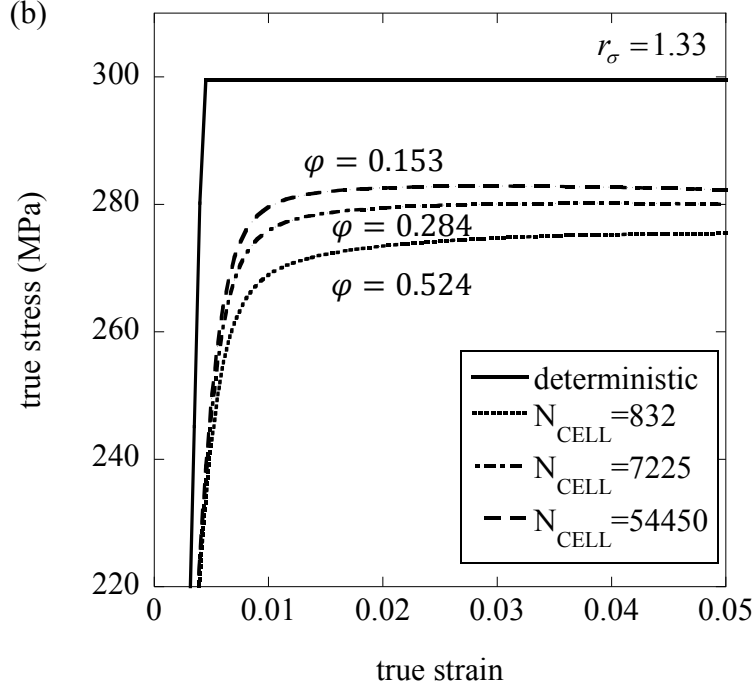


Figure 2.8 Effect of N_{CELL} on the macroscopic tensile (a) and compressive (b) response, for a given degree of plastic heterogeneity, $r_\sigma = 1.33$.

In the data presented in Figure 2.8 the aspect ratios of the SVE were kept constant. In a separate set of simulations ($r_\sigma = 1.33$, $r_E = r_H = 0$, $N_{FE} = N_{CELL}$) we varied the geometry of the SVE in a wide range, ranging from a chain of cells in series to an array of cells arranged in parallel; the corresponding uniaxial tensile strength varied from the mean yield stress (for the case of a parallel arrangement, in line with the upper bound derived in Section 2.2) to approximately one third of this value, for the case of a chain arrangement. Such variations are driven by the dependence of ϕ upon the geometry (aspect ratios) of the SVE, but also by different mechanisms of deformation and different stress triaxiality induced by the different specimen geometries.

Next we present, in Figure 2.9, analogous information as that in Figure 2.7 and Figure 2.8, for the case of a spatial variation of the hardening modulus alone ($r_H = 2$, $r_E = r_\sigma = 0$). Similarly to the case of variations of elastic modulus, the observed size effect is in this case very mild in the range of SVE sizes considered.

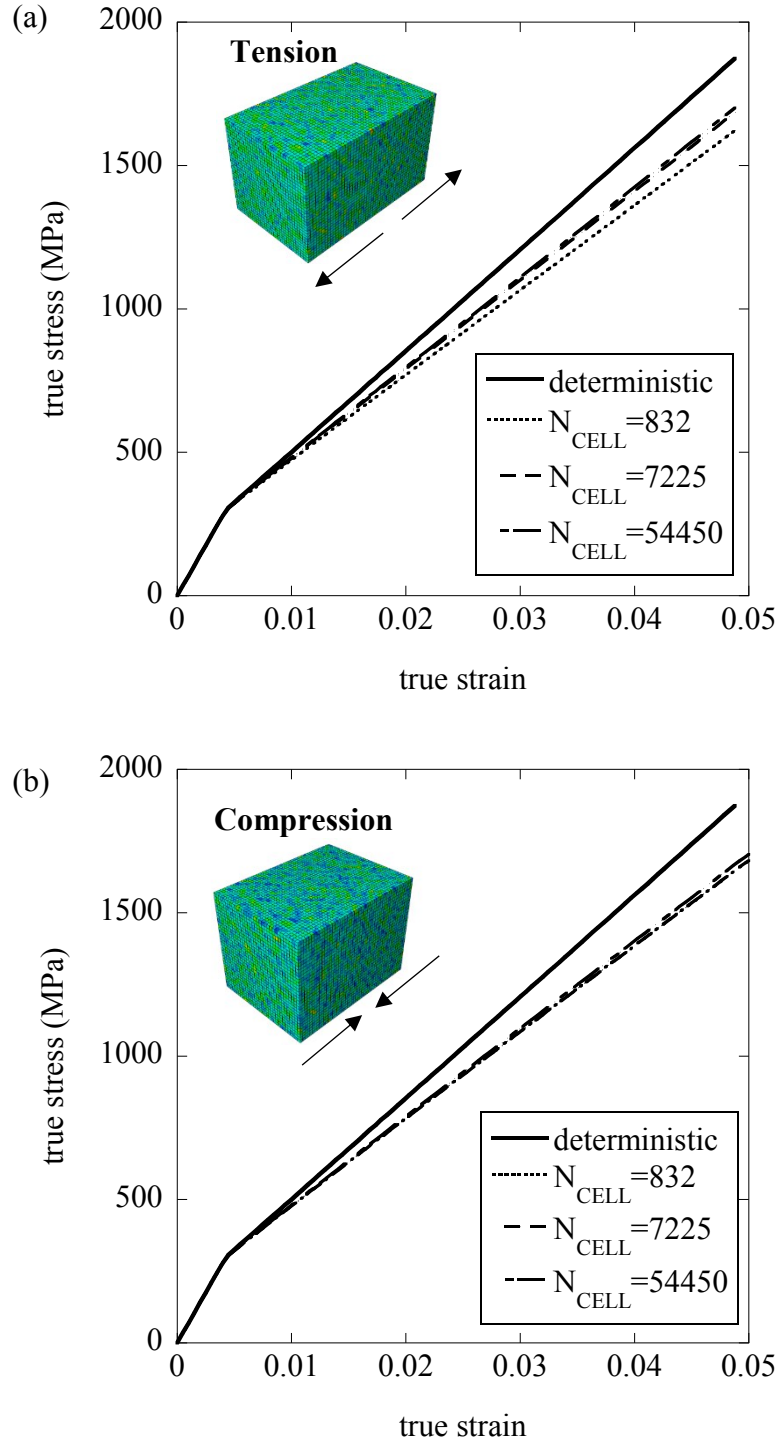


Figure 2.9 Effect of N_{CELL} on the macroscopic tensile (a) and compressive (b) response, for a given degree of heterogeneity in the hardening modulus, $r_H = 2$.

2.4.5 Multiaxial stress response

To illustrate the effects of material heterogeneity on the macroscopic response to multiaxial stress states, we use the numerical scheme presented above to construct yield surfaces of heterogeneous solids and compare with the homogeneous case. Cubic SVEs are generated with $V = 11.39 \text{ mm}^3$, $N_{FE} = N_{CELL} = 21952$. Macroscopic strain histories are imposed on the SVEs according to Eq. (2.19) and Table 1. Two sets of simulations were conducted varying either the elastic modulus or the yield stress at microscopic scale. Figure 2.10 shows the yield surface of a heterogeneous material featuring microscopic variations of the elastic modulus. In Figure 2.10(a) we present, for $r_E = 1.43$, the evolution of the yield surface.

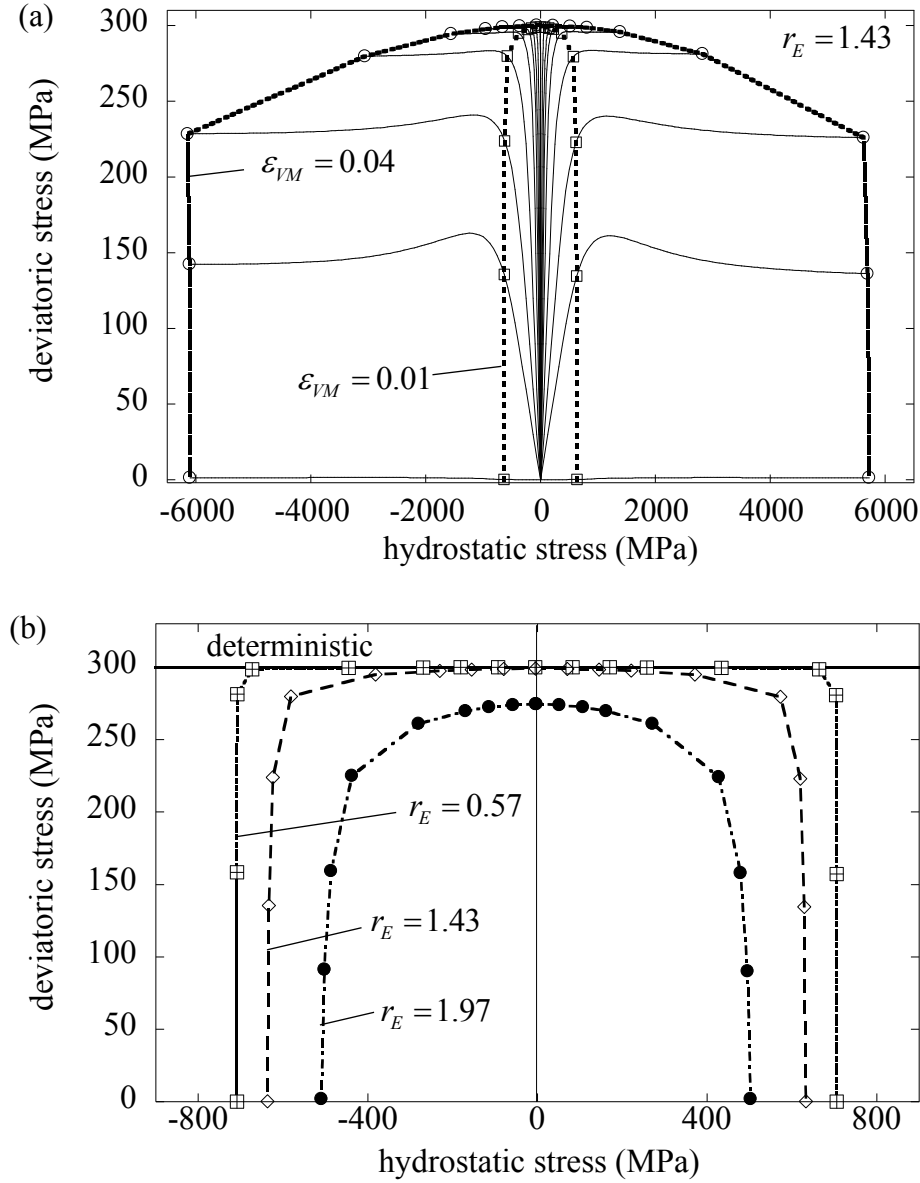


Figure 2.10 (a) Yield surface evolution for a given degree of elastic heterogeneity, $r_E = 1.43$ (b) Effect of r_E on the yield surface.

Trajectories of the hydrostatic and deviatoric stresses at different (initial) stress triaxiality are shown, and on each trajectory two points are marked, corresponding to von Mises equivalent strains of 0.01 (squares) and 0.04 (circles). Obviously, the macroscopic yield surface is pressure-dependent, although the microscopic material response is pressure-insensitive (obeying the von Mises criterion); this is due to the fact that a macroscopic hydrostatic stress results in deviatoric stress components at microscopic level, due to the elastic heterogeneity. The macroscopic material hardening can be observed in the figure and is neither isotropic nor kinematic (isotropic hardening is imposed at microscopic level). Figure 2.10(b) shows the

effect of the degree of heterogeneity r_E on the multiaxial response: clearly a higher heterogeneity gives a weaker response and enhances the pressure-sensitivity of the macroscopic response. Note that the yield surfaces in Figure 2.10(b) are obtained at von Mises equivalent strains of 0.01.

Figure 2.11 presents similar information for the case of microscopic variations of the yield stress; Figure 2.11(a) shows the evolution of the yield surface for $r_\sigma = 1.33$, while Figure 2.11(b) presents the effect of varying r_σ on the macroscopic yield. Clearly in this case the macroscopic response is pressure-insensitive; this is due to the fact that the material is elastically homogeneous and macroscopic hydrostatic stress components do not induce microscopic deviatoric components in this case. The macroscopic strain hardening is in this case isotropic; again a higher degree of heterogeneity results in a weaker macroscopic response (Figure 2.11(b)).

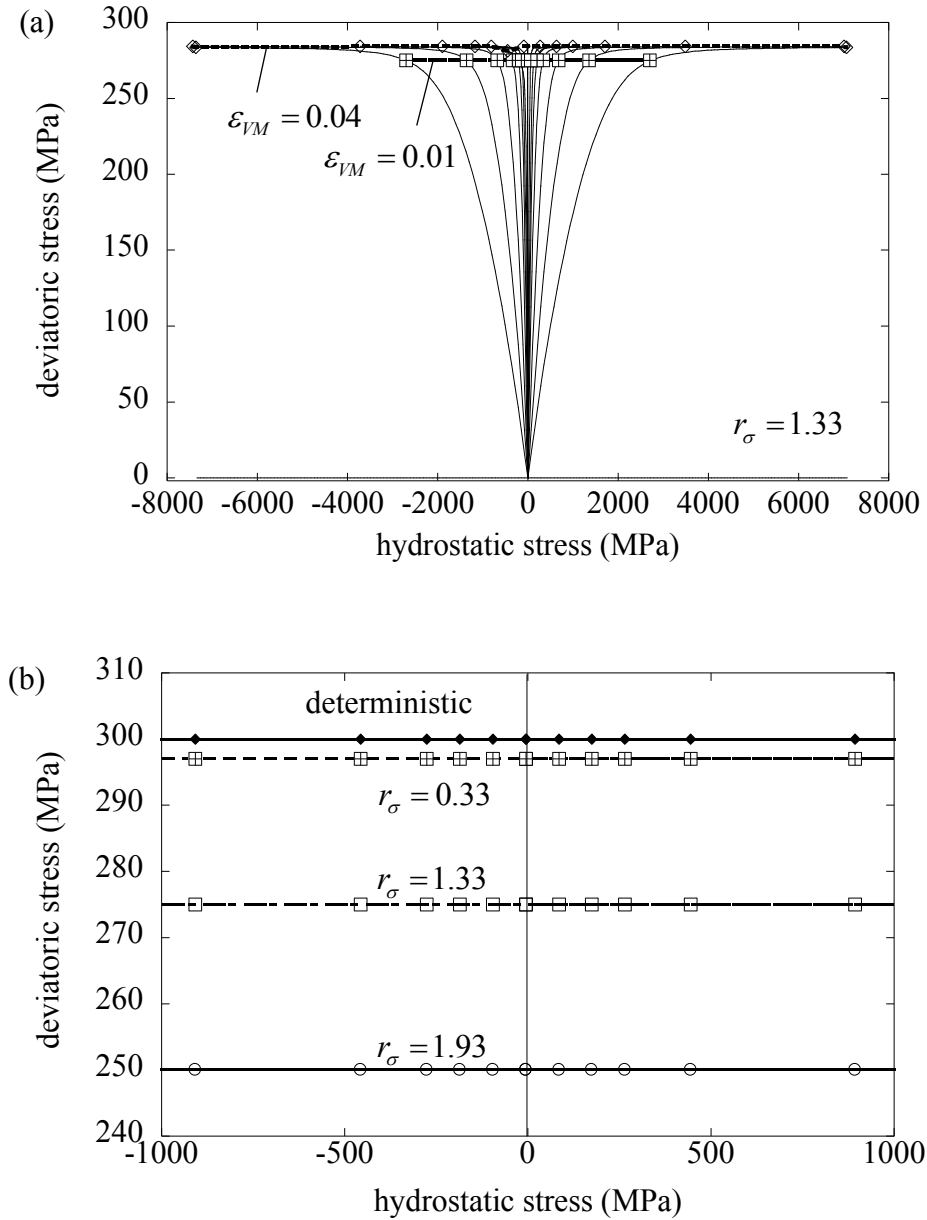


Figure 2.11 (a) Yield surface evolution for a given degree of plastic heterogeneity, $r_\sigma = 1.33$ (b) Effect of r_σ on the yield surface.

2.4.6 Case study: prediction of the fatigue endurance limit from the quasi-static response

The discussion of the results presented above has highlighted, among other things, the fact that in real polycrystalline materials, featuring a clear heterogeneity in the elasto-plastic properties, the onset of yield occurs at very low stresses, much lower than what is commonly referred as the material ‘yield stress’ (e.g. proof stress, or macroscopic flow stress at 0.2% plastic strain).

In addition, we found that the macroscopic response of heterogeneous materials featuring variations of the yield stress is close (recall Figure 2.5) to the predictions of the simple upper bound model developed in Section 2.2 (Eq. (2.14)). In principle, fitting Eq. (2.14) to the stress strain curve of a material of small strain hardening may be used to determine the macroscopic stress at the onset of plasticity $\sigma_y^{\min}$.

Such fitting exercise was conducted using uniaxial tension data in [114] on two types of Titanium alloys, considering only the stress-strain histories for strains less than 1%; an initial linear response is assumed, followed by a non-linear response (Eq. (2.14)) for $\sigma > \sigma_y^{\min}$. The value of $\sigma_y^{\max}$ was taken as the flow stress at total strain of 0.01 (this value approximately corresponds to the point at which the measured stress-strain curves attain a horizontal tangent). This fitting exercise yielded, for the two alloys considered (denoted as Ti-5553-1 and Ti-5553-3 in [114]) $\sigma_y^{\min} = 334$ MPa and $\sigma_y^{\min} = 312$ MPa, respectively. The authors also measured S-N curves for these two alloys (at relatively low stress ratio, $R=0.1$) and found that both alloys displayed a fatigue endurance limit, namely 330 MPa and 310 MPa for Ti-5553-1 and Ti-5553-3, respectively. These are remarkably close to the values of $\sigma_y^{\min}$ extracted from the uniaxial stress-strain curves.

It is well known that fatigue is a macroscopic phenomenon initiated by microscopic plasticity at relatively low stress, and supported by cyclic loading. Although the mechanisms are quite complex [115]-[118] and differ from material to material, it is logical to think that if the applied stress levels are low enough not to initiate microscopic plasticity, then the material will not fail by fatigue at such applied stresses. The data, in this case, support this notion; however more complex modelling techniques and a more extensive experimental campaign on different materials would be needed to confirm this hypothesis; this is left as a topic for future studies.

2.4.7 Model in practice

In practice the mechanical response of the material must be measured by conducting simple uniaxial tests. At the micro-level a bilinear response can be assumed and the variation of Young's modulus, yield stress and hardening modulus can be determined by calibrating the response with the measurement. Given the variation at the micro-level, the mechanical response at various stress triaxilities can be predicted. In the current chapter deformations were small. At higher strains, damage has to be incorporated in the model. One way to measure the damage for ductile solids is by repeating loading/unloading cycles on a uniaxial tensile specimen and measuring Young's modulus degradation as a function of strain.

2.5 Concluding Remarks

Monte Carlo analyses were conducted, with the commercial FE software ABAQUS/standard, to investigate the effects of microscopic variations in elastic modulus, yield strength and hardening modulus upon the macroscopic elasto-plastic response of heterogeneous solids. Random SVEs were generated and their multiaxial stress-strain response was predicted. The mechanical properties of the cells forming such SVEs was taken as linear elastic followed by incompressible elasticity with constant strain hardening modulus and isotropic hardening. Mechanical properties were different in each cell, according to random fields of uniform probability density. Microscopic variations of either the elastic modulus, the yield stress or the hardening modulus were imposed over a single length scale, and the macroscopic effects of such variations were investigated. The sensitivity of the macroscopic response to density of the FE discretisation and SVE size was explored, and predictions were compared to simple analytical Voigt/Reuss bounds. The main conclusions of the study are as follows:

- The response of an elastically heterogeneous elasto-plastic solid is softer than that of a homogeneous solid of average elastic modulus, with the reduction in stiffness proportional to the degree of heterogeneity. Similarly, the response of a plastically heterogeneous elasto-plastic solid is weaker than that of a homogeneous solid of average yield stress; the reduction in strength is proportional to the degree of heterogeneity. It follows that modulus and yield stress extracted from experiments do not, in general, coincide with spatial averages of their microscopic counterparts.

- The onset of yield in a heterogeneous material occurs at stresses much lower than the proof stress; the higher the degree of heterogeneity, the lower is the stress to cause first yield.
- Microscopic variation of stiffness or yield stress induce tension/compression asymmetry, strain localisation by shear banding and necking instability in uniaxial tension. The strain at which tensile necking occurs increases with the degree of heterogeneity, suggesting that material ductility must be related to such degree.
- For a plastically heterogeneous material strong size dependence of the response is observed, in line with experimental observations.
- An elastically heterogeneous material, comprising an array of plastically incompressible domains with isotropic hardening, displays a macroscopic response which is plastically compressible, pressure-sensitive and characterised by non-isotropic hardening.

2.6 APPENDICES

APPENDIX A

User-defined material model

Au user-material subroutine (UMAT) for elasto-plastic isotropic materials was implemented in the finite element software. The randomisation of material properties was employed within the UMAT via random number generated variables. Detailed description can be found below.

A mixed incremental and iterative approach was applied to model plasticity in a material which is being loaded past the yield stress of the material. The radial return method was used as the iterative solution, where the main components are an elastic predictor and a plastic corrector vector which are used in a Newton-Raphson iterative approach. According to Dunne and Petrinic (2011), the radial method is given by the following constitutive equations for the k th iteration:

$$\begin{aligned} r^k &= r_l + h\Delta p^k \\ d\Delta p &= \frac{\sigma_e^{tr} - 3G\Delta p^k - r^k - \sigma_y}{3G + h} \\ \Delta p^{k+1} &= \Delta p^k + d\Delta p \end{aligned}$$

Where

- $r = h \cdot p$ is the hardening part of the material stress-strain curve
- h is the hardening parameter
- p is the equivalent plastic strain
- r is the increment in equivalent stress
- G is the elastic shear modulus of material
- σ_e^{tr} is the elastic trial stress predictor
- σ_y is the initial yield stress

This is an explicit-type method in which the plastic corrector vector does not necessarily remain normal to the yield surface as the iteration process progresses (Fig. A.2), in 2D principal stress space.

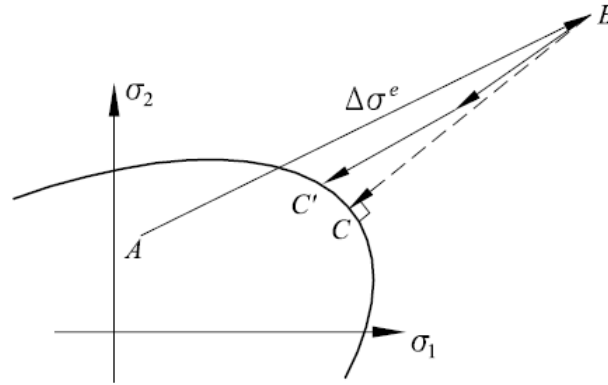


Figure. A.1 Visualisation in 2D principal stress space [119].

2.3 Synthesis of model

The subroutine is actually a UMAT central subroutine with small initial subroutines of UEXTERNALDB and SDVINI. Their use will be described below:

1. UEXTERNALDB

This simple routine just opens the file 'mat_cor.txt' containing the material property data for the stress-strain curve and transfers data to PROPERTIES vector. If there is a file-opening error, the intrinsic subroutine STDB_ABQERR is called. If there is an input-output error (IOSTAT variable) for the material property data, the program exits.

2. SDVINI

This subroutine assigns the randomised material properties to state variables (STATEV) which allow their use and manipulation/updating in the subsequent subroutine. It is necessary to employ SDVINI for this purpose in order that properties for the elements in the mesh that are defined in the initialisation step do not change in subsequent loading steps.

State variables 3 and 4 are used for Elastic modulus and Poisson's ratio, respectively, given that state variables 1 and 2 are reserved for equivalent plastic strain and stress, respectively, as described in UMAT section.

The randomisation is achieved using RANDOM_NUMBER with RANDOM_SEED Fortran intrinsic subroutines, with the seed based on the current time according to the computer. The

material property randomisation is realised using a semi-bandwidth which specifies the range of the uniform distribution of the property. The following construction is therefore used for randomised property E_i , based on mean value E and range ΔE .

$$E_i(r_i) = E_{\min} + r_i(E_{\max} - E_{\min}) = E_{\min} + r_i\Delta E$$

The hardening curve stress-strain data are then stored in state variables 5 and above.

3. UMAT

This section will deal with the substance of the radial return model and how it is synthesised in the Fortran code for the UMAT part of the subroutine. The ways in which the iteration stress vectors are applied are shown in Fig. A.2 for a typical linear-elastic-non-linear hardening curve.

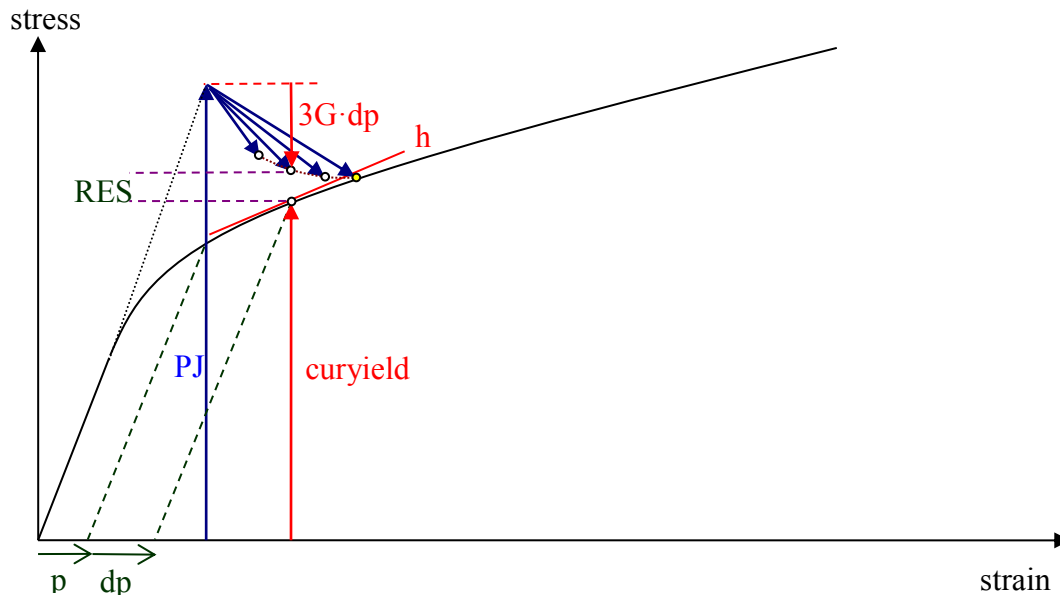


Figure. A.2 Radial return iteration method

With reference to Fig. A.2, there are some fundamental parameters which must be defined and employed henceforth:

- p : current value of equivalent plastic strain at the beginning of the increment (state variable 1).
- dp : increment in equivalent plastic strain

- PJ : equivalent trial elastic stress predictor
- G : elastic shear modulus of the material
- $3 \cdot G \cdot dp$: plastic corrector
- $curyield$: current value of the hardening function (state variable 2). This is equal to the sum of r and σ_y (initial yield stress).
- h : hardening function at the current increment
- RES : residual

It is clear from the locus of subsequent iterations, shown by red dotted line in Fig. A.2, the path taken by the algorithm until convergence is reached where the non-linear material hardening curve is reached, represented in Fig. A.2 by the yellow circle.

Iteration continues under this scheme until the convergence is achieved within the tolerance, TOL, that is the absolute residual is less than the tolerance:

$$RES = |PJ - 3 \cdot G \cdot dp - curyield| < TOL$$

The value of $curyield$ must be evaluated at every strain increment, dp , since it is a function of the hardening parameter, h , which is a function of equivalent strain, p .

For a given value of $p + dp$, the current value of $curyield$ is given as:

$$curyield = s_j + h \cdot (p + dp - e_j)$$

This accounts for the corresponding segment j of the multi-linear s-e hardening curve definition of the material which has been defined in the input data file, matcor.txt.

The hardening function, h , is simply the gradient corresponding to the level of equivalent plastic strain that is prevalent at that increment/iteration, and is evaluated from the s-e hardening curve definition:

$$h = \frac{s_{j+1} - s_j}{e_{j+1} - e_j}$$

A constant limit of the maximum stress is defined for p larger than that defined in the material input file.

Also the next increment in equivalent strain, dp_{i+1} , must be updated on each iteration:

$$dp_{i+1} = dp_i + \frac{RES}{3G + h}$$

The following fundamental steps of the UMAT are:

1. Define p and $curyield$ from current state variables.
2. Define Jacobian/elasticity (DSDDE) and identity (XIDEN) matrices.
3. Obtain stress predictor increment (STR) from strain increment.
4. Calculate deviatoric (DSTR) and equivalent (PJ) stress predictor.
5. Determine flow direction (XNDIR).
6. If yielding occurs, perform iterative procedure:
 - a. Determine current h from stress-strain curve
 - b. Determine current value of $curyield$
 - c. Evaluate RES and p
 - d. If convergence not achieved within tolerance, repeat.
7. Determine new dp , elastic strain and stress increment.
8. Current p is $p + dp$.
9. Store p and $curyield$ to state variables 1 and 2.
10. Evaluate Jacobian (DDSDDE).

Details of how the UMAT works in conjunction with ABAQUS can be found in [120].

CHAPTER 3

PREDICTIONS OF THE ELASTO-PLASTIC RESPONSE OF LOW-POROSITY SOLIDS

ABSTRACT

A numerical method is developed to model the macroscopic quasi-static mechanical response of solids with porosity in the range 0.01-0.3. A virtual material specimen is subdivided in small cubic cells by a regular tessellation; some of these cells are modelled as a plastically incompressible, rate-independent elasto-plastic solid, representing the parent material, while the remaining cells, representing the pores, are taken as a plastically compressible solid displaying densification behaviour at large strains. The sensitivity of the predictions to FE and statistical mesh density is explored, and a minimum size of the representative volume element (RVE) is determined. The yield surface is predicted for selected values of the porosity. The predictions are found in good agreement with previously published numerical studies in which the microstructural geometry was explicitly modelled.

3.1 Introduction

Many engineering materials display a non-negligible degree of porosity and this affects their mechanical response. Several phenomenological models have been proposed to date to describe the macroscopic yield response of a porous elasto-plastic solid, for example in [4, 12-14, 121], and more recently in [5-9, 11, 122, 123]. These models require extensive multi-axial testing of the material for their calibration and are unable to capture strain localisation triggered by microstructural inhomogeneity and possibly triggering fracture.

Other existing models have pursued a micromechanical approach; pioneering studies shown in [124-129], used variational methods to examine the elastic response of porous solids, while in recent years authors [69, 130-142] focused on the multi-axial yield behaviour of porous solids. A good discussion on different homogenisation techniques based on continuum micromechanics can be found in [143].

The microstructure of porous metals can be geometrically complex and several studies have analysed the mechanical response of periodic unit cells to predict the macroscopic response of the porous solid [63, 144-164]. Most of these studies considered unit cells comprising spherical voids in a continuum matrix.

In order to account for the stochastic nature of the microstructure, several recent studies focused on the generation and analysis of virtual microstructures of low-porosity solids; these typically consisted of random arrays of identical voids in a continuum matrix. Some authors focused on the elastic response [54-59] while others (e.g. [60-63, 165, 166]) examined the multi-axial yield behaviour. The technique for random generating periodic spherical particles is discussed in [64]. Other authors also accounted for the effects of pore size distribution [65-71] or of both pore size and shape [72-76]. Given the complexity and stochastic nature of the material microstructure, simulations of random material volume elements may provide greater accuracy than other deterministic modelling approaches. On the other hand, simulations of RVEs are computationally expensive, due to the geometric complexity of the microstructure and the necessity of performing repeated simulations; in addition, they cannot predict correctly the

large-strain material response unless computationally expensive self-contact algorithms are used.

In this chapter we present a different modelling strategy for low-porosity solids. We do not attempt explicit modelling of the geometry of the microstructure but we do account for the physical effects of the presence of the pores on the response of the material. After a regular tessellation, the material is treated as a rate-independent, two-phase composite comprising the solid parent material (modelled as a von Mises elasto-plastic continuum) and a fictitious, plastically compressible, soft and weak ‘pore’ material which mimics the effects of pore collapse and subsequent self-contact, avoiding the explicit use of expensive contact algorithms.

The structure of the chapter is as follows; in Section 3.2 we present the algorithm to generate the material microstructure and provide details of the numerical simulations conducted. Results are discussed in Section 3.3 and the main conclusions are summarised in Section 3.4.

3.2 Numerical Methods

In this chapter we attempt modelling of a porous solid comprising an elastic perfectly plastic matrix and a random array of identical pores. We shall compare our predictions to those in [61]; these authors generated periodic microstructures consisting of random arrays of identical spherical, non-overlapping voids embedded in a cubic RVE. The matrix was treated as elastic perfectly plastic and Monte Carlo analyses were conducted to determine the multi-axial elasto-plastic response of the porous solid at small tensile strains.

3.2.1 Generation of microstructures

Cubic material RVEs are considered; these are subdivided into identical cubic cells by a regular tessellation. The material is then treated as a two-phase composite: a certain fraction of the cubic cells are randomly flagged to represent the solid phase, while the remaining cells are flagged as pores, according to a uniform random spatial distribution. The algorithm employed does not prevent adjacent cells to be flagged as pores and this results in pores of different size and shape present in the microstructure (examples are shown in Figure 3.1). The proposed algorithm does not attempt controlling the distribution of pore sizes but it only reproduces the overall material porosity. The underlying assumption is that we expect, as observed experimentally, the overall porosity to be the dominant parameter governing the material response in the range investigated (porosity of 0.01-0.3). Further details of how the microstructures were produced can be found in APPENDIX A in Section 3.5.

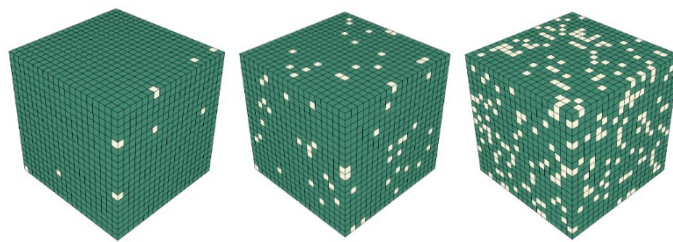


Figure 3.1 Non-periodic microstructures of different porosities (1%, 5% and 20% from left to right).

3.2.2 Constitutive models

The solid material phase is modelled using linear isotropic elasticity ($E_0 = 200$ GPa, $\nu = 0.3$) and incompressible J_2 plasticity, with yield stress $\sigma_F = 100$ MPa and vanishing strain hardening. The choice of material properties is dictated by that in [61].

To mimic the behaviour of pores in a solid matrix, the cells flagged as pores need to be able to experience high compressive or tensile volumetric strains without considerable energy absorption; they also need to lock (their stiffness needs to increase substantially) at sufficiently high compressive volumetric strains, in order to simulate the pore self-contact subsequent to compressive plastic collapse. In order to achieve these features without using computationally expensive contact algorithms, cells marked as pores are modelled as plastically compressible solids by the crushable foam model developed by Deshpande and Fleck [15] and implemented in ABAQUS standard, with the choice of isotropic hardening.

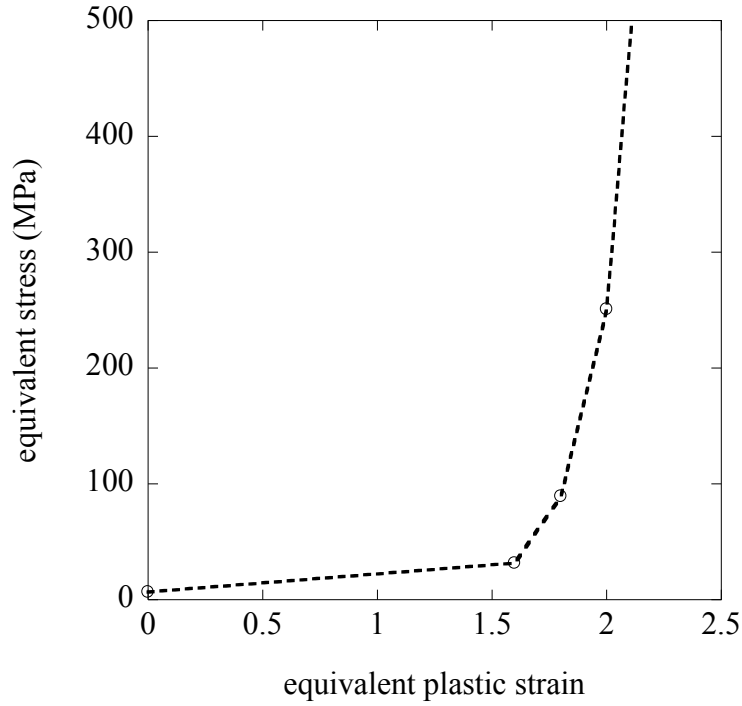


Figure 3.2 Plastic constitutive response of the fictitious pore material; prescribed history of the equivalent Deshpande-Fleck stress as a function of the corresponding equivalent plastic strain.

The pore material is taken as linear elastic and isotropic, with Young's modulus and Poisson's ratio of 2.9 GPa and 0.3, respectively, while the initial yield was set to $\sigma_{y_p} = 6.45$ MPa. These material properties were chosen to promote early "yield" of the pore material and to ensure fractions of stored and dissipated energy within the domain occupied by the pores of less than 1% of the total work done. Setting the values of stiffness and strength too close to zero would result in unstable FE simulations. Subsequent to first yield, a slight numerical strain hardening was imposed prior to densification, which was set to occur gradually at nominal compressive strains in the range 0.8-0.9. The plastic Poisson's ratio was set to zero and consequently the ratio k of the initial yield stresses in uniaxial and hydrostatic compression was set to $\sqrt{3}$, as dictated by the rule of normality of plastic flow. The prescribed history of equivalent stress versus equivalent plastic strain (as defined in Deshpande and Fleck [15]) for the pore material is presented in Figure 3.2. Preliminary simulations showed that the predicted macroscopic material response was scarcely sensitive to the choice of elastic modulus and initial stress of the pore material; specifically, a further reduction in σ_{y_p} or E_p by one order of magnitude reduced the macroscopic yield stress by less than 1 MPa and the macroscopic modulus by less than 3 GPa.

3.2.3 Boundary conditions

There is general consensus that periodic boundary conditions should be used in the FE analysis of periodic stochastic volume elements (SVEs) and representative volume elements (RVEs). The set of boundary conditions affects the predicted mechanical response of the material, as shown in [44, 61, 78, 79]. Several authors (e.g. [80, 81]) have shown that as the SVEs or RVEs get progressively larger in size, predictions obtained by imposing uniform displacement boundary conditions approach those made using periodic boundary conditions. Preliminary simulations confirmed this for the case of the SVEs analysed here and in our simulations, conducted on non-periodic microstructures, we impose uniform boundary conditions, forcing the faces of the cubic SVEs to remain planar as deformation proceeds, see for example [54, 67, 72, 75].

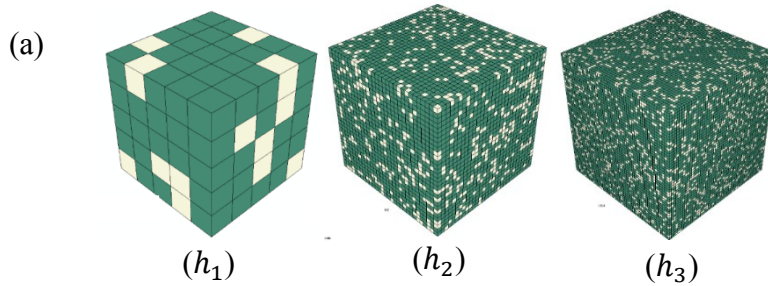
When simulating the uniaxial tensile or compressive response, one of the faces of the cubic SVE has normal displacements constrained while the opposite face is subject to normal displacements linearly increasing with simulation time, such to induce macroscopic tensile or compressive strain. The lateral faces are constrained to remain planar and the normal displacements on opposite lateral faces are forced to be equal and opposite; these constraints are imposed via the constraint equation tool of ABAQUS CAE, making use of appropriate dummy nodes.

In order to explore the multi-axial yield behaviour and to determine the material yield surface, different values of stress triaxiality were imposed in the elastic phase of loading. This was done by imposing macroscopic normal strains in the principal directions (denoted by 1,2,3) given by Eq. 2.19 (Section 2.3). In Eq. 2.19 the macroscopic strain rate was set to $\dot{\epsilon} = 5 \text{ s}^{-1}$ and t represents the simulation time; nine pairs of parameters (α, β) were chosen, in line with those in [61], to give 18 different values of stress triaxiality, of which 9 positive (loading cases 1-9) and 9 negative (loading cases 10-18). A summary of the parameters corresponding to each of the 18 loading cases is provided in Table 1 (Section 2.3). Histories of true principal stresses were extracted from each simulation and allowed determining the corresponding histories of hydrostatic stress and equivalent von Mises stress, as well as the volumetric and equivalent von Mises strains, as shown in Eqs. 2.20 - 2.23 (Section 2.3).

3.2.4 Meshing and Monte Carlo analyses

The SVEs, of volume V , were meshed using regular arrays of simple cubic, 8-noded brick elements, of type C3D8 in ABAQUS/standard, with a full integration scheme. Monte Carlo analyses were conducted: repeated FE simulations were conducted on 10 realisations of each microstructure to obtain the average and spread of the predicted outputs.

The sensitivity of the predictions to FE mesh density (or number of FE used, $N_{FE} = V / L_e^3$, where L_e is the size of the cubic FE used) and to density of the cell tessellation (or number of cells used, $N_{CELL} = V / V_{CELL}$, where V_{CELL} is the volume of one cell of the tessellation) was determined by conducting repeated simulations at increasing N_{FE} and N_{CELL} , to determine the minimum values of N_{FE} and N_{CELL} which made the predictions insensitive to these two parameters. Such sensitivity analyses are presented below.



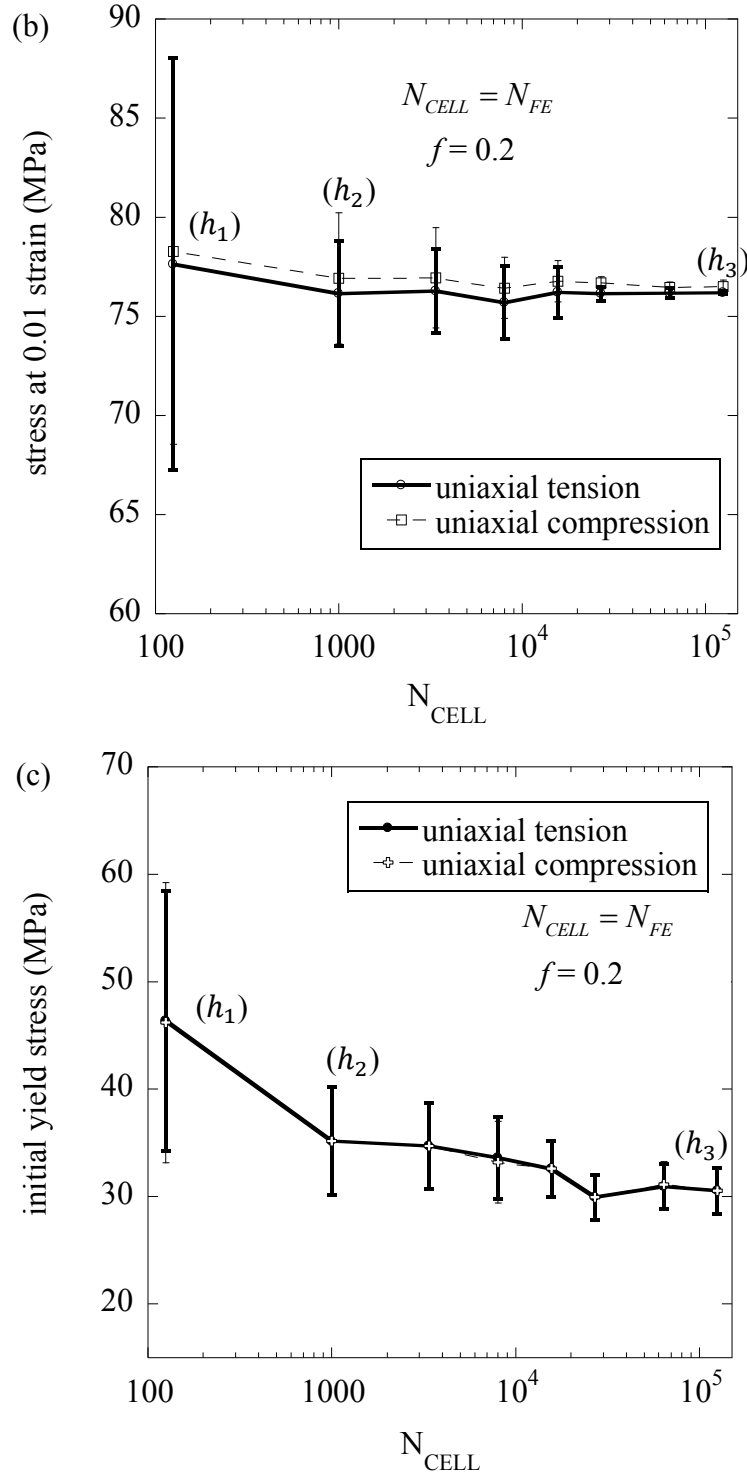


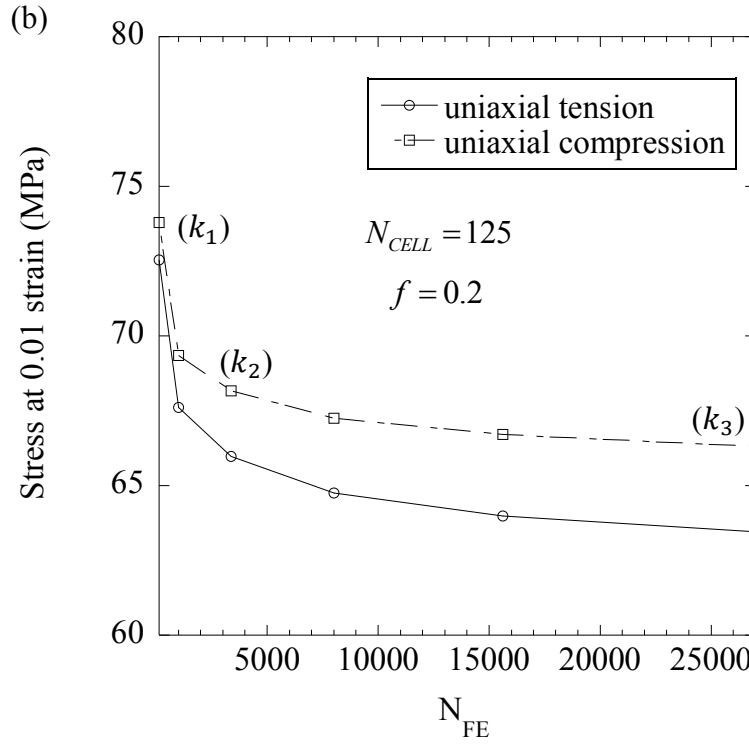
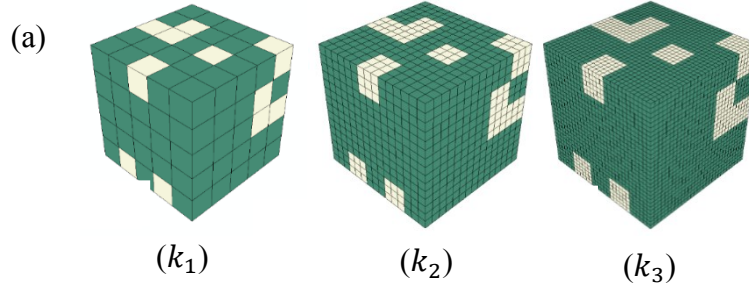
Figure 3.3 (a) Example of SVEs at increasing N_{CELL} , for the choice $N_{CELL} = N_{FE}$. (b) Sensitivity of compressive and tensile flow stress at a strain of 0.01 to the parameter N_{CELL} ; (c) Sensitivity of the macroscopic compressive or tensile stress at first yield to N_{CELL} ; error bars indicate the range of the outputs.

3.2.5 Sensitivity of predictions to the density of the statistical and FE meshes

We proceed to analyse the sensitivity of the FE simulations to N_{CELL} , for a porosity $f = V_p / V = 0.2$, where V_p is the total volume of pores. Different microstructures with N_{CELL} in the range 125-125000 were generated (examples are shown in Figure 3.3(a)); for each choice of N_{CELL} , 10 realisations of the microstructures were analysed. The FE mesh was chosen such that each statistical cell was meshed by a single linear finite element ($N_{CELL} = N_{FE}$). All the microstructures were subject to loading in uniaxial tension and compression; the simulations were interrupted when a total strain of 1% was reached and the corresponding flow stress was recorded; its sensitivity to N_{CELL} is shown in Figure 3.3(b). The average tensile and compressive flow stresses at 0.01 strain were found to be scarcely sensitive to N_{CELL} for $N_{CELL} > 1000$. The scatter decreased, as expected, with increasing N_{CELL} , and becomes less than 8% of the average for $N_{CELL} > 1000$. Irrespective of the value of N_{CELL} , the predicted compressive response was stronger than the tensile response, indicating a strength asymmetry. In addition to the flow stress at a strain of 0.01, we extract the macroscopic stress which causes first yield in the parent material. Figure 3.3(c) shows the sensitivity of this stress to N_{CELL} ; the macroscopic stress which causes first yield is identical in tension and compression; this stress is scarcely sensitive to N_{CELL} for $N_{CELL} > 27000$. As expected, the scatter in this quantity initially reduces with increasing N_{CELL} but becomes scarcely sensitive to this parameter for $N_{CELL} > 27000$.

In Figure 3.4(a)-(c), we present the sensitivity of the FE predictions to N_{FE} for a porosity $f = 0.2$ and the choice $N_{CELL} = 125$. Simulations are conducted by progressively refining the FE mesh (increasing N_{FE}) on a single realisation of the material microstructure, as illustrated in Figure 3.4(a). Figure 3.4(b) shows that the flow stress at total strain of 0.01 becomes approximately mesh insensitive for $N_{FE} > 8000$, corresponding to having 64 finite elements meshing each of the 125 cells, $N_{FE} / N_{CELL} = 64$. Again, the predicted compressive response is stronger than the tensile response, indicating a strength asymmetry. The macroscopic stress at initial yield is identical in compression and tension, as shown in Figure 3.4(c); this becomes

mesh insensitive for $N_{FE} > 166370$, corresponding to having 1331 (11^3) finite elements meshing each of the 125 cells, $N_{FE} / N_{CELL} = 1331$.



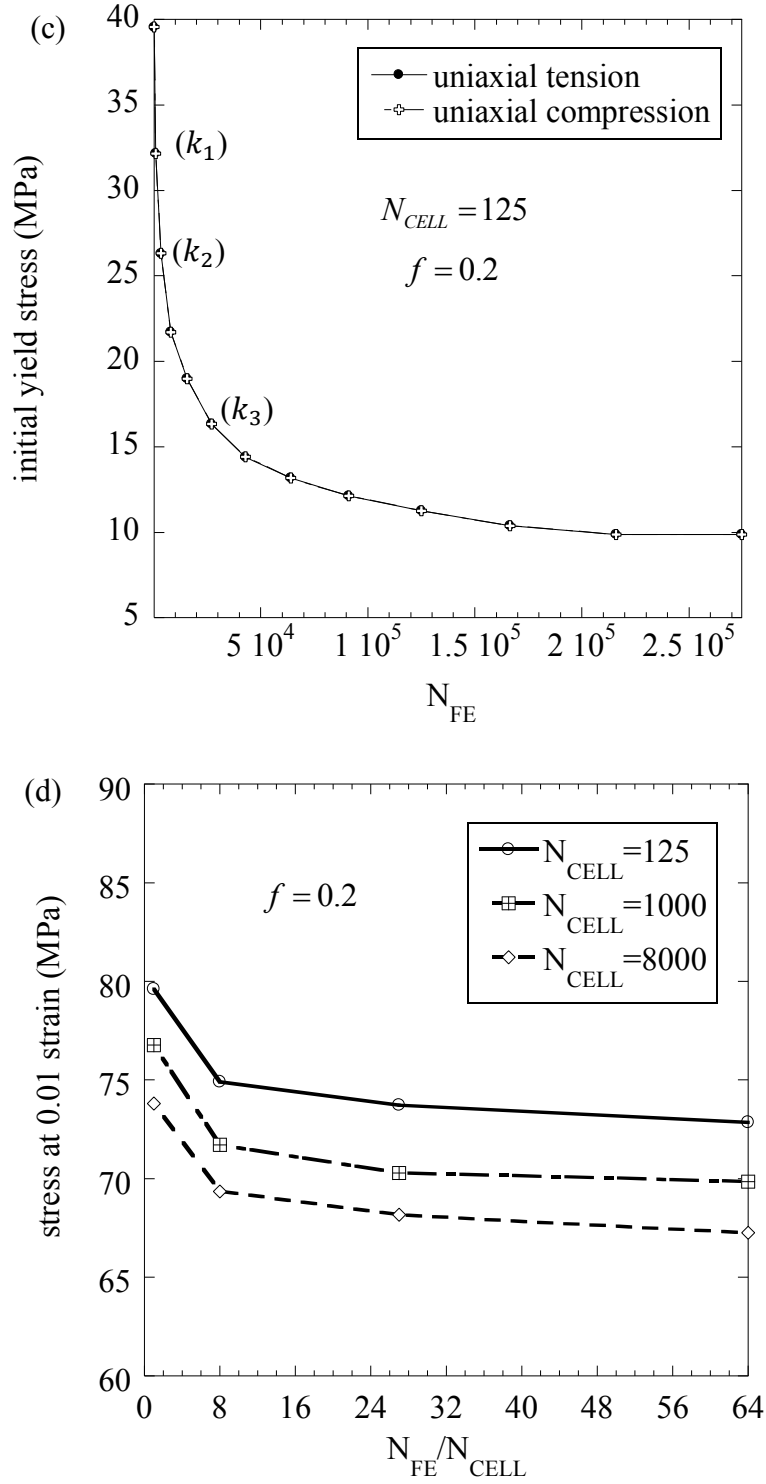


Figure 3.4 (a) Examples of SVEs at increasing N_{FE} , for the choice $N_{CELL} = 125$. (b) Sensitivity of compressive and tensile flow stress at a strain of 0.01 to the parameter N_{FE} . (c) Sensitivity of macroscopic compressive or tensile stress at first yield to N_{FE} . (d) Sensitivity of the compressive strength to N_{FE} / N_{CELL} .

The predicted material strength is found to decrease monotonically with increasing mesh density, although the rate at which it decreases reduces with increasing N_{FE} ; this can be explained observing that progressively refining the mesh allows capturing the high stress concentration around the sharp pores; as the mesh is refined, the maximum values of stress around the pores tend to increase, giving earlier yield. Figure 3.4(c) suggests an effective “stress concentration factor” increasing from around 2.5 to 10 as the mesh is progressively refined.

In Figure 3.4(d) we present predictions of the compressive strength for the choices $N_{CELL} = 125, 1000$ and 8000 and for different mesh densities, N_{FE} / N_{CELL} ($f = 0.2$). It is clear that, for each choice of N_{CELL} , the prediction are scarcely sensitive to N_{FE} for $N_{FE} / N_{CELL} > 64$.

3.3 Results and discussion

We proceed to analyse in detail the predictions, to construct yield surfaces at increasing porosity and to compare our results to those obtained in [61]. Simulations are conducted on ten realisations of the microstructures and average stress versus strain histories are calculated. The parameters N_{CELL} and N_{FE} are chosen to be sufficiently large that predictions are insensitive to them ($N_{FE} / N_{CELL} = 64, N_{CELL} = 1000$). This choice guarantees results independent of size and FE mesh, for all porosities analysed, and a low scatter in the predictions, of order 6%. This RVE contains approximately $2 \cdot 10^5$ degrees of freedom (DOFs). We note here that in the analyses of [61] the predictions became mesh-insensitive only for very large RVEs, corresponding to a number of DOFs of order 10^6 .

We will compare our predictions to corresponding sets of predictions in [61]; these were conducted using meshes with $2 - 6 \cdot 10^5$ DOFs, and gave a scatter in strength of order 5-10%, similar to what found in the present study with a smaller number of DOFs.

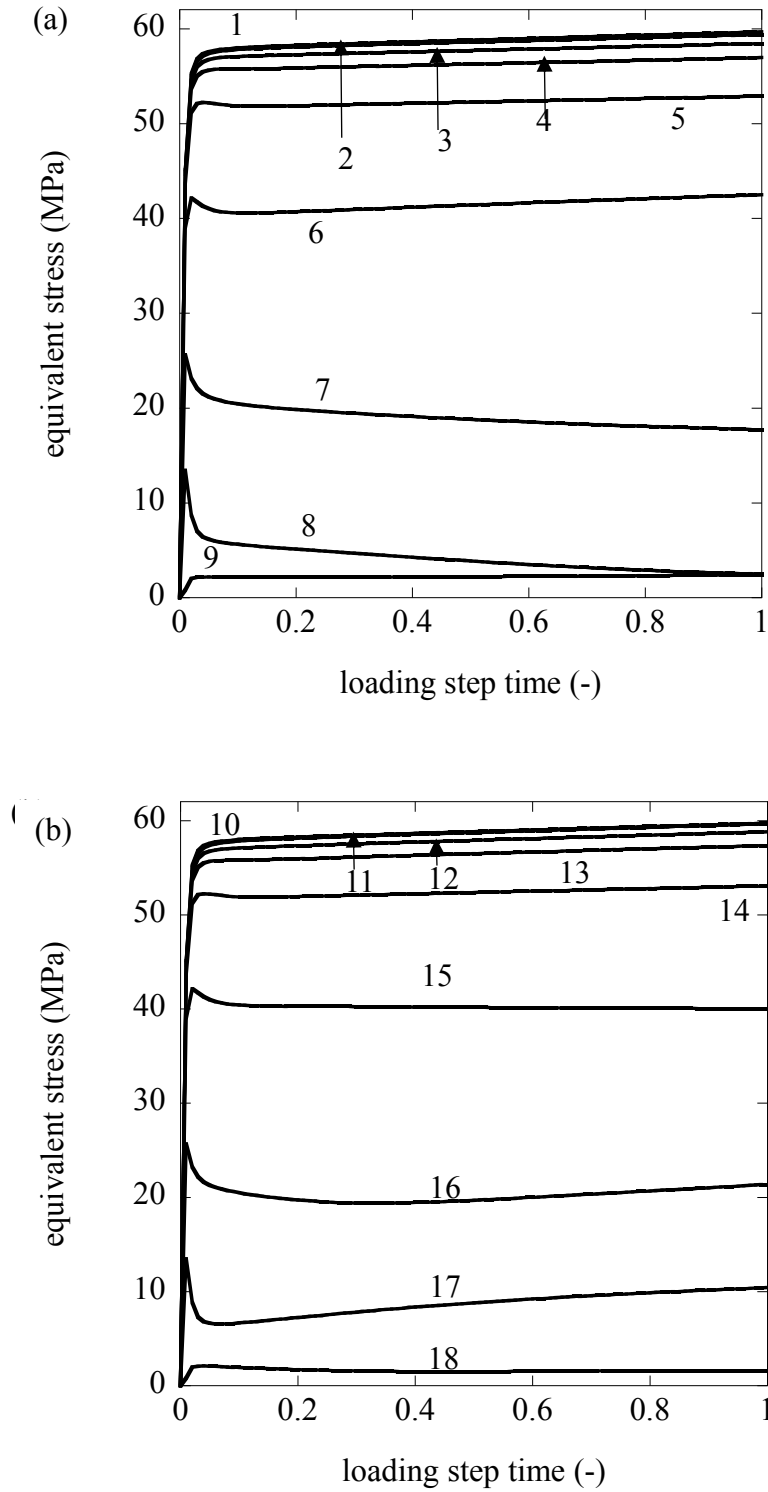


Figure 3.5 (a) Time history of von Mises stress for loading cases 1-9; (b) Time history of von Mises stress for loading cases 10-18.

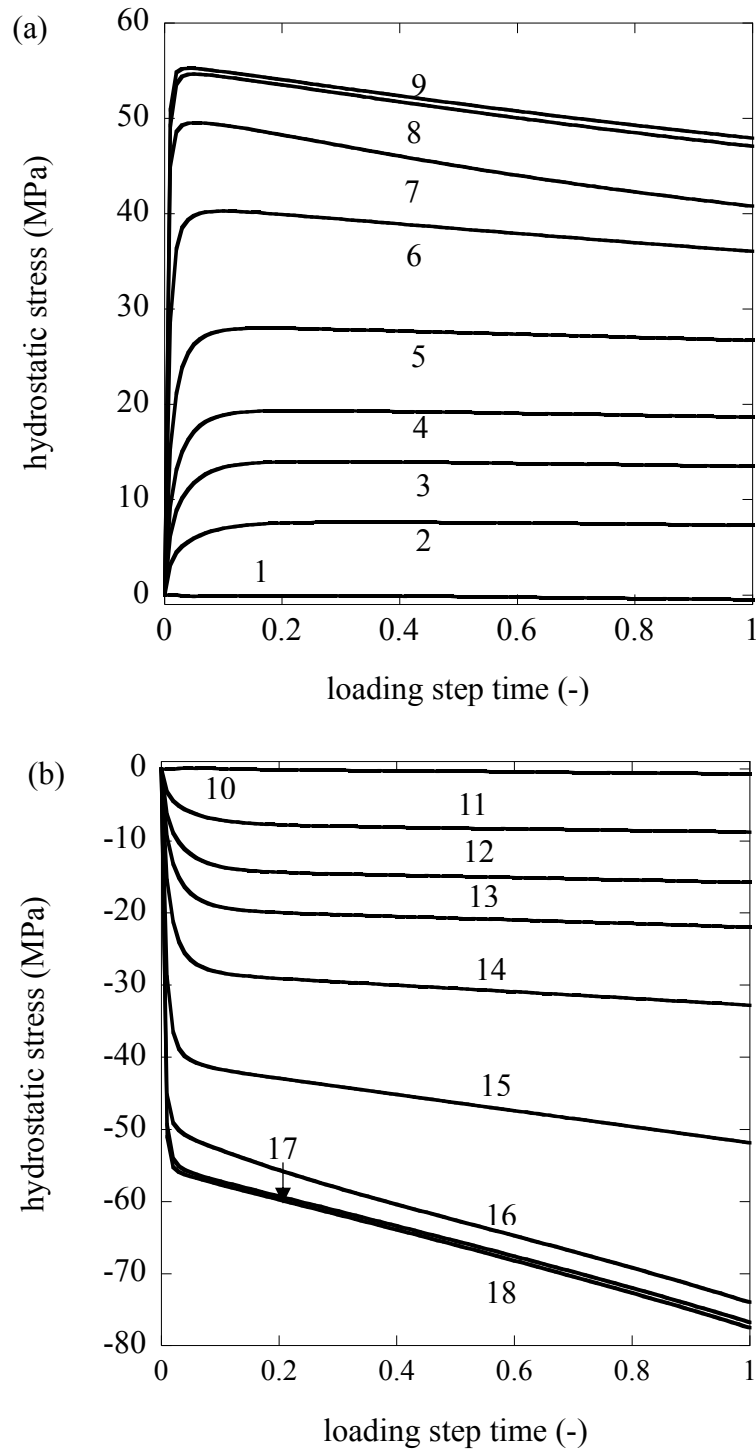


Figure 3.6 (a) Time history of hydrostatic stress for loading cases 1-9; (b) Time history of hydrostatic stress for loading cases 10-18.

3.3.1 Analysis of deviatoric and hydrostatic stress histories

Figure 3.5 (a) and (b) present the time histories of equivalent von Mises stress for loading conditions 1-9 (tensile hydrostatic stress) and 10-18 (compressive hydrostatic stress), and for the choice $f = 0.3$; Figure 3.6 present the corresponding time histories of hydrostatic stress (1-9 for tensile hydrostatic stress and 10-18 for compressive hydrostatic stress). All data in Figure 3.5 and Figure 3.6 were obtained by analysing a single realisation of the microstructure. The porosity was chosen to match the results presented in Fig. 9 of Fritzen et al. [61]. These authors modelled the geometrical details of the material microstructure and predicted a plateau in the von Mises stress history, at strains in excess of a small threshold ($t = 0.2$); we predict very similar histories with our simplified modelling approach, as seen from Figure 3.5. Let us now focus on the histories of hydrostatic stress presented in Figure 3.6. Fritzen et al. [61] again predicted that such histories should display a plateau phase at simulation times in excess of 0.2. We indeed observe this plateau for loading cases characterised by low hydrostatic stress (1-5 and 10-14); in contrast, for loading cases 6-9 and 15-18, associated to high hydrostatic stress states, we observe a strain-hardening or a strain-softening response in presence of high compressive or tensile hydrostatic stress, respectively, as a consequence of the anisotropic plastic deformation of the pores.

3.3.2 Yield surface and strain hardening

In Figure 3.7 we present, for the case $f = 0.3$, the trajectories described by the progressively increasing hydrostatic and equivalent von Mises stress corresponding to each of the 18 loading conditions analysed; we mark, along each of these trajectories, the points that correspond to an equivalent von Mises strain of 0.01 (empty squares) and 0.04 (full circles), to visualise the yield surface (indicated by the dashed lines) and its evolution with continued straining. The results are obtained by averaging the predictions of 10 repeated simulations on 10 realisations of the microstructure.

It is evident that the initial yield surface (at von Mises strain of 0.01) is slightly asymmetric especially for loading cases associated to high hydrostatic stresses. With continued plastic straining the tension/compression asymmetry becomes more pronounced, this is a direct consequence of the strain dependence reported in Figure 3.6(a) and Figure 3.6(b). While the

initial yield point (macroscopic stress at first yield) is symmetric in tension and compression (as shown in Figure 3.3(c) and Figure 3.4(c) and suggested by basic stress analysis), the material develops a tension/compression asymmetry with continued plastic deformation, as shown in Figure 3.7.

The model predicts a pressure-sensitive yield response; the load triaxiality is constant in the elastic regime but as macroscopic plasticity intervenes, elongation of the pores introduces anisotropy and loss of the initial triaxiality. The asymmetry in the yield strength is governed by the change in volume of the pores (positive in tension and negative in compression). In our simulations we do not attempt modelling material damage, however in real porous materials this asymmetry may be accentuated by intervening damage mechanisms.

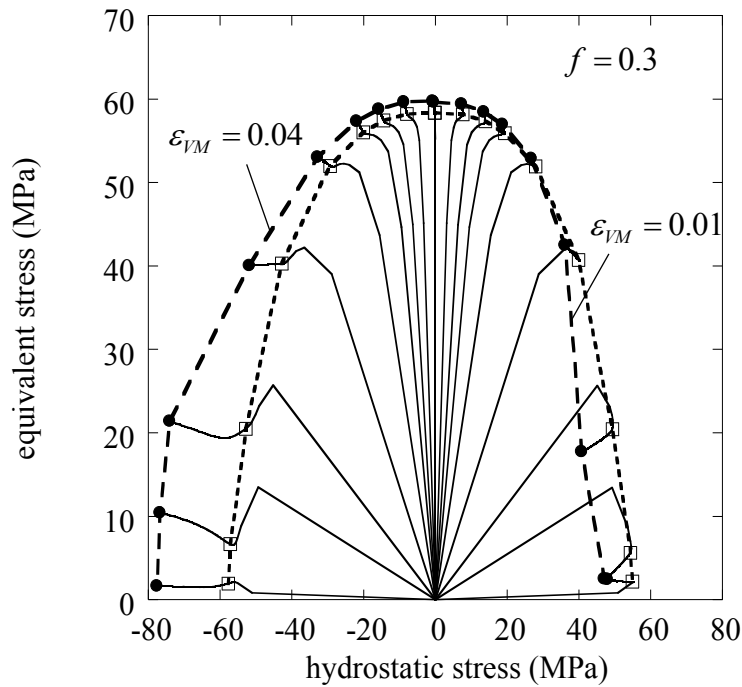


Figure 3.7 Yield surface and its evolution for a 30% porous solid. Squares correspond to an equivalent von Mises strain of 0.01, circles correspond to an equivalent von Mises strain of 0.04.

3.3.3 Effect of increasing porosity on the initial yield surface

In Figure 3.8 we analyse the sensitivity of the initial yield surface to the degree of porosity. Our predictions are compared to those in [61]. We note initially that these authors construct

their initial yield surfaces using the plateau values of hydrostatic and von Mises equivalent stress, and such plateau is achieved at time in excess of 0.2, corresponding to strains of order 0.01. In contrast, in our simulations, the hydrostatic and von Mises stresses did not always reach a plateau phase at a time of 0.2. The predictions presented below are obtained by pairs of hydrostatic and von Mises stress values evaluated at either an equivalent von Mises strain of 0.01 or a volumetric strain of 0.01, whichever occurred first in the simulations. For porosities in the range 0.01 to 0.3, the numerical predictions of [61] are presented in Figure 3.8, fitted by the Gurson-Tvergaard-Needleman (GTN) model [14]; we note that Fritzen et al. [61] only analysed loading cases with tensile hydrostatic stress, however the (symmetric) GTN model is shown also for negative hydrostatic stress. The figure includes predictions obtained with the current modelling approach; clearly, the presented approach matches the yield surfaces predicted by Fritzen et al. [61] for positive hydrostatic stress. In addition, we are able to predict a tension/compression asymmetry in line with experimental observations, see for example [11]. Such asymmetry, as expected, becomes more pronounced as the porosity increases.

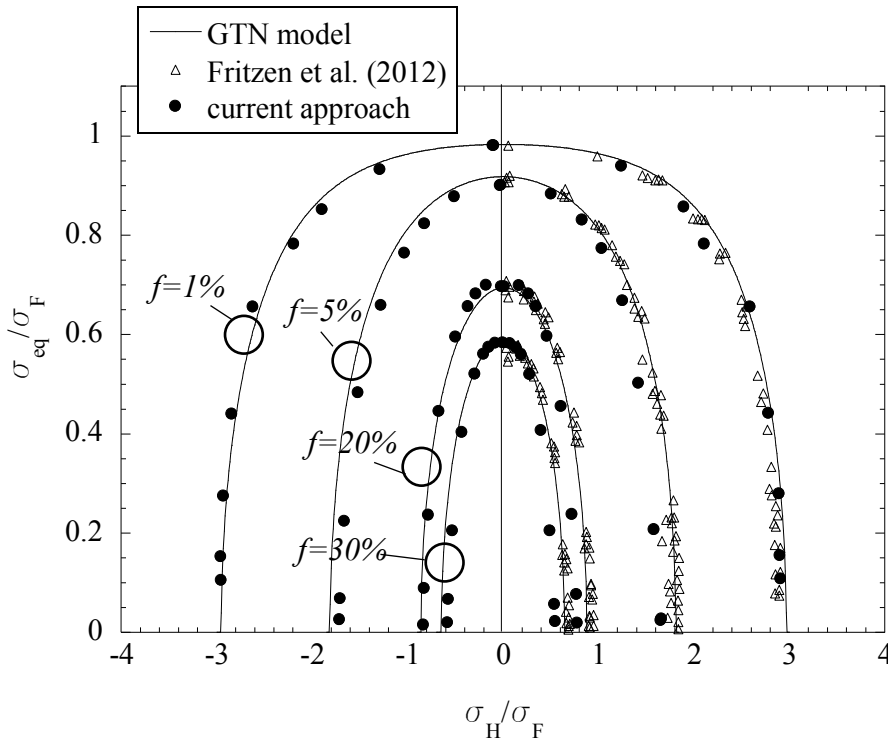


Figure 3.8 Predicted initial yield surfaces at different porosity. Results by Fritzen et al. [61] are fitted by the GTN model and compared to the predictions from the current study. Here, σ_F denotes the yield stress of the parent material.

3.3.4 Uniaxial tensile and compressive response at large strains

To demonstrate the predictive capability of the proposed model at large strains, we show in Figure 3.9 the uniaxial tensile and compressive stress/strain curves for materials of different porosities, up to a large strain. We note that the imposed macroscopic strains are not large enough to trigger pore densification in tension. For very low porosity (0.01), the material response is nearly symmetric in tension/compression and close to that of a perfectly-plastic material, with yield stress just below the yield of the parent material ($\sigma_F = 100 \text{ MPa}$). As the porosity increases, the tensile and compressive responses start diverging with increasing strain, with the compressive response always stronger than the tensile response; such asymmetry is more pronounced at high porosity. In Figure 3.10 we present heavily deformed SVEs obtained from simulations of a porous solid ($f = 0.2$) at a macroscopic tensile or compressive nominal strain of 0.4; the meshes include contours of the equivalent von Mises plastic strain. We observe that in compression some of the pores have completely collapsed, while in tension they have considerably expanded. The irregularity of the geometry results in localisation of plastic strain similar to what reported in [61].

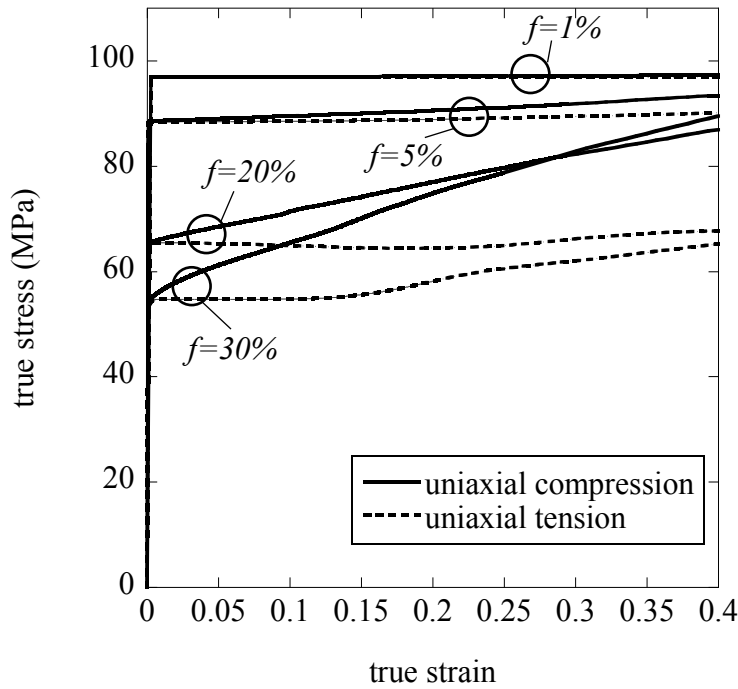


Figure 3.9 Uniaxial tensile and compressive response of a material at increasing porosity.

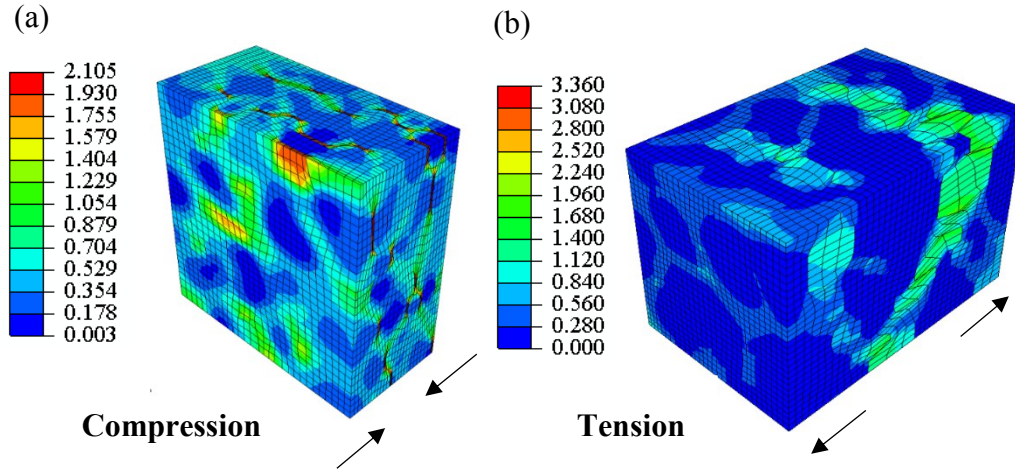


Figure 3.10 Contours of the equivalent von Mises plastic strain for a porous material ($f = 0.2$) subject to a nominal strain of 0.4 in uniaxial compression (a) or uniaxial tension (b).

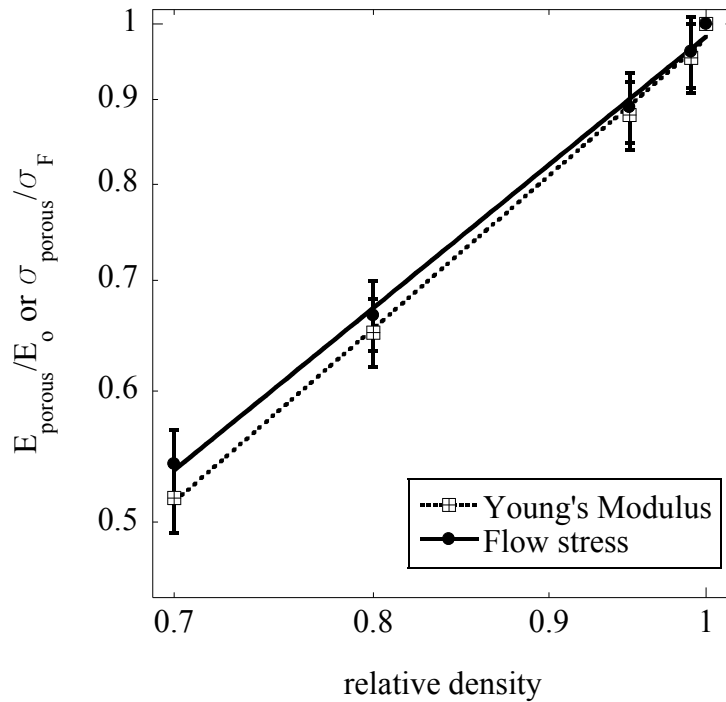


Figure 3.11 Compressive Young's modulus and flow stress at 0.01 strain as a function of relative density.

3.3.5 Scaling of compressive modulus and strength

The compressive data presented in Figure 3.9 is now used to determine scaling laws for the compressive modulus and strength of low-porosity solids. The modulus and flow stress (at a compressive strain of 0.01) are plotted in Figure 3.10 as a function of relative density, $\bar{\rho} = 1 - f$. The figure includes a least-square fit through the data of the power-law expressions

$$\frac{E_{porous}}{E_0} = C_E \bar{\rho}^n; \quad \frac{\sigma_{porous}}{\sigma_F} = C_\sigma \bar{\rho}^m \quad (3.1)$$

which provided $C_E = 0.98$, $n = 1.81$, $C_\sigma = 0.98$, $m = 1.69$ (with residuals of order $R = 0.998$). Power-law scaling of the strength and modulus of low-porosity metals has been reported in several experimental studies by several authors, for example in [167-170]. Typical values found in literature are $C_E = C_\sigma = 1$, $n = 1-3$, $m = 1-2.5$; the proposed models therefore predict reasonably well the scaling of compressive stiffness and strength with relative density.

3.4 Concluding Remarks

We attempt modelling the multi-axial elasto-plastic response of solids of moderate porosity by a micro-mechanical approach. The material is treated as a two-phase composite comprising an incompressible elasto-plastic solid and voids. The voids are modelled as plastically compressible solids of negligible stiffness and strength, but including a strain-locking behaviour at high strains to simulate self-contact of the pore. We explore the mesh dependence of the predictions and determine the minimum size of an RVE. Predictions are in agreement with the results of previously published studies in which the geometrical details of the pores were explicitly modelled, as a random array of identical spherical voids. The main conclusion are as follows:

- The proposed modelling approach is computationally efficient and able to predict the elasto-plastic response of ductile solids of porosity in the range 0.01-0.3.
- The model yields predictions nearly identical to those of more detailed simulations which account explicitly for the geometry of the microstructure [61] and for this reason need to use substantially more degrees of freedom. The effectiveness of the simple proposed approach confirms that the details of pore shape and pore size distribution have only a minor effect on the response of porous ductile solids, while the overall porosity has the most prominent effect (for $f = 0.01-0.3$).
- The models predict that the onset of plasticity is symmetric in uniaxial tension and compression, but porous solids rapidly develop a tension/compression asymmetry with continued plastic deformation; this is mainly due to the different macroscopic hardening displayed by the material in uniaxial tension and compression.
- The models correctly predict scaling laws for the Young's modulus and yield strength of porous solids.

3.5 APPENDICES

APPENDIX A

Algorithm I

1. *Initialise and define parameters for domain:*

- Relative density for material $\bar{\rho}$
- Number of cells in x, y and z coordinate directions ($n_{lex}, n_{ely}, n_{elz}$)
- $\mathbf{E}$, the matrix of dimensions $\mathbf{E}$ ($n_{lex}, n_{eley}, n_{elz}$). This matrix assumes a value of 0 for solid and 1 for void.
- Degree of numerical sub-discretisation given by parameter ns in each coordinate direction.
- Global cell counter, $counter=0$.

2. *Sweep through entire 3D domain, cell by cell, using a uniform random variable to determine if a void or metal (solid) phase is assigned to each cell:*

WHILE $counter \leq n_{lex} \times n_{eley} \times n_{elz}$

- Draw a random number from a standard uniform distribution, $R \sim U(0, 1)$, and if $R < \bar{\rho}$, THEN assign a solid element, ELSE assign a void.

3. *Sub-discretise the cell into $p \times p \times p$ finite elements:*

- The new global element number, e , for elements of the sub-discretised mesh are given by

$$e = i + (j - 1)n_{lex} \cdot p + (k - 1)n_{lex} \cdot n_{eley} \cdot p^2 + (ii - 1)p + (jj - 1)p^2 \cdot n_{lex} + (kk - 1)p^3 \cdot n_{lex} \cdot n_{eley} \quad (A.1)$$

where i, j, k are the local coordinates within the cell and ii, jj, kk are the global coordinates within the domain.

4. ABAQUS input file:

Assign each cell an element set '*Elset' for the ABAQUS input deck file. This also meant that corresponding '*Solid Section' and '*Material' definitions for each element set specifying the deterministic/randomised material properties were outputted by the algorithm.

Flow chart of Algorithm I is shown in Fig. A.2.

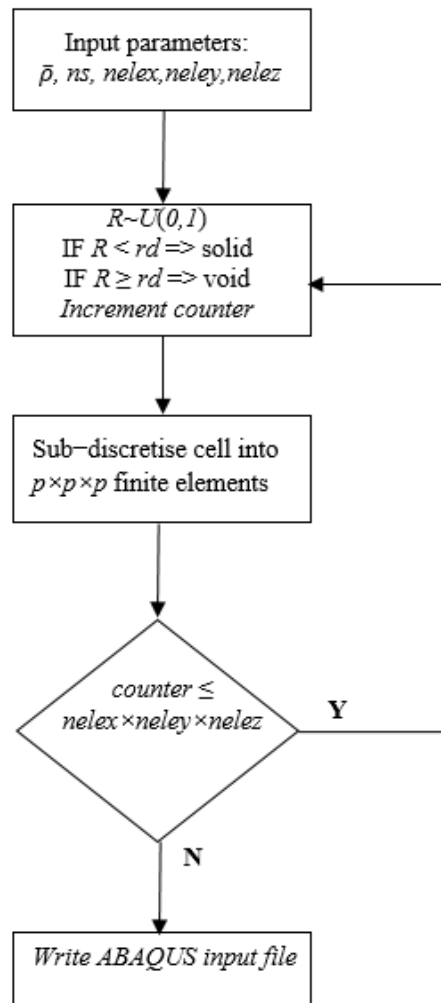


Figure. A.2 Flow chart for Algorithm I.

CHAPTER 4

MODELLING THE MECHANICAL RESPONSE OF CELLULAR SOLIDS MADE FROM SINTERED TITANIUM POWDERS

ABSTRACT

Two algorithms are developed to generate virtual microstructures of Titanium foams of medium relative density, in the range 0.37 – 0.48; one of the algorithms captures the effect of pore shape and size distribution, while the other algorithm only accounts for the relative density of the material. Foams are modelled as two-phase composites consisting of a solid material and voids; the elasto-plastic and damage response of the parent material is deduced from its measured mechanical responses in tension and compression, while the material occupying the voids is assigned a plastically compressible constitutive response, to mimic the effects of pore collapse and subsequent self-contact. Finite Element (FE) simulations are conducted to predict the measured macroscopic material response in uniaxial tension and compression, as well as in pure shear; a mesh convergence study is performed and the minimum RVE size is determined. The simulations are found in good agreement with measurements and can predict accurately and effectively the material's mechanical response up to large strains, as well as the scaling of mechanical properties with relative density.

4.1 Introduction

Metal foams are widely used in a variety of applications including the aerospace, automotive, naval, defence and medical industries due to their low specific weight and high energy absorption capacity. Numerous authors have conducted modelling work on the response of these materials, adopting both phenomenological and micro-mechanical approaches. Previously published phenomenological modelling work attempted describing the macroscopic material response using appropriately calibrated homogeneous constitutive models, such as Deshpande and Fleck [15]. A comparison of several phenomenological models for metal foams is provided in [171]. This approach requires extensive testing of the material and neglects heterogeneity and strain localisation, which may lead to fracture.

Several authors provided estimates of the elastic properties and strength, or constitutive equations for different types of foams by micromechanical approaches, as in [133, 135]. Other authors analysed the mechanical behaviour of simplified structure cells representative of different types of foams and derived analytical predictions of the elastic and plastic properties, reported in [172, 173].

The response of metallic foams is strongly dependent upon its relative density; as these materials are attractive for their low weight, much of the research has focussed on foams of very low relative density, while relatively less research exists on foams of medium density, like those examined in this study. Irrespective of the density, the microstructure of foams is highly irregular and several studies have attempted determining the effect of geometric and material randomness upon the macroscopic response, with the aid of stochastic FE simulations or analytical models.

For foams of very low density, several micromechanical modelling approaches were conducted; for example Schraad and Harlow [174] investigated the compressive response of random cellular materials up to high strains, considering the ensemble average of the response of a random cell, providing a non-linear mechanical response specifically devised to represent the macroscopic effects of plastic collapse and densification. In [175, 176] unit-cell models were employed to predict the yield surface or the compressive stress-strain behaviour by

incorporating periodic boundary conditions. In [177] the surface evolver technique was employed, on models of different sizes to predict the crushing behaviour of open cell low-density foams with ligaments modelled by beam elements. In [178], again investigating a light open-cell foam with $\bar{\rho} = 0.08$, contact between the ligaments was also explicitly modelled. Similar stochastic FE models were presented by other authors, see for example [179]; the geometry was generated via 3D Voronoi tessellations and FE simulations were used to predict the macroscopic elastic response. In [180] virtual foam microstructures were generated using Voronoi tessellation in Laguerre geometry. Repeated FE simulations were performed on small-scale models (or “testing volume elements”), similar to [181, 182]. In [180] the parent solid was meshed by shell elements and the elastic response of solid foams of density $\bar{\rho} < 0.2$ was predicted; later in [183] the predictions were extended to the post-yield response

Generation of virtual, but realistic foam microstructures of porous metals of high relative density has been performed by several authors such as in [54, 61, 66]. These authors used arrays of mono-disperse spherical or cubic voids in a solid matrix and performed Monte Carlo analyses to determine the macroscopic response of statistical volume element (SVE). Their approaches modelled the parent material by continuum elements, but the predictions were limited to low strain, due to lack of appropriate contact algorithms.

Other researchers investigated the response of low density foam microstructures by performing X-ray tomography on material samples, meshing the scanned geometry and performing FE analyses on several porous solids, in order to predict their compressive response [184-186]. These approaches were computationally expensive, due to the geometric complexity demonstrated by real materials.

Relatively little research was conducted on foams of medium relative density, such as those investigated here. Recent studies by our research group [75, 187, 188] focussed on predictions of the response of the same Titanium foams examined in this study. Virtual foam geometries were generated based on a Voronoi tessellation, to obtain virtual microstructures very close to those observed by X-ray tomography. FE simulations were conducted on small SVEs of the foam and meshed with solid elements; these SVEs were subjected to loading of different

triaxiality and up to high strains, in order to obtain the yield surface and examine its evolution under increasing strain. The response of the parent material was calibrated against compression tests, absent any damage model, and self-contact algorithms were implemented to capture self-contact of the pore walls upon collapse at large macroscopic strains. The contact models made the simulations computationally intensive, such that only small SVEs (cubes of side length of approximately 1 mm) could be analysed, and consequently the scatter in strength predictions was high (of order 100%). In addition the simulations could predict the compressive response to reasonable accuracy but largely over-predicted the measured tensile and shear responses.

In this chapter we focus on materials with medium relative density and present a modelling approach that does not necessitate self-contact algorithms to model the pore closure (with the objective of reducing the computation power), and we introduce damage in the response of the parent material to increase the accuracy in predictions in comparison to those such as in [75]. We propose two algorithms to generate virtual microstructures of the foam examined; the first algorithm is capable of modelling the material's average porosity, while the second algorithm also captures the effects of the pore size distribution and of irregular pore shapes. The material is treated as a two-phase composite comprising solid Titanium (modelled as a von Mises elastoplastic solid with continuum ductile damage) and a fictitious, plastically compressible, 'pore' material which mimics the effects of pore collapse and subsequent self-contact, avoiding the explicit use of contact models in the simulations.

The structure of the chapter is as follows; in Section 4.2 we describe the material investigated and summarise the measurements performed. In Section 4.3 we present the algorithms to generate the material microstructure and provide details of the numerical simulations. Results are discussed in Section 4.4. In Section 4.5 we outline the main conclusions of this chapter.

4.2 Materials and Methods

4.2.1 Materials

The Foam that is examined in the current chapter is made from sintered powders by using a foaming agent and a polymeric binder. Additional information regarding the manufacturing of the foam is provided in [189]. To summarize the manufacturing method, a pure Ti powder was mixed with a foaming agent and a polymeric binder to produce a dry mixture. When a low heat was applied to the polymeric binder it started to foam, once the heat was increased pyrolysis of the binder was achieved. Finally, once the heat was increased even further, sintering of the metallic powder was completed.

Figure 4.1 shows optical micrographs of a foam of medium relative density 0.42, at different magnifications. It can be seen that the material comprises large pores, of diameter of order 100 μm , forming an irregular porous structure. The solid fraction of this foam is made from sintered powder particles of approximately spherical shape and initial size of order of few microns; incomplete sintering of such powder particles causes a secondary micro-porosity in the material, with pores of diameter of around 10 μm . In this chapter we examine the response of the parent material (sintered Titanium, of relative density of 0.95, made by sintering Titanium powder in absence of foaming agent and polymeric binder) as well as that of foams of different relative densities, obtained from this parent material by sintering in presence of a foaming agent and a polymeric binder.

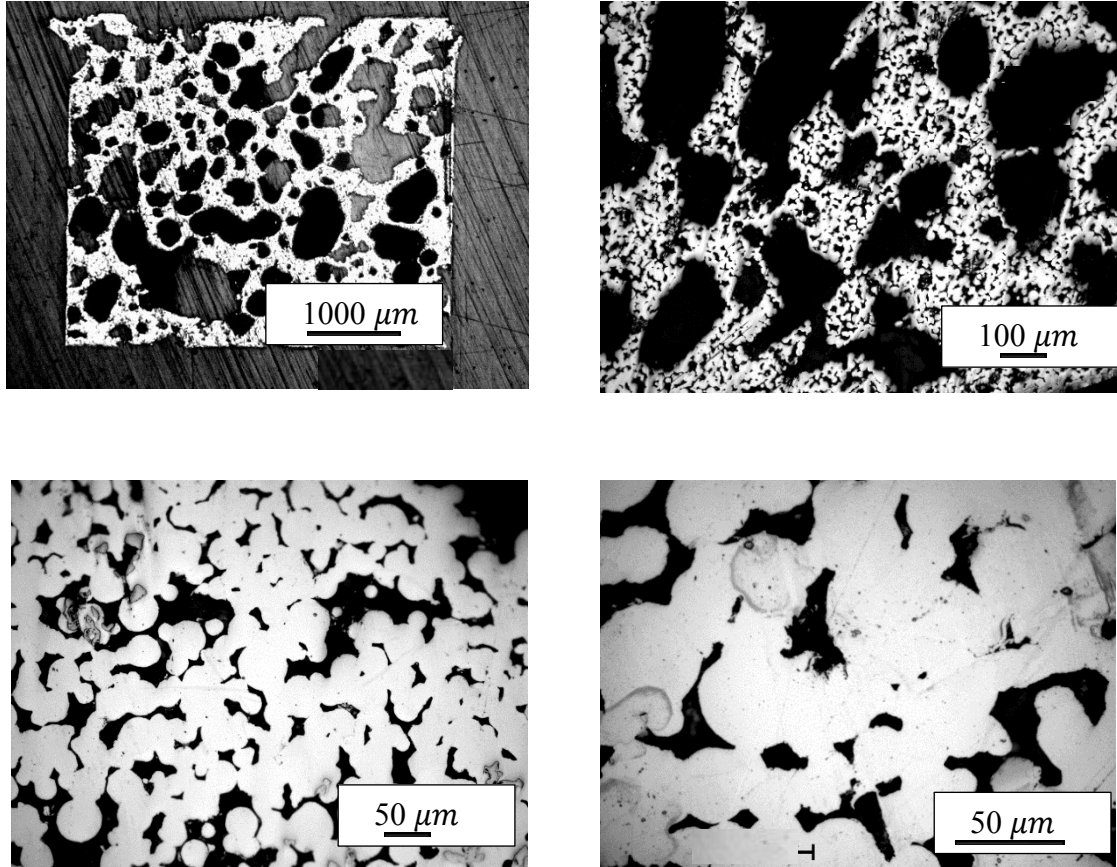


Figure 4.1 Optical microscope images of a titanium foam with $\bar{\rho} = 0.42$, at four different magnifications.

The material possess a cellular structure comprising arrays of pores and relatively large region of fully-dense solid, connected by relatively thinner and irregular ligaments. It is clear from Figure 4.1 that the parent material cannot be modelled effectively by arrays of shell and beam elements due to its irregular geometry, which suggests a continuum-type modelling approach for these medium density foams.

4.2.2 Mechanical tests

In order to measure the compressive response of foams and parent material uniaxial quasi-static compression and tension experiments were conducted. For the compression experiments cylindrical specimens of 11mm diameter and 13mm height were employed. A laser extensometer was used to measure the deformation in the direction of loading, whereas the lateral deformation was measured using a video camera via digital image correlation. The compressive force was measured using a resistive load cell. For the tensile experiments dog-bone specimens of 8mm gauge length, 5mm width, 5mm thickness and 12mm shoulder radius were employed. Deformation was measured by a high resolution camera using image analysis. In addition, to measure the lateral deformation a laser extensometer was also used. The tensile force was measured using a resistive load cell. Shear experiments were performed by Siegkas et al. [75] on a foam of relative density 0.37. The shear experiment is described in [75].

Figure 4.2 presents representative stress versus strain histories for a foam subject to tension, compression and shear deformation. The response was initially elastic, followed by a strain hardening phase; the material displayed a ductile response in compression but was brittle in shear and tension, fracturing in both cases at strains less than 1%. In compression, formation of micro-cracks was observed for strains higher than 0.2; while in tension, *in-situ* tests revealed formation of micro cracks at strains of less than 1%, typically initiating at the voids . The tensile, compressive and shear tests were repeated 3 times and the scatter in strength was of 7% in compression and 15% in tension and shear.

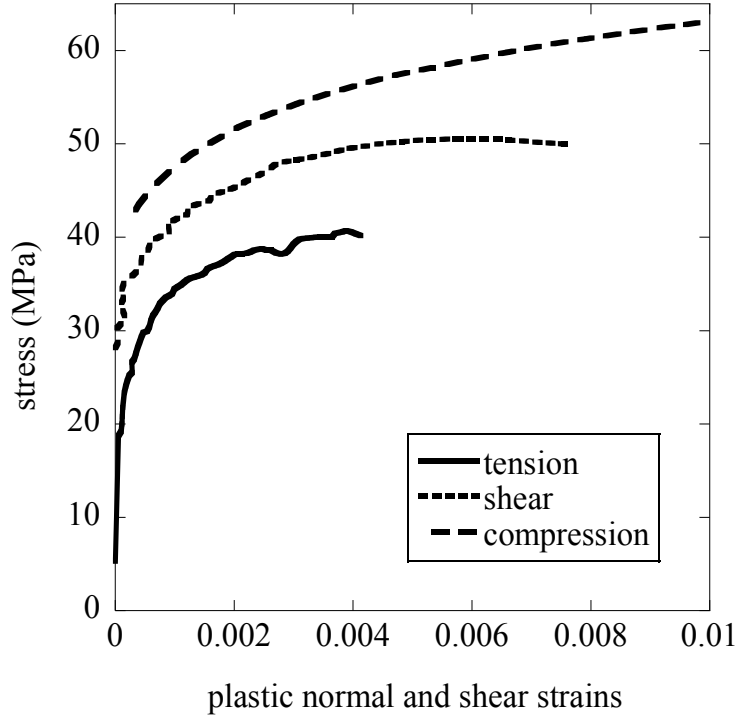


Figure 4.2 Measured responses of titanium foam ($\bar{\rho} = 0.37$) in uniaxial tension, compression and shear.

Figure 4.3 presents the response of the Titanium parent material in uniaxial tension and compression, in term of true stress versus true plastic strain histories. We note that only the information in these tests was used to calibrate the constitutive models used in FE simulations. The material responds in both tension and compression with an elastic behaviour (Young's Modulus 100 GPa, Poisson's ratio 0.1) followed by pronounced strain hardening; the tensile and compressive responses diverge at plastic strains in excess of 0.003; from this point on, the compressive response is stronger than the tensile response. In compression the test was terminated at a total strain of 0.3, while in tension the specimen fractured at a strain of order 10% in a brittle fashion, by propagation of a crack perpendicular to the loading direction. The repeatability of the flow stress in these tests was within 3% in compression and 5% in tension.

It is well known that metallic alloys display a symmetric response in tension and compression, and it is also accepted that porous metals may display a tension/compression asymmetry, due to the details of the plastic deformation mechanisms induced by the pores; however, the asymmetry observed in Figure 4.3 is too large to be due to the plasticity only, considering the small porosity of only 5%. This indicates that the observed tension/compression asymmetry may be due to damage mechanisms activated in tension but not in compression.

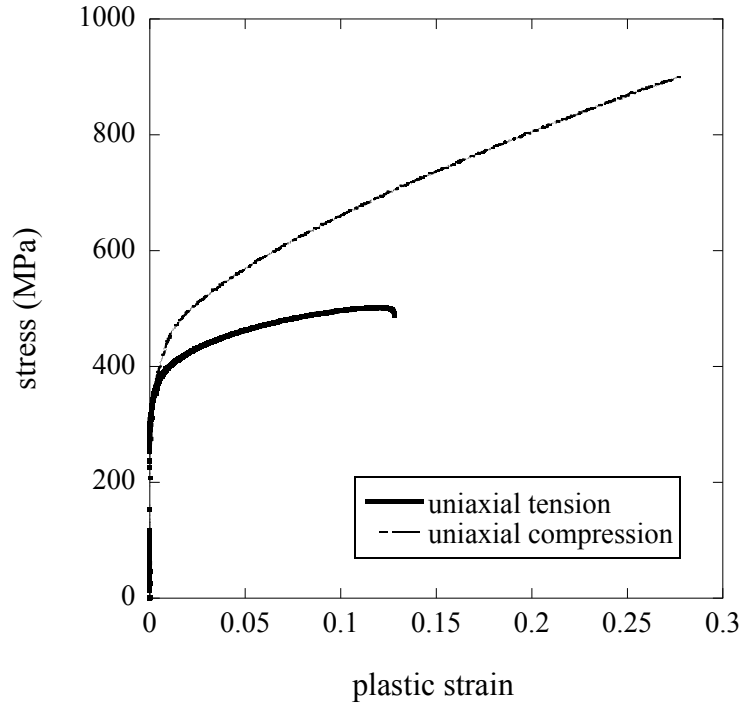


Figure 4.3 Measured stress-strain response of the parent material ($\bar{\rho} = 0.95$) under uniaxial tension and compression.

In order to shed light on such hypothesis, optical microscopy was conducted, as shown in Figure 4.4. Figure 4.4(a) presents optical micrographs of the as-received material at different magnifications. At each magnification it is possible to observe an initial porosity of approximately 5%. Figure 4.4 (b) shows a micrograph conducted on a polished portion of a tensile specimen after final fracture, such that the material shown has undergone a macroscopic tensile plastic strain of order 0.1; it is clear that voids have grown substantially, such that the porosity of the material has increased to around 15%. Analysis at greater magnification showed that micro-cracking at the sintering necks and material plasticity were the primary mechanisms to drive pore growth in presence of tensile stress. In Figure 4.4(c) we present micrographs of the material after a uniaxial compression test, such that the material has experienced a macroscopic plastic compressive strain of order 0.2; the compressive deformation has induced plastic collapse of many of the pores, such that the material now appears to have porosity of order 1%. In-situ SEM observations showed that fracture mechanisms also intervene in compression but only at strains in excess of 0.2. These observations suggest a different micromechanical behaviour in tension and compression, as it is common for porous metals.

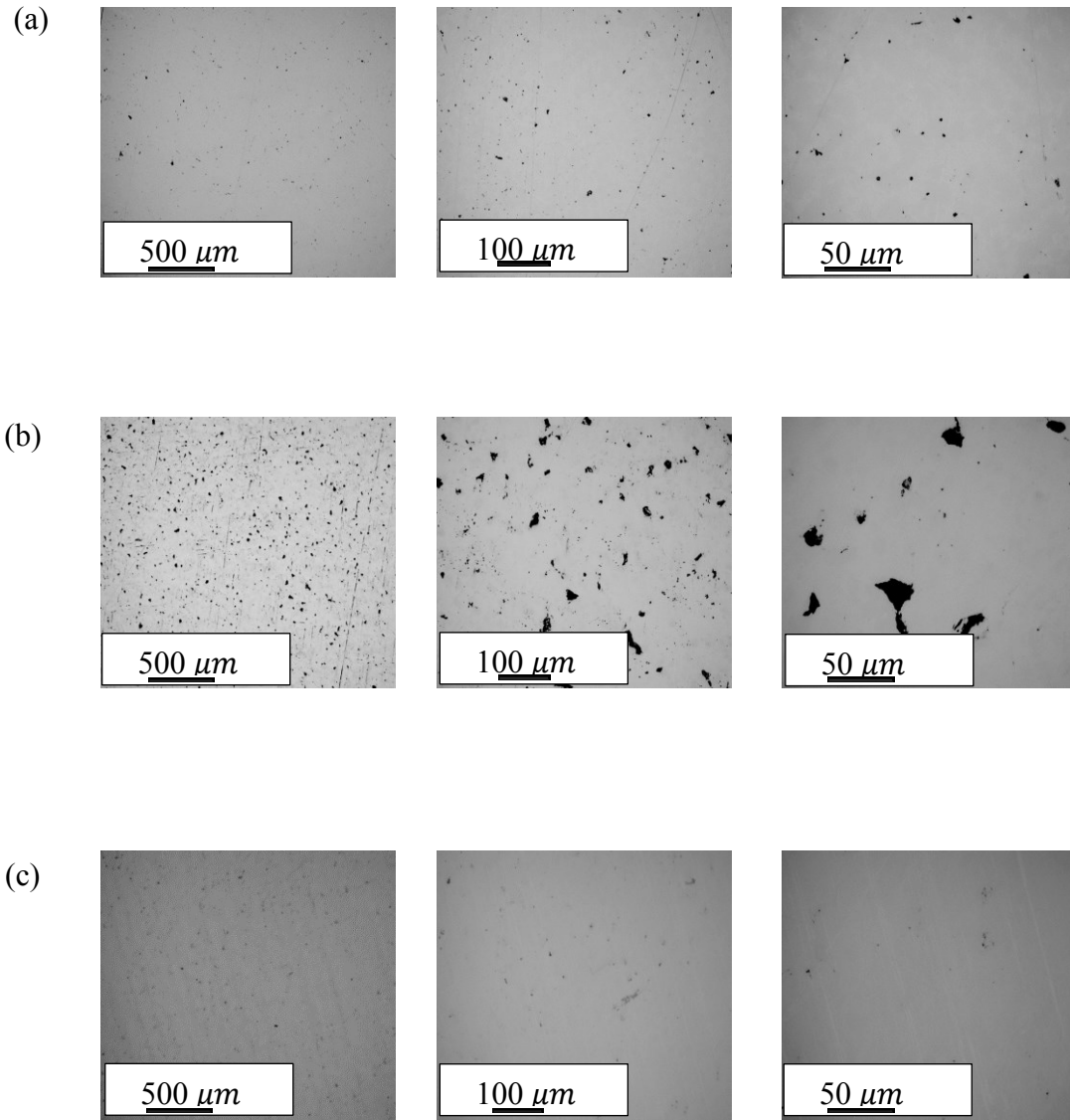


Figure 4.4 Optical microscope images of parent material at three different magnifications. (a) Untested specimen; (b) Specimen having experienced a macroscopic tensile plastic strain of 0.12, and (c) Specimen after compressive plastic strain of 0.2.

To further investigate the differences in the compressive and tensile responses of the parent material, this was tested, in both tension and compression, using a special test protocol, aimed at measuring the material stiffness as a function of the imposed macroscopic strain. This involved super-imposing to the monotonic loading of the specimen a series of N unloading/reloading cycles of strain amplitude chosen to ensure that loading and unloading occurred at the same strain rate (this was chosen to be 0.0002 s^{-1} ; N was typically 7 loading/unloading cycles for each 1% increment in total strain). The corresponding measured responses were very close to those obtained by simple monotonic loading, apart from the presence of the unloading/reloading cycles. A numerical algorithm was developed to extract

the unloading material stiffness at different strains; this information is presented in Figure 4.5 for tension and compression.

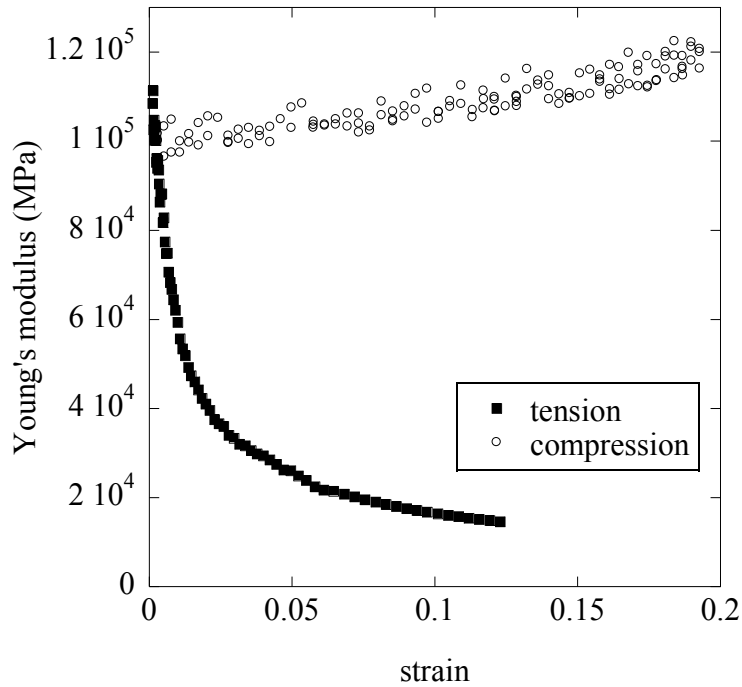


Figure 4.5 Young's Modulus as a function of total strain for repeated unloading/reloading tension and compression tests of the parent material.

In compression, the stiffness is insensitive to strain until the imposed plastic strain exceeds the value 0.1, after which closure of the small pores results in a slight material stiffening. In tension, in contrast, the modulus decreases monotonically with strains when these exceed a value of approximately 0.003. Such reduction is a consequence of both pore cavitation and nucleation and growth of micro-cracks, also observed in *in-situ* tests. Figure 4.6 reports SEM micrographs of the tensile fracture surface of the parent material; a large porosity and evidence of pore growth and coalescence is observed.

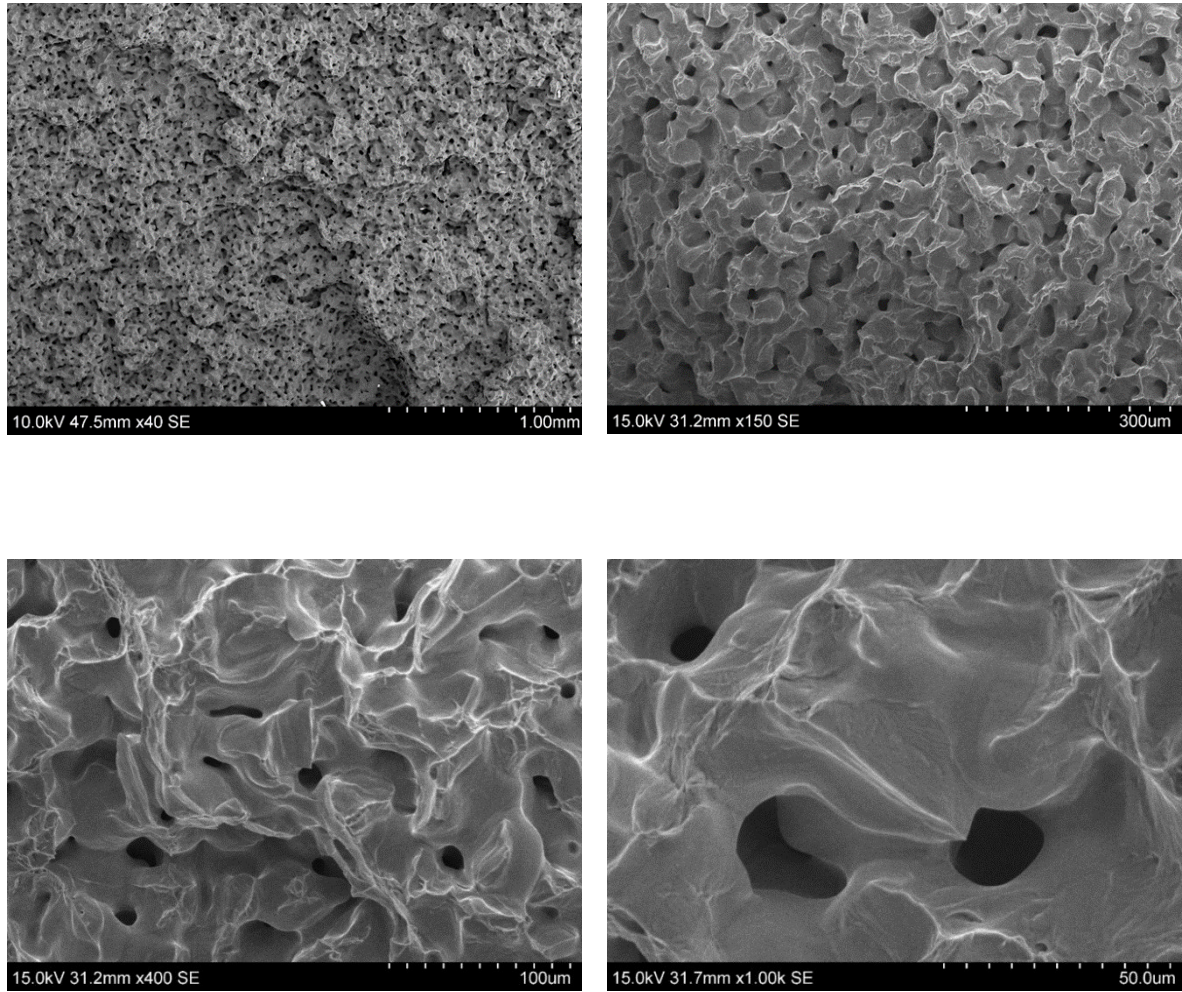


Figure 4.6 SEM images of a fracture surface of the parent material after tensile failure, at four different magnifications.

4.2.3 X-ray tomography

X-ray tomographic scans were conducted on selected foam specimens (small cubes of side length 5 mm) to deduce the distribution of pore size and observe the geometric features of the material microstructure. An example of the measured cumulative pore distribution is given in Figure 4.7 for a foam of relative density 0.42. This data is used as an input for the generation of material microstructures in FE simulations, described below.

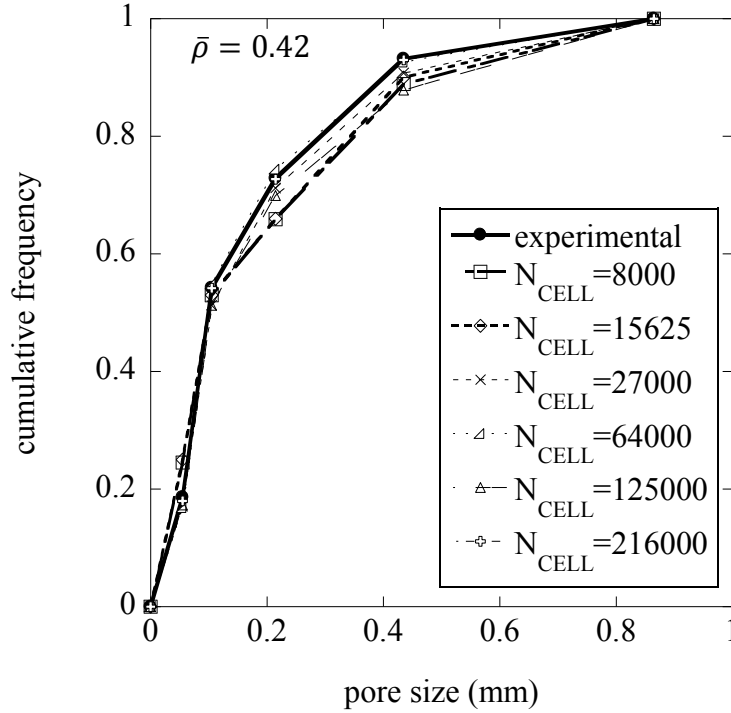


Figure 4.7 Comparison of measured and virtual (Algorithm II) cumulative pore size distribution for a titanium foam with $\bar{\rho} = 0.42$. The effect of number of cells on virtual pore size distribution is shown.

4.3 Numerical Methods

4.3.1 Generation of foam microstructures

In our previous modelling attempt of this material [75], we constructed virtual foam microstructures by making use of a Voronoi tessellation of the specimen's domain. This resulted in microstructures very similar to the real ones, which were observed via X-ray tomography. In this study we follow a different modelling strategy; rather than pursuing microstructures representing all the geometric features of the real material, we focus on modelling effectively the physical mechanisms which control deformation of the material, namely pore collapse, emergence of damage in the presence of tensile stress components, and densification at high compressive stress. Two different algorithms are implemented to describe the foam microstructure and examples of two realisations obtained via these two algorithms are given in Figure 4.8(a) (white elements represent the pores while green elements represent the parent material). Neither of the two algorithms imposes geometrical periodicity on the microstructures generated.

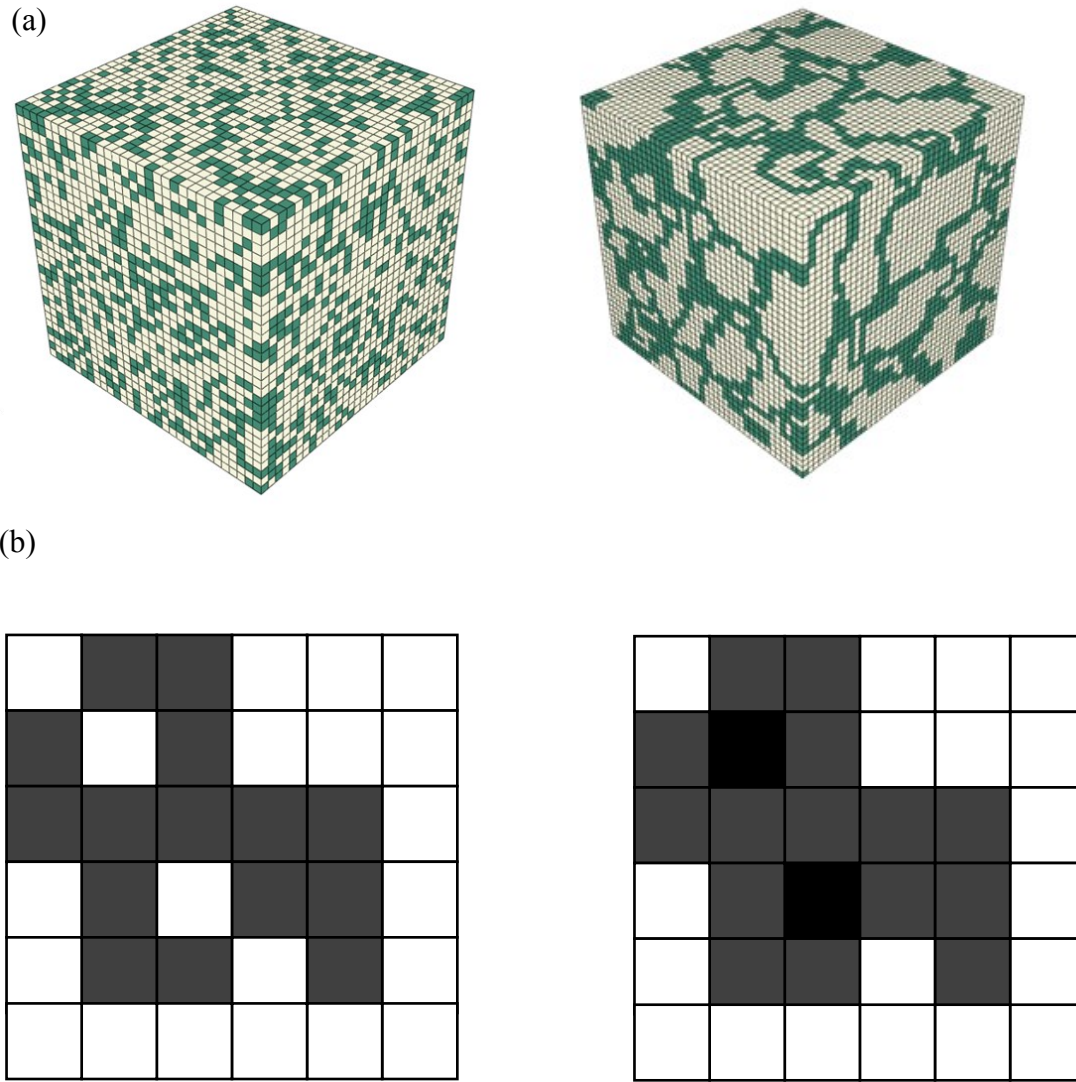


Figure 4.8 (a) Representative microstructures obtained via Algorithm I (left) and Algorithm II (right) for a foam of relative density 0.42. (b) Schematics of removal of isolated solid material.

4.3.1.1 Algorithm I

This algorithm can capture the effect of porosity on the mechanical response of the material, under the hypothesis of pores of equal size. Cubic foam specimens are considered and discretised into cubic cells by a uniform tessellation. The volume of cells, V_{CELL} , is considered as a variable and simulations are repeated at different values of V_{CELL} , to determine the sensitivity to this parameter. Some of the cells are randomly chosen to represent the parent

material of the Ti foam, while the remaining cells are flagged as pores and their constitutive response is chosen to mimic the behaviour of the pores; the volume fractions of solid cells and pores are dictated by the relative density of the foam examined. Each cell was assigned the status of ‘solid element’ or of ‘pore element’ by generation of a pseudorandom number from a uniform distribution. It is possible that this algorithm results in adjacent cells being flagged as pores, resulting in the fact that not all pores have cubical shape. Further details of the Algorithm I can be found in APPENDIX A in Section 3.5.

4.3.1.2 Algorithm II

This algorithm aims at capturing not only the material porosity but also the distribution of pore size and the irregular pore shape. Again, a solid cubic volume is discretised into small cubic cells by a regular, arbitrary tessellation. The total volume occupied by pores, V_p , is obtained from the specimen volume V and its relative density $\bar{\rho}$ as $V_p = (1 - \bar{\rho})V$. The cumulative distribution of pore size is now considered (see for example the distribution shown in Figure 4.7 for a relative density of 0.42); the range of possible pore sizes is divided into a discrete number of bins (typically 5), following which it is possible to calculate, for each bin (index i), the fraction of pore volume having a certain pore size, $V_{pi} = p_i V_p$. Knowledge of the average pore volume V_i allows calculation of the number of pores (of each size) to include in the microstructure, i.e. $N_{pi} = V_{pi} / V_i = p_i (1 - \bar{\rho})V / V_i$.

Each pore is then sequentially included in the microstructure, starting from the largest and then progressively moving to the smaller pore sizes. In order to obtain pores of random shape, each pore originates at a random cell, chosen as a seed point; subsequently, the pore is grown around this cell, occupying adjacent cells; this growth process is based on a random walk originated at the seed cell; we note that only horizontal and vertical movements are possible for this random walk. By this process closed-cell or open-cell geometries can be produced. Further details of the Algorithm II is in APPENDIX A in Section 4.6.

The material under investigation possesses a porous structure with a non-uniform degree of percolation; in this study however we choose to represent the material microstructure as closed-

cell. Pores of arbitrary shape and prescribed volume are progressively inserted into the microstructure; in order to preserve the overall value of relative density and the distribution of pore size, a criterion of non-coalescence is enforced between the pores. This results in a closed-cell foam microstructure; we expect that the assumed absence of percolation in the pore network will have negligible effects on the predicted mechanical response. Due to the non-coalescence constraint, it is possible that a certain pore cannot grow to the desired size; if this is the case, the algorithm grows the pore as much as possible and then moves to the next pore.

In the process of pore growth it may occur that solid cells are generated in positions such that they are surrounded by cells flagged as pores, as illustrated in Figure 4.8(b) (left); as these isolated solid cells would not participate in the mechanical response of the material, when this is detected these cells are removed and flagged as pore material (as shown in Figure 4.8(b) - right). If, at the end of the pore generation phase, the relative density does not achieve the target value, the entire process is repeated until the target relative density is achieved to within a certain threshold.

For sufficiently high values of the ratio $N_{CELL} = V / V_{CELL}$ it is possible to model the actual distribution of pore size; Figure 4.7 shows that, for a relative density of 0.42, the accuracy with which Algorithm II captures the measured pore distribution increases with increasing number of cells. When $N_{CELL} = 64000$ or greater, the pore size distribution achieved by Algorithm II nearly coincides with the measured one.

4.3.2 Constitutive models

4.3.2.1 Constitutive response of the parent material

Elasticity of this solid was modelled as linear isotropic, with $E = 100 \text{ GPa}$ and $\nu = 0.1$ as measured. The parent material of the foams considered in this study is a sintered Titanium powder characterised by a small micro-porosity, of order 5-10%. Strictly, such material should be modelled as a plastically compressible solid; however we have shown in our previous modelling study [75] that the predicted foam response is scarcely sensitive to the plastic compressibility of the parent material; consequently we model the parent material as a J_2 ,

plastically incompressible solid. The plastic material response is calibrated according to the measured *compressive* response of the porous titanium, shown in Figure 4.3. To account for the weaker *tensile* response measured for this material, a continuum ductile damage model is also adopted, as implemented in ABAQUS Standard. The rationale for this is provided by the observations provided in Figure 4.3 - Figure 4.5, discussed in Section 4.2.2; the damage model is calibrated exclusively by the uniaxial test data presented in Figure 4.3, as follows.

The chosen damage model allows specifying an equivalent (von Mises) plastic strain at initiation of damage and the subsequent damage evolution as a function of the applied equivalent plastic displacement of the element. The damage initiation strain can be specified as a function of stress triaxiality η , and is defined as the ratio of hydrostatic to deviatoric (equivalent Von Mises) stress, $\eta = \sigma_H / \sigma_{VM}$. For all values of stress triaxiality, it was assumed that $d(\bar{\epsilon}_{PL}) = 1 - \sigma_T(\bar{\epsilon}_{PL}) / \sigma_C(\bar{\epsilon}_{PL})$; in other words, the compressive response $\sigma_C(\bar{\epsilon}_{PL})$ is considered as the undamaged elasto-plastic material response; the tensile response $\sigma_T(\bar{\epsilon}_{PL})$ is considered to be weaker than the compressive response due to intervening damage mechanisms, as observed in experiments. Experiments only provide the damage evolution law up to the strain at which the material fails in tension; beyond such strain, it is assumed that the damage evolves linearly until it reaches a value of 1; the slope of the $d(\bar{\epsilon}_{PL})$ curve in this phase is taken equal to the measured slope at the point of fracture.

In uniaxial tensile loading the damage variable d starts assuming positive values when the applied plastic strain exceeds 0.003; this strain can therefore be considered as the damage initiation strain in uniaxial tensile loading. The assumed variation of the damage initiation strain as a function of triaxiality is presented in Figure 4.9. At triaxiality $\eta \geq 1/3$ the damage initiation strain was taken as independent of triaxiality and equal to 0.003. At triaxiality $\eta = 0$ (pure shear), the equivalent plastic strain at damage initiation was taken as the equivalent Von Mises plastic strain corresponding to a maximum tensile principal strain of 0.003, namely $\bar{\epsilon}_{PL} = 3.46 \cdot 10^{-3}$. A linear interpolation was used to calculate the damage initiation strain at triaxiality $0 < \eta < 1/3$. In presence of compressive hydrostatic stress, and for $\eta \leq -1/3$, the damage initiation strain was arbitrarily set to a large constant value ($\bar{\epsilon}_{PL} = 0.2$), in line with

the fact that no stiffness degradation was measured for the material in compression at applied strains less than 0.2. A linear interpolation was used to determine the damage initiation strain in the range $-1/3 < \eta < 0$.

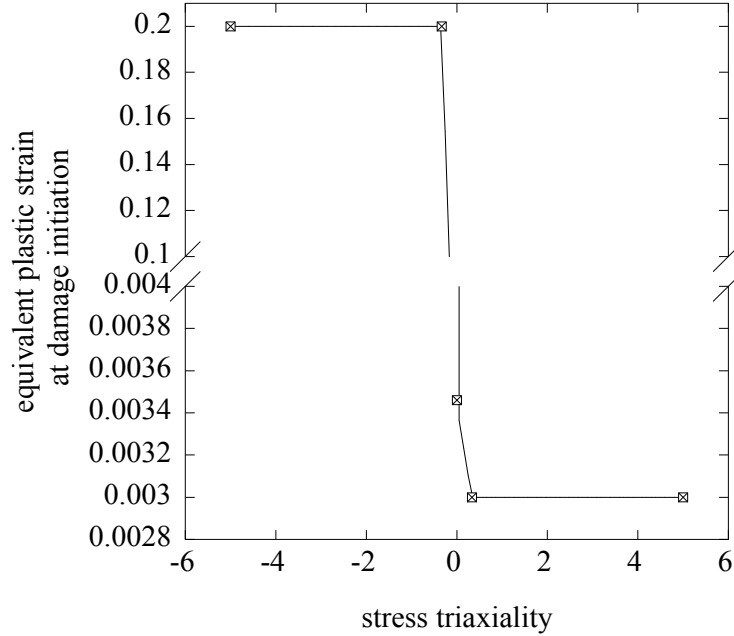


Figure 4.9 Equivalent plastic strain at damage initiation as a function of stress triaxiality for the Titanium parent material ($\bar{\rho} = 0.95$).

The damage evolution has to be provided to ABAQUS in the form of damage variable d versus element plastic displacement, while our measured data are expressed in terms of plastic strain. The plastic displacement was obtained from the plastic strain by multiplying by the element size L_e of the finite elements employed, as in [190]. Note that only uniform grids of cubic FEs were employed in the simulations.

4.3.2.2 Constitutive response of the fictitious pore material

In order to mimic the behaviour of pores in a solid matrix, the cells flagged as pores need to be able to experience high compressive or tensile volumetric strains without considerable energy absorption; they also need to lock (their stiffness needs to increase substantially) at sufficiently high compressive volumetric strains, in order to simulate the pore self-contact subsequent to compressive collapse. In order to attribute these features to their mechanical response while

avoiding computationally expensive contact algorithms, cells marked as pores are modelled as plastically compressible solids by using the crushable foam model implemented in ABAQUS standard, with the choice of isotropic hardening.

The ‘pore’ material was taken as linear elastic and isotropic, with arbitrary chosen Young’s modulus and Poisson’s ratio of 2.9 GPa and 0.1, respectively. The plateau collapse stress was arbitrarily set to 7 MPa; a slight strain hardening was imposed prior to densification, which was set to occur gradually at nominal compressive strains of 0.8-0.9. The plastic Poisson’s ratio was set to zero and consequently the ratio k of the initial yield stresses in uniaxial and hydrostatic compression was set to $\sqrt{3}$ as dictated by the flow rule of Deshpande and Fleck [15]. The history of equivalent stress versus strain for the fictitious pore material is presented in Figure 4.10. Preliminary simulations showed that the global foam response was insensitive to the choice of elastic modulus and plateau stress provided that these were substantially less than the corresponding values for the parent material (< 5%). Setting the values of stiffness and strength too close to 0 would result in unstable FE simulations.

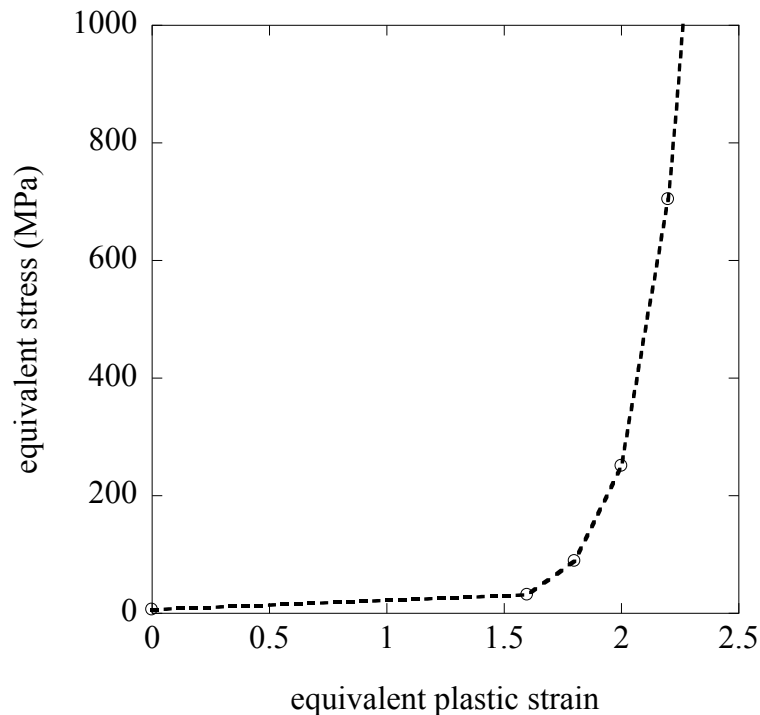


Figure 4.10 Assumed Deshpande-Fleck equivalent stress versus plastic strain response for the virtual pore material.

4.3.3 Boundary conditions

There is general consensus that periodic boundary conditions should be used in the FE analysis of stochastic volume elements (SVEs) and representative volume elements (RVEs). The set of boundary conditions affect the mechanical response of the material, as shown in [78]. On the other hand, several authors such as in [80, 81] have shown that for sufficiently large SVEs or RVEs, predictions obtained by imposing periodic boundary conditions tend to yield identical results to those obtained using uniform displacement boundary conditions. Preliminary simulations confirmed this fact for the case of our SVEs and in our simulations, conducted on non-periodic microstructures, we employ uniform boundary conditions to model uniaxial and pure shear loading as in [54].

In uniaxial tension and compression, one of the faces of the cubic SVE has normal displacements constrained, while the opposite face is subject to linearly ramped normal displacements, such to induce axial tensile or compressive strain. The lateral faces are constrained to remain planar and the normal displacements on opposite lateral faces are forced to be equal and opposite; these constraints are imposed via the constraint equation tool of ABAQUS CAE, making use of dummy nodes.

In order to simulate shear deformation, a uniform tensile strain is imposed in one direction by constraining one of the faces of the cubic SVE to have vanishing normal displacements, while the opposite face is subject to outwards normal displacements, such to induce a uniform tensile strain ε . A compressive strain $-\varepsilon$ is imposed along the perpendicular direction by application of appropriate inwards normal displacements. The simulation is run and the stress and strain histories along the 3 principal directions are recorded. The shear stress versus shear strain curve is then extracted from the definitions of equivalent von Mises stress and strain, provided below

$$\begin{aligned}\sigma_{VM} &= \left[\frac{(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_3 - \sigma_2)^2}{2} \right]^{1/2} = \sqrt{3} \tau \\ \varepsilon_{VM} &= \frac{\sqrt{2}}{3} \left[(\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_1 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_2)^2 \right]^{1/2} = \gamma / \sqrt{3}.\end{aligned}\tag{4.1}$$

4.3.4 Meshing and Monte Carlo analyses

In all cases, the SVEs were meshed using regular arrays of cubic, linear (constant strain) 3D finite elements, of type C3D8 in ABAQUS Standard, with a full integration scheme. Monte Carlo analyses were conducted on the microstructures generated by both Algorithm I and Algorithm II; repeated FE simulations are conducted on 10 realisations of each microstructure and the average and spread of the simulation outputs were analysed.

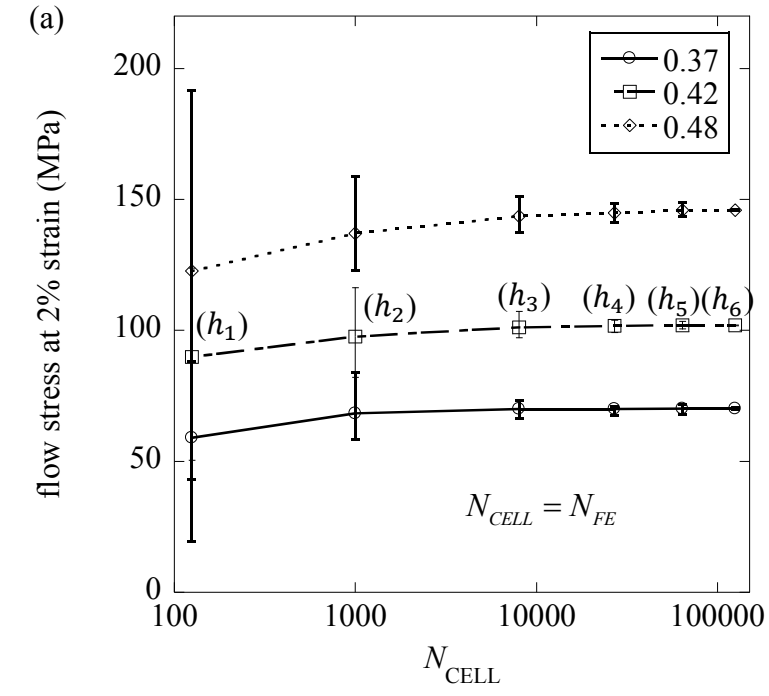
The sensitivity of the predictions to FE mesh density (or number of FE used, $N_{FE} = V / L_e^3$) and to density of the cell tessellation (or number of cells used, $N_{CELL} = V / V_{CELL}$) was determined by conducting repeated simulations at increasing N_{FE} and N_{CELL} , in order to determine the minimum values of N_{FE} and N_{CELL} which made the predictions insensitive to these two parameters. We note that conducting simulations at different N_{CELL} is equivalent to exploring the size dependence of the material's response. As N_{CELL} increases, while the main geometric length-scale – the average pore size - remains unchanged, we effectively increase the physical size of the RVE simulated. The model is therefore capable, in principle, of capturing scale effects such as those induced by the surface of the porous solid. The sensitivity of the predictions to both N_{FE} and N_{CELL} is discussed in the following Section.

4.3.5 Sensitivity of predictions to the density of the statistical and FE meshes

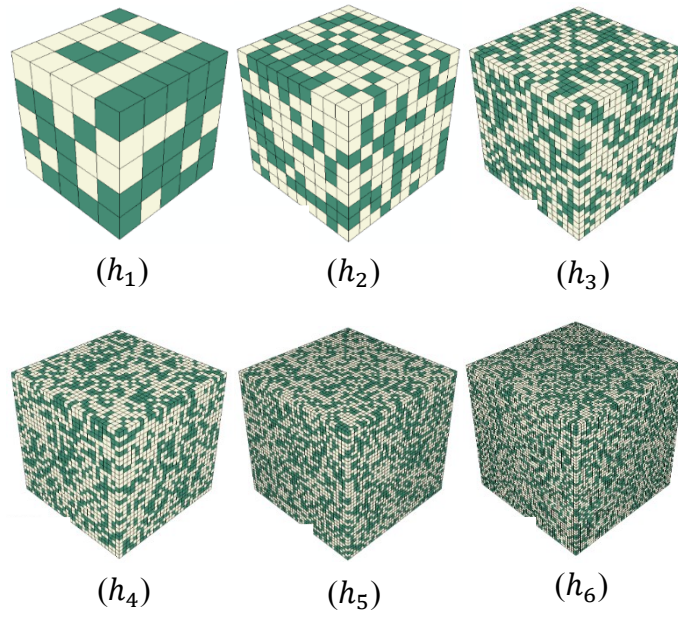
4.3.5.1 Algorithm I

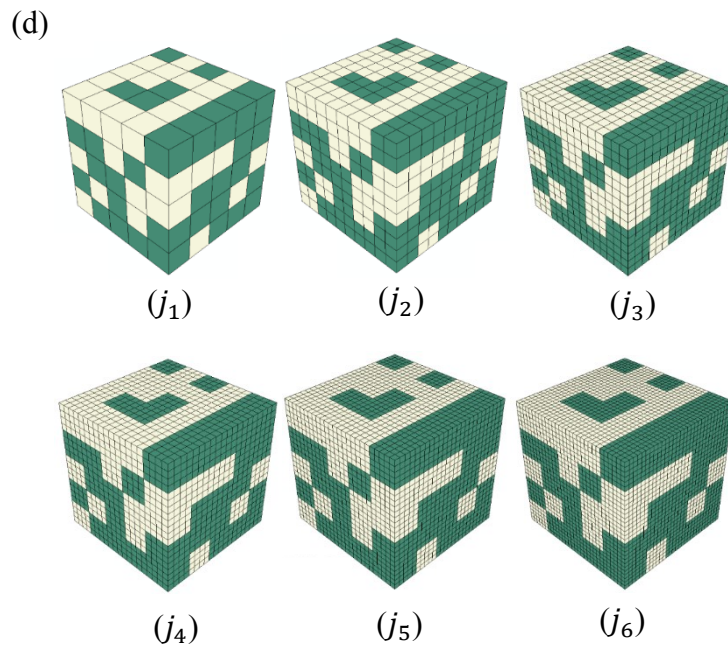
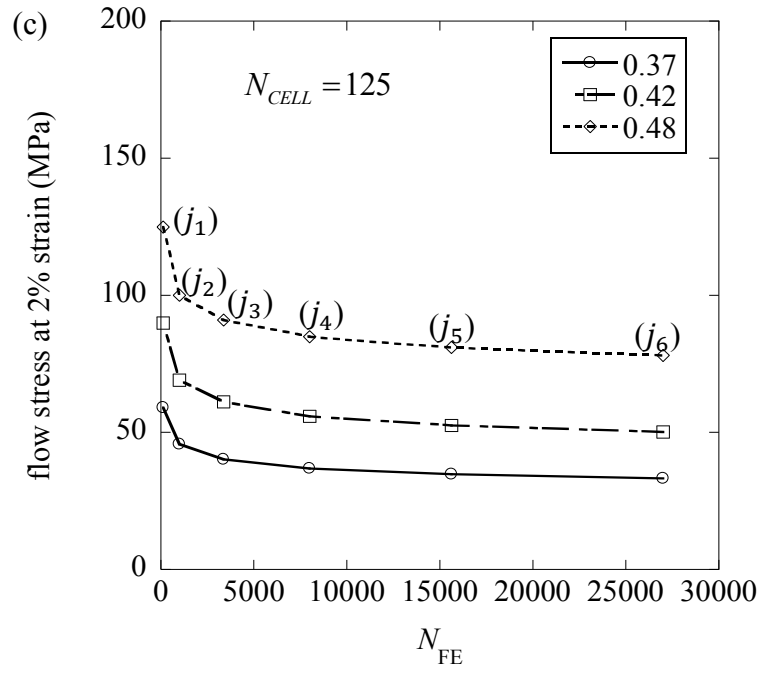
We proceed to analyse the sensitivity of the FE predictions to N_{CELL} , for microstructures generated using Algorithm I. As summarised in Figure 4.11(a), Algorithm I was employed to generate different microstructures with N_{CELL} varying in the range 125-125000; for each choice of N_{CELL} , 10 realisations of the microstructures were generated. The FE mesh was chosen such to have $V_{CELL} = L_e^3$, i.e. each statistical cell was meshed by a single linear finite element. All the microstructures were subject to loading in uniaxial compression; the simulations were interrupted when a total compressive strain of 2% was achieved and the corresponding flow stress was recorded. The study was repeated for 3 different relative densities and results are summarised in Figure 4.11(a). Irrespective of relative density, average predictions were found

to be scarcely sensitive to N_{CELL} for $N_{CELL} > 1000$. For $N_{CELL} < 1000$ the flow stress increases with increasing N_{CELL} , indicating a size dependence of the compressive response, such that smaller foam samples are softer than larger ones, as reported also by other authors in [191-193]. We argue that this is a consequence of the small value of N_{CELL} , resulting in a microstructure which is not truly random. The scatter in the predictions decreases, as expected, with increasing N_{CELL} , as shown in Figure 4.11(a). Such scatter becomes less than 5% for $N_{CELL} > 8000$. Figure 4.11(b) shows examples of the different microstructures analysed, corresponding to the data presented in Figure 4.11(a) for the case $\bar{\rho} = 0.42$.



(b)





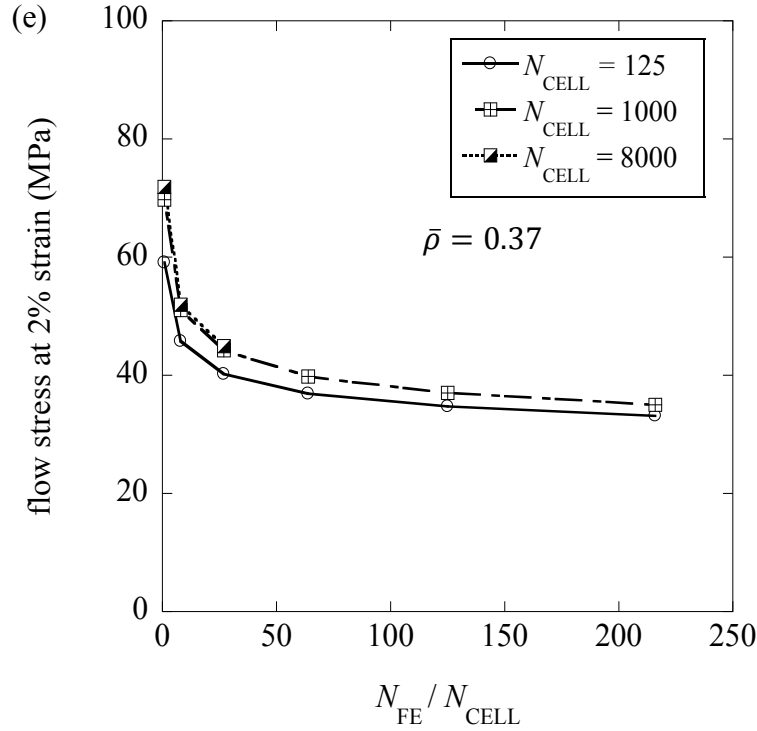


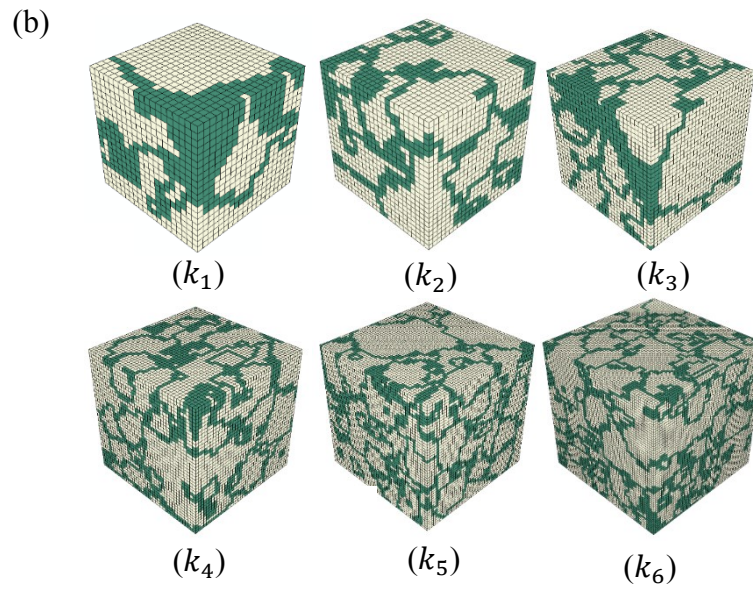
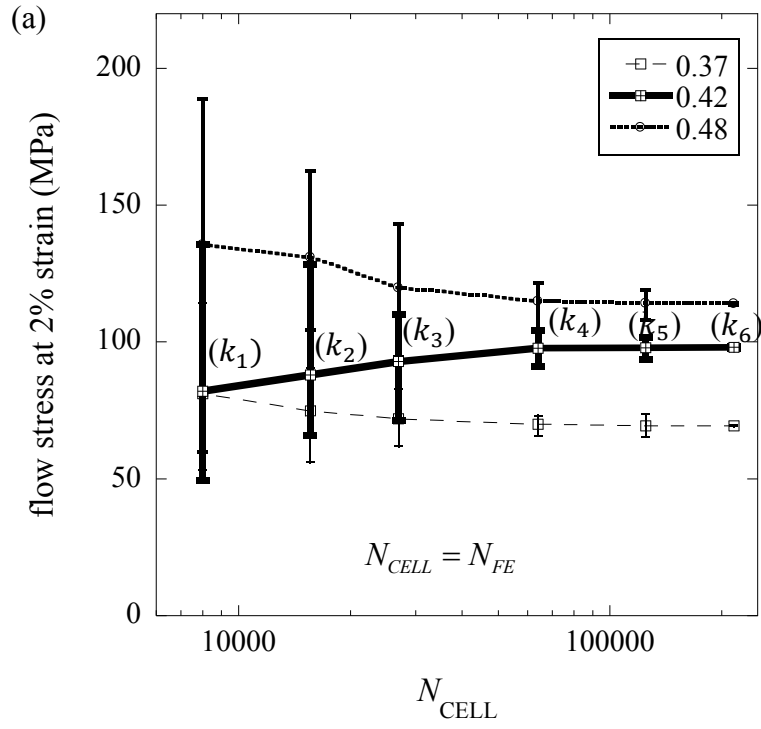
Figure 4.11 (a) Sensitivity of the predictions to N_{CELL} for different values of relative density; (b) example of SVEs at increasing N_{CELL} ; (c) mesh convergence study, or sensitivity of the predictions to N_{FE} ; (d) example of SVEs at $N_{CELL} = 125$ and increasing N_{FE} ; (e) Sensitivity of the predictions to the number of finite elements per cell, N_{FE} / N_{CELL} .

In Figure 4.11(c) the sensitivity of the predictions to the FE mesh density is determined. For the choice $N_{CELL} = 125$, simulations are conducted by progressively refining the FE mesh (or increasing N_{FE}) on a single realisation of the microstructure. Figure 4.11(d) shows examples of the different meshes analysed for this single realisation. It is found that predictions become approximately mesh insensitive for $N_{FE} > 8000$, corresponding to having 64 finite elements meshing each of the 125 cells ($N_{FE} / N_{CELL} = 64$). The material response is found to decrease monotonically with increasing mesh density; this can be explained observing that progressively refining the mesh allows capturing the high stress concentration around the cubic pores; as the mesh is refined, the maximum values of stress around the pores tend to increase, giving earlier yield and a lower macroscopic compressive flow stress at 2% strain.

In Figure 4.11(e) we present predictions for the choices $N_{CELL} = 125, 1000, 8000$ and different mesh densities N_{FE} / N_{CELL} , for a selected relative density. The compressive flow stress at 2% strain is provided as a function of the number of FE per cell, N_{FE} / N_{CELL} . It is clear that, for every choice of statistical mesh (value of N_{CELL}), the predictions become scarcely sensitive to N_{FE} for $N_{FE} / N_{CELL} > 64$.

4.3.5.2 Algorithm II

We now present similar information as in Section 4.3.5.1, for the case of Algorithm II. Figure 4.12(a) shows the sensitivity of predictions to N_{CELL} , for the case $N_{FE} = N_{CELL}$. Figure 4.12(b) shows examples of the different microstructures analysed, corresponding to the data presented in Figure 4.12(a) for the case $\bar{\rho} = 0.42$. The compressive flow stress at 2% strain monotonically increases with increasing N_{CELL} only for the case $\bar{\rho} = 0.42$, while it decreases for the other two densities considered. This inconsistent behaviour is due to the fact that at low values of N_{CELL} Algorithm II only provides microstructures with a small number of pores, not really representative of the material microstructure. The sensitivity analysis shows that the flow stress is scarcely sensitive to N_{CELL} for $N_{CELL} > 27000$.



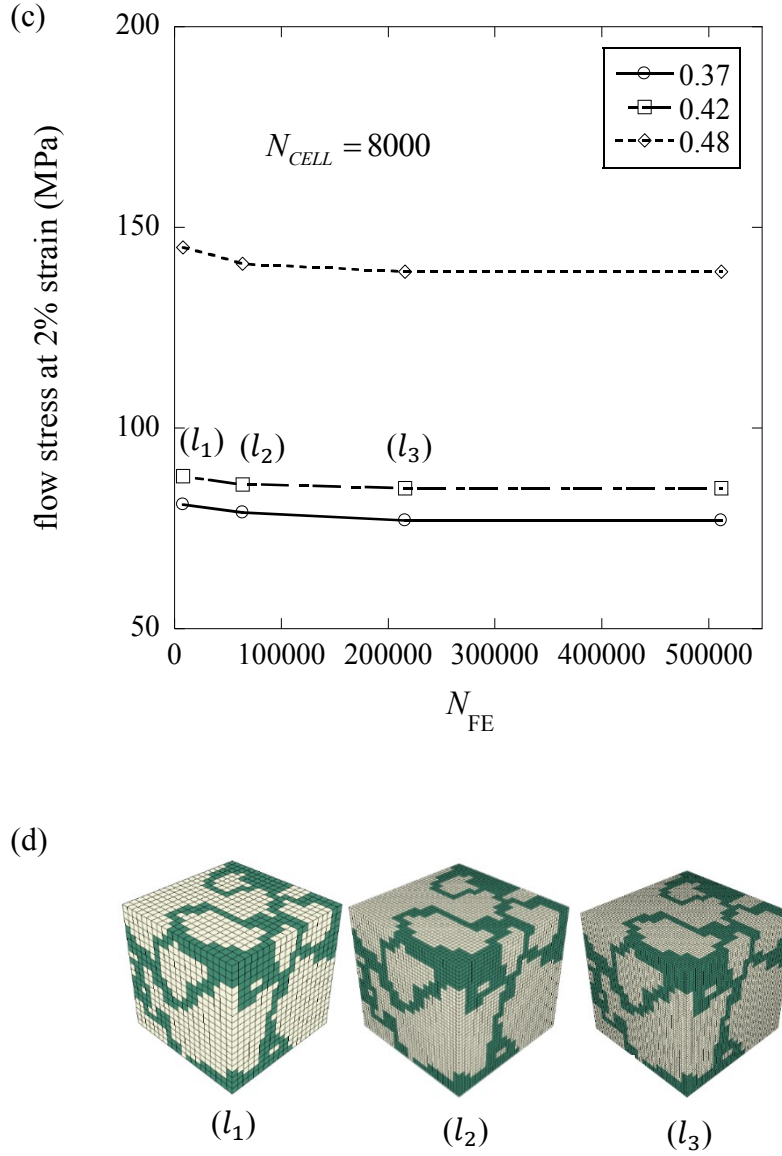


Figure 4.12 (a) Sensitivity of the predictions to N_{CELL} for different values of relative density; (b) example of SVEs at increasing N_{CELL} ; (c) mesh convergence study, or sensitivity of the predictions to N_{FE} ; (d) example of SVEs at $N_{CELL} = 8000$ and increasing N_{FE} .

Figure 4.12(c) show a FE mesh convergence analysis conducted on one realisation of a microstructure ($N_{CELL} = 8000$). Figure 4.12(d) shows examples of the different microstructures analysed, corresponding to the data presented in Figure 4.12(c) for the case $\bar{\rho} = 0.42$. For the three relative densities considered, predictions appear to be scarcely sensitive to the FE mesh density in the whole range considered, i.e. $N_{FE} > 8000$. This is due to the fact that Algorithm II produces foam microstructures with pores of smoother shape than those obtained via

Algorithm I; this results in a lower stress concentration, which can be resolved with a relatively smaller number of elements. In other words, meshing each cell with one single FE ($N_{FE} / N_{CELL} = 1$) is sufficient to obtain mesh-insensitive predictions.

4.3.5.3 Sensitivity of the response to the number of pores and surface effects

We now examine the sensitivity of predictions obtained with both algorithms to the total number of pores N_p , for a given relative density. The FE mesh density for algorithms I and II were chosen based on the mesh-sensitivity studies presented above, such that predictions are mesh-insensitive. The comparison, presented in Figure 4.13, show that both algorithms predict a material response scarcely sensitive to N_p when this is large. The scatter in the response of the SVEs decreases, as expected, with increasing number of pores; at every value of N_p , predictions from Algorithm I always display greater scatter than those from Algorithm II.

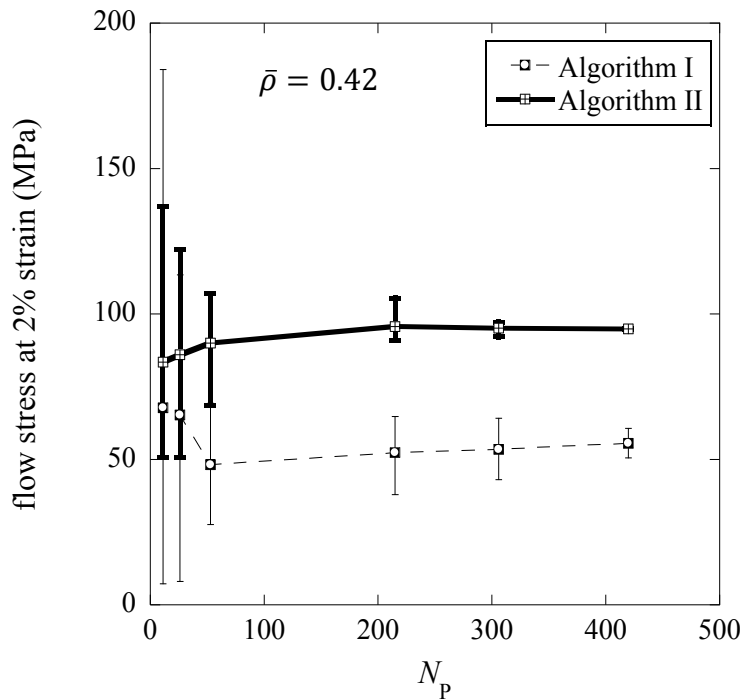


Figure 4.13 Comparison of Algorithms I and II; the predicted compressive flow stress at 2% strain from the two algorithms is shown as a function of the total number of pores modelled, N_p .

In Table 2 we provide details of the parameters N_{CELL} and N_{FE} employed in the simulations shown in Figure 4.13. It is obvious that Algorithm I is computationally less expensive than Algorithm II, in the sense that, in order to model a given number of pores N_P , Algorithm II requires a number of finite elements larger than what required by Algorithm I. Algorithm I is also associated to a weaker response than that of Algorithm II, due to its modelling of pores with sharper corners, as discussed above. It will be shown below that predictions of Algorithm II are more accurate than those from Algorithm I, but we will also show that with appropriate modifications Algorithm I can yield predictions of the same accuracy as Algorithm II making use of substantially less computational power.

<u>Algorithm I</u>				
N_P	N_{CELL}	N_{FE} / N_{CELL}	N_{FE}	Scatter range (%)
11	27	64	1728	130.38
26	64	64	4096	80.59
53	125	64	8000	43.18
215	512	64	32768	25.61
306	729	64	46656	19.76
420	1000	64	64000	reference
<u>Algorithm II</u>				
N_P	N_{CELL}	N_{FE} / N_{CELL}	N_{FE}	Scatter range (%)
11	8000	1	8000	51.57
26	15625	1	15625	41.69
53	27000	1	27000	21.47
215	64000	1	64000	7.50
306	125000	1	125000	2.70
420	216000	1	216000	reference

Table 2 Details of the FE simulations presented in Figure 4.13.

Figure 4.13 shows that Algorithm II presents a strength increasing with the number of pores; since the average pore size is unchanged, a growth in the number of pores (or equivalently, physical specimen size) reduces the fraction of pores which lies on the external surface. As such surface pores tend to yield earlier than pores in the bulk of the RVE (this is due to the different stress state, always comprising one vanishing principal stress), it follows that the mechanical strength increases with increasing number of pores.

4.4 Results and discussion

We proceed to analyse in detail our numerical predictions and to compare these to corresponding measurements. Simulations are conducted on ten realisations of the microstructures obtained via Algorithm II and average predicted stress versus strain histories are calculated, for three selected loading cases corresponding to the experiments performed in this study (uniaxial tension, compression, pure shear). The parameters N_{CELL} and N_{FE} are chosen to be sufficiently large that predictions are insensitive to them ($N_{FE} = N_{CELL}$, $N_{CELL} = 64,000$).

4.4.1 Stress versus strain histories

Figure 4.14(a) presents compressive nominal stress versus strain histories for three relative densities. The figure includes predictions obtained with and without modelling of damage. Very good agreement between measurements and predictions is found for all relative densities; modelling of the material damage is necessary, even in compression, in order to capture the measured response of the foams at strains exceeding 5%; as shown in Figure 4.5, degradation of material stiffness under tensile stresses begins at much lower strains than 5%, however its effect upon the macroscopic material response is negligible. The predicted sensitivity of the stress/strain curves to foam density matches accurately the measurements reported by Siegkas et al. [75]. The inserts of Figure 4.14(a) show the deformed mesh ($\bar{\rho} = 0.42$) at a total compressive nominal strain of 0.2. We stress that our simulations, unlike those from all previous studies, can be conducted up to very large plastic strains, as shown by Figure 4.14(b), showing a very good agreement between measurements and predictions up to the densification regime.

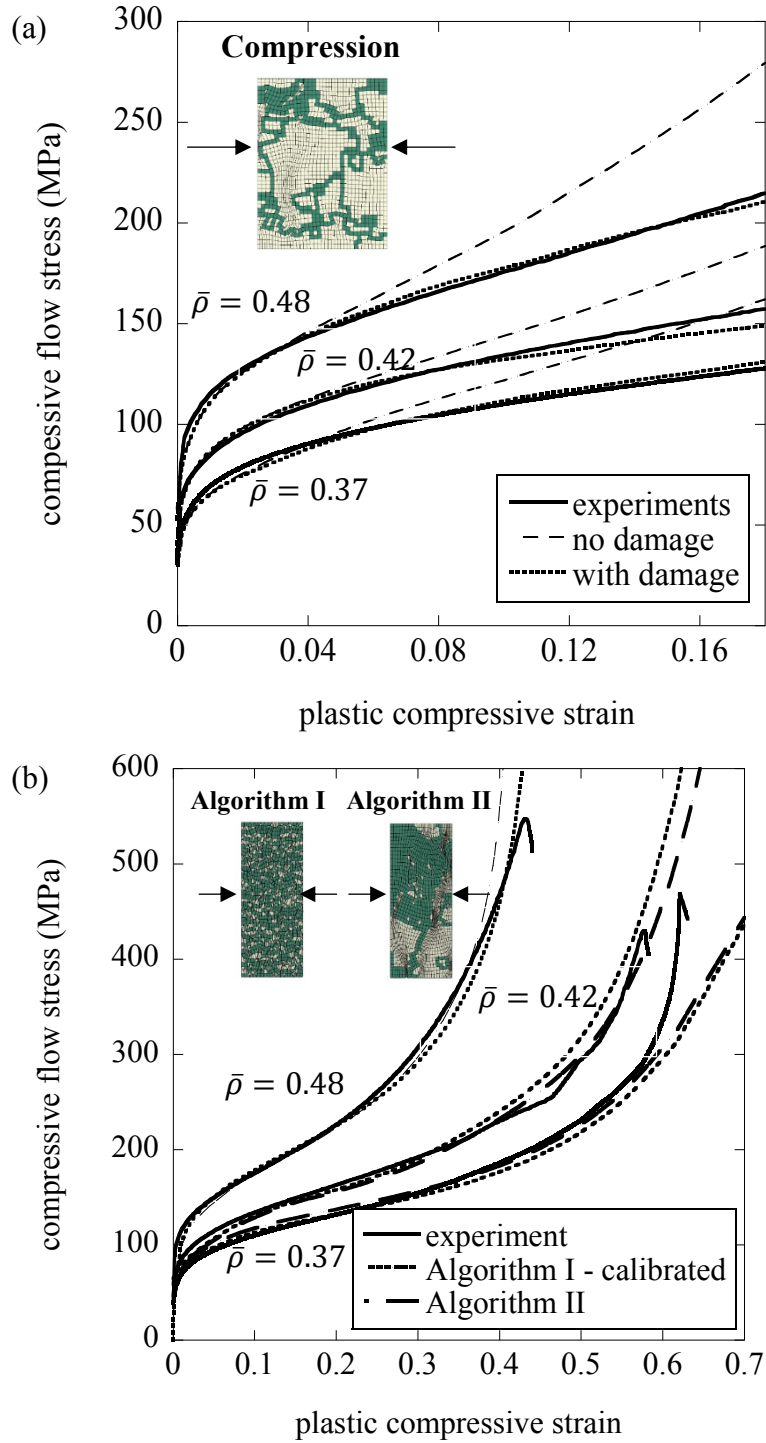


Figure 4.14 (a) Comparison of measurements and predictions of the uniaxial compressive response of three selected foams. The inserts show the deformed mesh ($\bar{\rho} = 0.42$) of a planar section at a total compressive nominal strain of 0.2. (b) Predictions of the uniaxial compressive response of three selected foams up to large plastic strains. Inserts show the deformed mesh ($\bar{\rho} = 0.42$) of a planar section at a total nominal compressive strain of 0.6 for Algorithm I (calibrated) and for Algorithm II.

In Figure 4.15 we present similar information for the case of uniaxial tension. For this loading case, the predicted macroscopic material's response is affected by material damage since the early stages of deformation, at macroscopic tensile strains less than 1%. The simulations predict an initial strain hardening response of the foams, followed by a strain softening, due to growth of the pores. Measurements of the tensile response are available only for the case $\bar{\rho} = 0.37$ and again, predictions are found in good agreement with the experiment. On the other hand, in the tests the specimens failed catastrophically at strains less than 1%, by unstable propagation of a macroscopic crack perpendicular to the loading direction. The inserts of Figure 4.15 show the deformed mesh ($\bar{\rho} = 0.42$) at a total tensile nominal strain of 0.08.

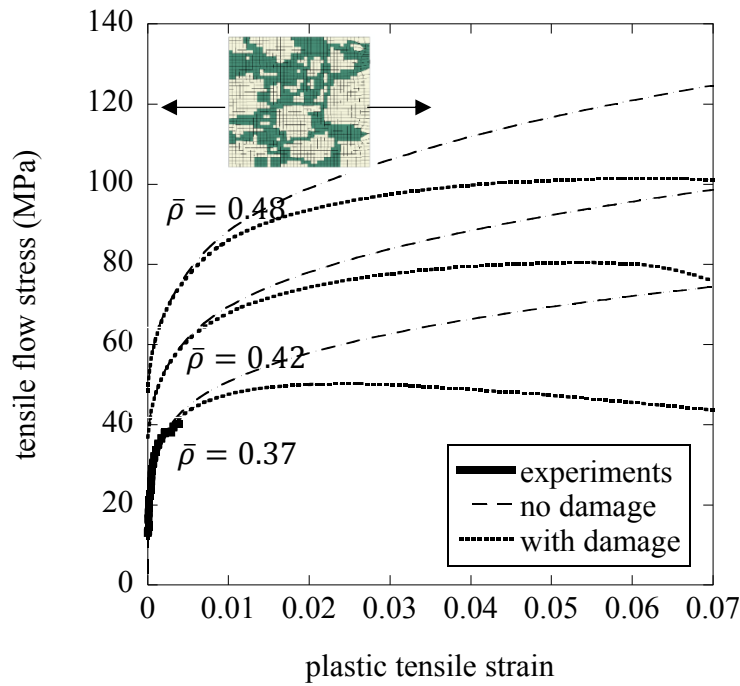


Figure 4.15 Comparison of measurements and predictions of the uniaxial tensile response of three selected foams. The inserts show the deformed mesh ($\bar{\rho} = 0.42$) of a planar section at a total tensile strain of 0.08.

Figure 4.16 presents predictions of the shear response of three selected foam densities; the measured shear response of a foam of density $\bar{\rho} = 0.37$ is included for comparison. The stress strain histories were obtained from the equivalent von Mises stress and strains (σ_{eff} , ε_{eff} , respectively, Eq. (4.1)) as

$$\varepsilon_{xy} = \gamma_{xy} / 2 = \sqrt{3} \varepsilon_{eff} / 2 \quad (4.2)$$

$$\tau_{xy} = \frac{1}{\sqrt{3}} \sigma_{eff} \quad (4.3)$$

The FE predictions are found in good agreement with the experiments (the curve shown is an average of three stress/strain histories from 3 repeated test), however clearly the simulations cannot capture the unstable shear fracture observed in the experiments at a plastic shear strain of approximately 2% (for the case $\bar{\rho} = 0.37$). The inserts in Figure 4.16 show the deformed mesh ($\bar{\rho} = 0.42$) of a planar section lying on one principal plane, at macroscopic plastic shear strain of 0.1. The quasi-static simulations are unable to capture the dynamic events leading to unstable brittle fracture in tension and shear tests, but predict a softening material response at similar stress levels as in the measurements.

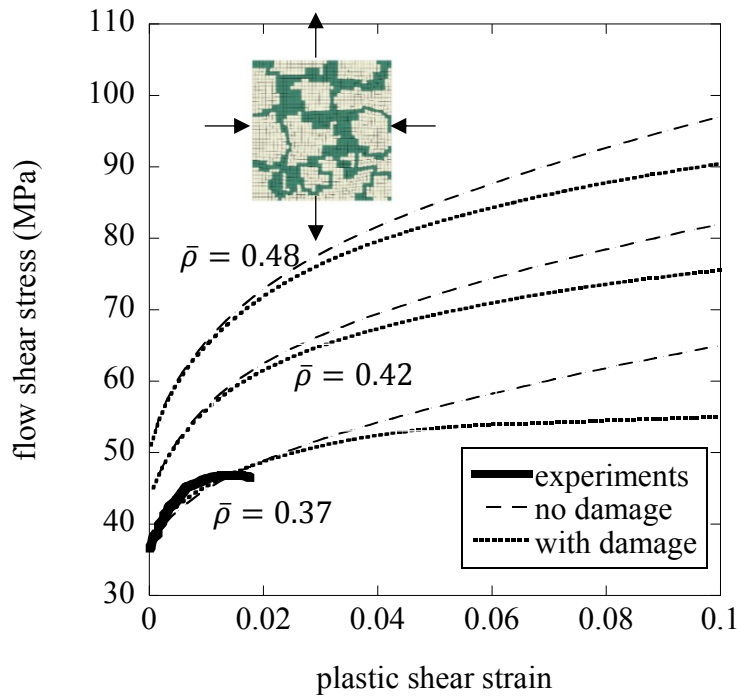


Figure 4.16 Comparison of measurements and predictions of the shear response of three selected foams, in terms of histories of shear stress versus shear strain ($\varepsilon_{xy} = \gamma_{xy} / 2$). The inserts show the deformed mesh ($\bar{\rho} = 0.42$) of a planar section lying on one principal plane, at plastic shear strain of 0.1.

4.4.2 Yield surface of the Titanium foam

Figure 4.17 presents a portion of the yield surfaces for two selected foams of different relative densities. The coordinates of the data points represent the predicted or measured macroscopic hydrostatic and deviatoric (equivalent von Mises) stresses in the foams, at an effective von Mises strain, $\varepsilon_{eff} = 0.05$; this specific value was chosen to allow direct comparison of our predictions with those in [75]. Data from experiments is included in the figure; note that in the tensile and shear test the material catastrophically failed at effective strains lower than 0.05; for these 2 tests the deviatoric and hydrostatic stresses are extracted at the peak stress in the measured stress/strain curves presented in Figure 4.15 and Figure 4.16.

The simulations in [75] grossly over-predict the fracture stress of the Titanium foam in the case of tension and shear; their agreement with measurements in the case of compression is also not completely satisfactory. On the contrary, our predictions are in very good agreement with the measurements in all loading cases (see also Figures 4.14 - 4.16). The simulations performed in this chapter predict a strong tension/compression asymmetry, in line with what observed in our tests (and widely reported in the literature for porous materials). A comparison of the predicted responses of the two foams shows that the yield surface grows in an approximately self-similar fashion with increasing relative density. The scaling of strength with relative density is predicted correctly by our simulations but not by those in [75].

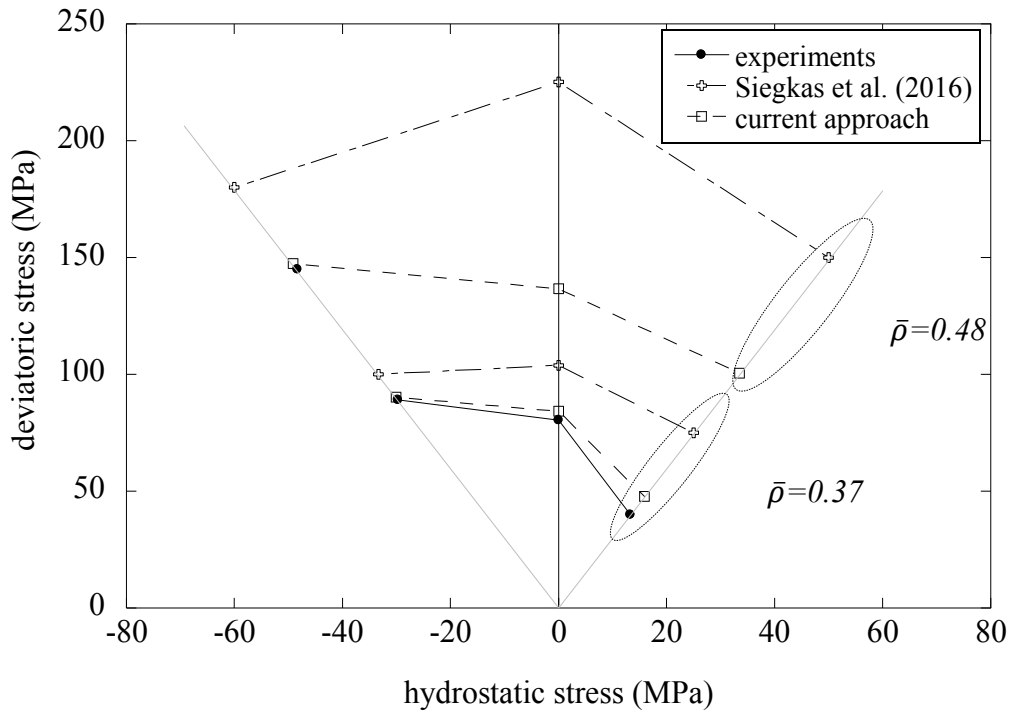


Figure 4.17 Partial yield surfaces for two selected foam densities. Our predictions are compared to those by Siegkas et al. [75] on the same material and to available measurements.

In the work of [75] the geometry of the SVEs considered was very close to the actual foam geometry observed by X-ray tomography. On the other hand their simulations did not account for material damage and were computationally expensive, due to the large number of contact pairs needed to capture correctly the self-contact of the pores. They analysed cubic SVEs of volume of order 1 mm^3 and each simulation lasted an average of 10 hours on a PC with an Intel i7 processor. In contrast, in our modelling approach we do not attempt capturing the geometrical details of the foams' microstructures, but we aim at modelling correctly the overall relative density and the mechanical response of the pores, by assigning a non-linear, plastically compressible response to the pore regions. Our approach compares favourably to that in [75] both in terms of computational cost (we analyse cubic SVEs of volume around 12 mm^3 and each simulation lasts around 1 hour on a similar PC with an Intel i7 processor) as well as accuracy, as it is evident from Figure 4.17.

4.4.3 Calibration of Algorithm I

We have shown above that Algorithm I is computationally much more effective than Algorithm II; on the other hand, it underestimates the flow stress due to the fact that, essentially, it is modelling pores with sharp corners, promoting early local yielding of the parent material; for this reason we employed Algorithm II in the previous Sections.

We illustrate this in Figure 4.18, which shows measurements and predictions (of both algorithms) of the compressive flow stress at a compressive plastic strain of 0.02, at three selected relative densities; clearly the predictions made via Algorithm II are in excellent agreement with experiments but those made via Algorithm I are not. We note that the SVEs employed for the simulations shown in this figure had equal number of nodes. We include in the figure an additional set of predictions, obtained via Algorithm I by employing a different constitutive response for the parent material. In this additional set of predictions, the history of stress versus plastic strain for the parent material was obtained by multiplying by a constant value the measured stress at every strain, such that this modified response is stronger than the measured one. The behaviour of the pore materials and the damage algorithms are not modified for this additional set of predictions. The multiplicative constant is determined by fitting the data in Figure 4.18 by a linear relationship of type $\sigma_c(\varepsilon^{pl} = 0.02) = A + B\bar{\rho}$ and considering the ratio of the intercept A associated to the predictions of Algorithm II and the corresponding intercept predicted by Algorithm I. After this calibration, Algorithm I yields predictions coincident to those obtained via Algorithm II and therefore in good agreement with experiments; we have included in Figure 4.14(b) predictions from this ‘calibrated’ version of Algorithm I to highlight that agreement with experiments is not lost up to very large strains.

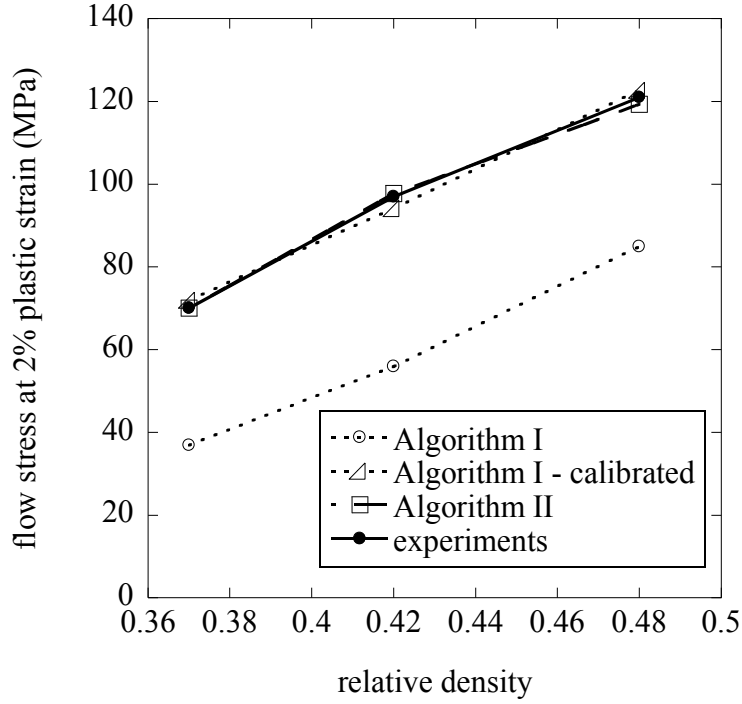


Figure 4.18 A comparison of measurements and FE predictions of both algorithms, for uniaxial compression. The nominal stress at 0.02 compressive plastic strain is plotted for selected relative densities.

An alternative method of calibration of Algorithm I such that it predicts accurately the measured stress/strain curves is to use a smaller value of the FE mesh density N_{FE} / N_{CELL} , as illustrated in the following. For a relative density of 0.37, experiments predict a compressive flow stress (at plastic strain 0.02) of about 70 MPa. In Figure 4.11(a) we showed that predictions of Algorithm I are insensitive to N_{CELL} for $N_{CELL} = 1000$. Now consider Figure 4.11(e); this shows that by choosing $N_{FE} / N_{CELL} = 1$ the simulation provide a flow stress of about 70 MPa, for $N_{CELL} > 1000$. Repeating the simulations in compression with $N_{FE} = N_{CELL} = 1000$, one obtains predictions of the compressive strength identical to those of Algorithm II, or those of Algorithm I when a stronger parent material is used. Physically, choosing $N_{FE} / N_{CELL} = 1$ (rather than $N_{FE} / N_{CELL} = 64$ for a mesh-insensitive prediction) corresponds to modelling smoother pores.

4.5 Concluding Remarks

Two algorithms were developed to construct representative microstructures of sintered Titanium foams; Algorithm I correctly represents the overall relative density of the foams; Algorithm II also models the distribution of pore size within the microstructure and capture the pore shape. The mechanical response of corresponding SVEs was predicted via FE simulations and the sensitivity of the predictions to FE mesh density, statistical mesh density and size of the SVEs was determined. Monte Carlo analyses were conducted on SVEs of different size and the size of an appropriate RVE was established, for both types of microstructures considered. The RVEs were then used to predict the measured response of a Titanium foam in uniaxial compression and tension, as well as shear. Relative densities of 0.37, 0.42 and 0.48 were considered in order to predict scaling laws for the strength of these foams. The predictions were found in good agreement with measurements and were compared to the results of FE analyses conducted in [75] for the same materials. A damage model was used to represent stiffness degradation of the parent material of the foams and was calibrated exclusively against the available uniaxial stress versus strain response of the parent material, rather than obtained via a curve-fitting exercise. The main conclusions from this study are as follows:

- The proposed modelling approach is computationally inexpensive compared to similar approaches for the same material, and is able to capture the stress versus strain responses of sintered Titanium foams in compression, tension and shear up to large strains, as well as the dependence of these responses upon relative density. The models are calibrated using exclusively measured data.
- It was found that the response of the foams analysed is scarcely size-dependent as long as the specimen volume contains at least 50 pores.
- Comparisons with the predictions in [75] showed that it is not necessary to capture all geometrical details of the foam microstructure (such as pore shape) in order to obtain accurate predictions.
- Our approach did not explicitly model the self-contact of the cell walls but introduced the effect of such self-contact by assigning a non-linear, plastically compressible response to the pores; such approach proved effective.
- Algorithms I and II yield similar, effective predictions of the response of the foams examined, if Algorithm I is appropriately calibrated. Algorithm I is more computationally effective than Algorithm II.

4.6 APPENDICES

APPENDIX A

Algorithm II

1. *Initialise and define parameters for domain:*

- Relative density for material $\bar{\rho}$
- Number of cells in x, y and z coordinate directions ($nlex, nely, nelz$)
- E , the matrix of dimensions E ($nelex, neley, nelez$). This matrix assumes a value of 0 for solid and vno for a void of a given reference number.
- Degree of numerical sub-discretisation given by parameter ns in each coordinate direction.
- Void size element counter, n , and global void element counter, $N=0$.

WHILE $N \leq \bar{\rho} \times nelex \times neley \times nelez$

2. *Randomly place a **void seed** within domain only where there are already no void elements immediately adjacent to the proposed site:*

- Initialise adjacency flag, $adj = 0$ and $n=0$.
- Draw randomly coordinates of proposed seed location, (x,y,z) , from $x \sim U(1, nelex)$, $y \sim U(1, neley)$, $z \sim U(1, nelez)$.
- Loop through all 26 adjacent elements within the **cube** formation around (x,y,z) , i.e. from $x-1$ to $x+1$, $y-1$ to $y+1$, $z-1$ to $z+1$. IF any element is already a void, set $adj = 1$.
- IF there is no void at (x,y,z) AND $adj = 0$, place seed at location: $E(x,y,z) = vno$, increment N , increment n , and proceed to void growth stage.

3. *Void growth stage: Determine randomised size (in elements), Nfv , of void according to Inverse-CDF; this is done using the histogram 'bins' data from experimental observations together with a single random uniform variable. Then grow:*

WHILE $n \leq Nfv$

- A single scanning variable **sweeps** alternately forwards and backwards through the entire domain. When it 'finds' the location (x,y,z) of the current void, vno , we draw a random integer from $G \sim U(1,6)$ to determine the randomised growth direction (1=left,

2=right, 3=down, 4=up, 5=front, 6=back). A destination growth position vector, pos , is then calculated from:

$$pos_x = \{ x - 1, x + 1, x, x, x, x \} \quad (A.2)$$

$$pos_y = \{ y, y, y - 1, y + 1, y, y \} \quad (A.3)$$

$$pos_z = \{ z, z, z, z, z + 1, z - 1 \} \quad (A.4)$$

- Vectors falling outside the domain are corrected to remain at the domain boundaries.

Similarly with stage 2, grow void only where there are no void elements belonging to other voids immediately adjacent to the proposed cite:

- Set adjacency flag, $adj = 0$.
- Loop through all 26 adjacent elements within the cube formation around (x,y,z) , as before. IF any element is already assigned as belonging to another void, set $adj = 1$.
- IF there is no void at (x,y,z) AND $adj = 0$, grow void at location: $E(x,y,z) = vno$, increment N and increment n .

4. *Void integrity procedure: A void integrity sub-algorithm is then implemented to remove any islands that may have been unintentionally created inside the voids. Thus, to identify and remove a fully-enclosed matrix island inside the void of any shape, the following algorithm is performed employing “abstract matrices” (Example shown in Fig. A.1):*

- Set **Ecol** ($nelex, neley, nelez$) and **Erow** ($nelex, neley, nelez$) ‘abstract’ matrices to zero.
- Loop through all x - y planes in E ($nelex, neley, nelez$), k : 1 to $nelez$.
- For each x - y plane loop through all rows in the plane, j : 1 to $neley$: Each row is then scanned to identify left and right limits of the current void, vno . WHILE $E(i,j,k) \neq vno$, increment i within limits of domain width, UNTIL $left=i$ limit; Repeat WHILE condition but now decrement i UNTIL $right=i$ limit. Check for any “row-gaps” between these limits. An *abstract row-gaps matrix* is created, Fig. 1(b): i : left to right, IF $E(i,j,k) = 0$, THEN set $Erow(i,j,k) = 1$.
- Loop through all columns in the plane, i : 1 to $nelex$: Each column is then scanned to identify external top and bottom limits of the current void, vno : WHILE $E(i,j,k) \neq vno$, increment j within limits of domain width, UNTIL $top=j$ limit; Repeat WHILE

condition but now decrement j UNTIL $bottom=j$ limit. An *abstract col-gaps matrix* is created, Fig. 6(c): j : top to bottom, IF $E(i,j,k) = 0$, THEN set $Ecol(i,j,k) = 1$.

- Where there are *common elements* in both row-gaps and col-gaps abstract matrices, a ‘true island’ may exist, Fig. 1(d): Loop through all elements in x - y plane. IF $Erow(i,j,k)=1$ AND $Ecol(i,j,k)=1$, THEN check if adjacent elements to the “island” are either the void itself or matrix.
- Set adjacency flag, $adj = 0$; test 26 adjacent elements as before and if *another void* ($\neq vno$) is detected set $adj = 1$. Then removal is not performed and the island is not a true island. If a true island is found then this is removed, $E(i,j,k) = 1$, and n and N are incremented.
- Repeat entire procedure looping through all y - z planes in the domain. i : 1 to $nelex$, and for x - z planes, j : 1 to $neley$. In this way, the 3 dimensional void structures in the domain are checked that it are simply connected.

5. *Sub-discretise cells of entire domain entire domain into $p \times p \times p$ finite elements:*

- The new global element number, e , for elements of the sub-discretised mesh is given by equation (A.1).

6. *ABAQUS input file*

Assign each cell an element set ‘*Elset’ for the ABAQUS input deck file. This also meant that corresponding ‘*Solid Section’ and ‘*Material’ definitions for each element set specifying the deterministic/randomised material properties were outputted by the algorithm.

Flow chart of Algorithm II is shown in Fig. A.2.

0	1	1	0	0	0
1	0	1	0	0	0
1	1	1	1	1	0
0	1	0	1	1	0
0	1	1	0	1	0
0	0	0	0	0	0

(a) Initial void structure (vno=1)

0	0	0	0	0	0
0	1	0	0	0	0
0	0	0	0	0	0
0	0	1	0	0	0
0	0	0	1	0	0
0	0	0	0	0	0

(b) Row-gaps abstract matrix

0	0	0	0	0	0
0	1	0	0	0	0
0	0	0	0	0	0
0	0	1	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

(c) Column-gaps abstract matrix

0	1	1	0	0	0
1	1	1	0	0	0
1	1	1	1	1	0
0	1	1	1	1	0
0	1	1	0	1	0
0	0	0	0	0	0

(d) Final void structure. Red indicate internal holes that have been filled.

Figure. A.1 Schematic illustration of void integrity sub-algorithm for a given plane to fill remove islands inside voids.

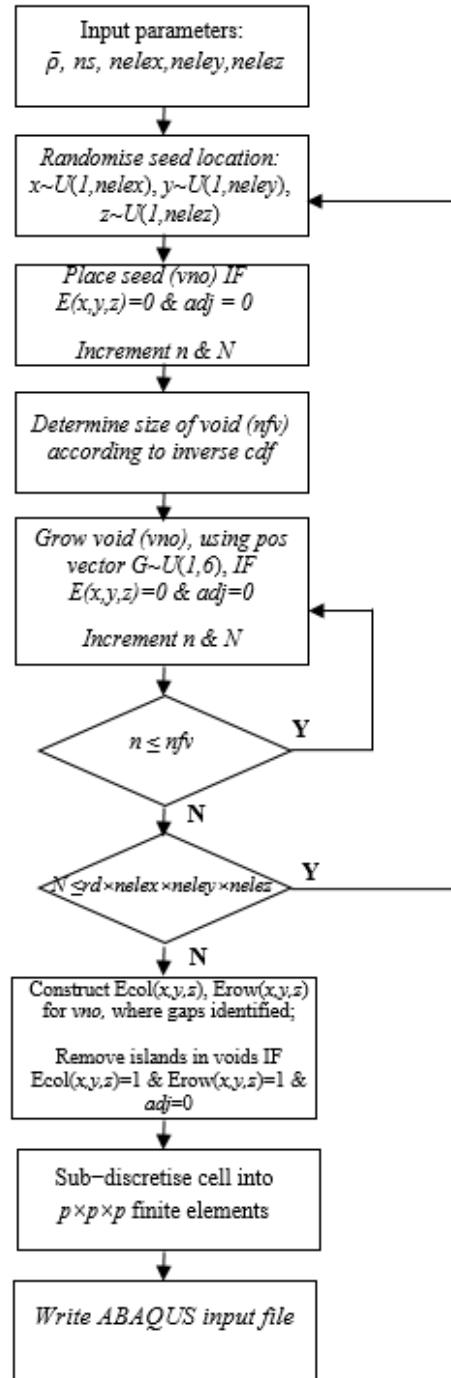


Figure A.2 Flow chart for Algorithm II.

CHAPTER 5

PREDICTIVE MODELLING OF THE FRACTURE TOUGHNESS OF A SINTERED TITANIUM ALLOY

ABSTRACT

A simple stochastic theoretical model and accompanying stochastic FE simulations are used to predict the fracture response of a notched beam in three-point bending, using as an input only stress-strain data measured in repeated uniaxial tension and compression tests. The material investigated is a solid made from sintered Ti powder, which coincides with the parent material of the Ti foams discussed in Chapter 4. This is modelled as an array of stochastic, elasto-plastic volume elements including a softening damage response. A comparison of theoretical predictions to experiments provides the length-scale for softening-induced strain localisation, as well as the statistical details of the material properties of the stochastic volume elements, which are used as inputs for stochastic FE simulations. Results suggest that, for this solid, tensile strength and fracture toughness are different expressions of a single physical property, the mechanical cohesion of the material. The details of the solid's heterogeneity establish a link between strength and toughness.

5.1 Introduction

Damage mechanics is often used in numerical modelling of engineering materials, to predict the mechanical behaviour and fracture. Although damage initiation depends only on stress, the evolution of damage requires a certain amount of energy called fracture energy. Several finite element (FE) simulations have been conducted by employing the concept of strain softening, but the solution was found to be strongly dependent on the choice of mesh density [194, 195].

Several authors such as in [196-199] have studied fracture problems and proposed ways of theoretically determining the fracture energy from (hypothetical) displacement-controlled uniaxial tension test. Their approach assumes that after the peak stress a section of the specimen under tension starts to localise. While the deformation of the specimen increases the strain of the section within the damage zone increases, while the strain in the other sections of the specimen decreases. In their analysis a characteristic length scale was defined which was associated with the size of the damage zone. Although in theory the authors claim that uniaxial tension is the most direct way of measuring fracture energy, in practice, due to experimental difficulties, three point bending tests were conducted to determine the fracture energy.

Various authors [200-203] have conducted experimental work to measure the damage evolution as a function of strain. Common to all methods is that uniaxial tension tests have been conducted under a special protocol where repeated unloading/reloading cycles were imposed to a monotonic loading in order to determine the damage parameter as a function of strain. Alternative approaches for measuring the damage are discussed elsewhere [204, 205].

The approach used by several authors (e.g. [206, 207]) is based on phenomenological models, and damage models are calibrated to match experimental measurements.

Several researchers [49-52, 208] have employed Monte Carlo FE simulations to predict the fracture response, but these studies were limited to quasi-brittle materials. Common to this approach is that heterogeneity is introduced by spatially varying the fracture properties and assigning them to all elements. Fracture properties are not measured by experiments but are

calibrated based on tension tests. This approach results in capturing realistic crack paths and an accurate macroscopic response.

In the current study we perform experiments to determine the mechanical response of a sintered titanium solid; uniaxial tension, compression and three point bending tests were conducted. By employing a special test protocol, involving super-imposing to the monotonic loading of the specimen a series of N unloading/reloading cycles of strain amplitude, we measured the stiffness degradation as a function of the imposed macroscopic strain, under uniaxial tension and compression. Furthermore, an analytical model was developed to predict the tensile experiment. The gauge section of the tensile specimen was modelled with random heterogeneous material properties. The undamaged response of each element was calibrated with the compressive response of the titanium obtained from experiments. Hence by matching the macroscopic tensile response predicted by the analytical model to the measured tensile response, we determined the variation range of the fracture properties at local level as well as the length scale of heterogeneity. By employing this length scale and the variation range of fracture properties obtained from the analytical model, we performed FE simulations using the Monte Carlo analysis, and predicted the fracture toughness of the material. Predicted fracture toughness was then compared to the three-point bending measurements.

The structure of this chapter is as follows; in Section 5.2 we describe the experiments conducted and summarise the measurements performed. In Section 5.3 we present the analytical model employed to predict the length scale of heterogeneity. In Section 5.4 we provide details of the numerical FE simulations. In Section 5.5 we outline the main conclusions of this chapter.

5.2 Experiments

5.2.1 Introduction

This section describes the experimental results on the mechanical behaviour of titanium with 5% porosity. The main tests that were conducted are the following:

- Monotonic uniaxial tension tests under displacement control on dogbone specimens (T1 and T2)

- Stiffness-sensing uniaxial tension tests under displacement control on dogbone specimens (T3 and T4)
- Monotonic uniaxial compression tests under displacement control on cylindrical specimens (C1 and C2)
- Stiffness-sensing uniaxial compression tests under displacement control on cylindrical specimens (C3 and C4)
- Monotonic three-point bending tests under deflection control on prismatic specimens with rectangular cross section and prescribed notch at mid-span (B1 and B2)
- Stiffness-sensing three-point bending tests under deflection control on prismatic specimens with rectangular cross section and prescribed notch at mid-span (B3 and B4)

Testing parameters for the aforementioned tests are summarised in Table 3.

Specimen	$\Delta\varepsilon$ or $\Delta\delta$	Test
T1	n/a	Tension
T2	n/a	Tension
T3	0.0004	Tension
T4	0.002	Tension
C1	n/a	Compression
C2	n/a	Compression
C3	0.004	Compression
C4	0.004	Compression
B1	n/a	3PB
B2	n/a	3PB
B3	0.036 mm	3PB
B4	0.048mm	3PB

Table 3 Experimental parameters.

5.2.2 Mechanical tests

5.2.2.1 Monotonic tension and compression

“Quasi-static compression and tension tests were performed to measure the compressive response of titanium. Cylinders of diameter 10 mm and height 13 mm were forced to deform in uniaxial compression by a pair of lubricated loading platens. The compressive force was measured by a resistive load cell, while the specimen shortening was measured by a laser extensometer. The specimen deformation was recorded with a video camera in order to

measure the Poisson ratio via digital image correlation. Tensile tests were conducted on flat titanium specimens of dog-bone geometry, machined from rectangular, prismatic samples to have gauge length 6 mm, width and thickness of 4 mm and shoulder radius of 6 mm. Specimens were clamped by mechanical grips and loaded at quasi-static rates of strain by a screw-driven machine in displacement-control. The tensile force was measured by a resistive load cell and the elongation of the sample was measured by a high resolution camera and accompanying image analysis” Siegkas et al. [75].

Figure 5.1(a) presents the response of the material in uniaxial tension and compression, in terms of true stress versus true strain histories. The material responds in both tension and compression with an elastic behaviour (Young’s Modulus 100 GPa, Poisson’s ratio 0.1) followed by pronounced strain hardening; the tensile and compressive responses diverge at approximately strains in excess of 0.003; from this point on, the compressive response is stronger than the tensile response. In compression the test was terminated at a total strain of 0.3, while in tension the specimen fractured at a strain of order 10% in a brittle fashion, by propagation of a crack perpendicular to the loading direction (Siegkas et al. [75]). Both tensile and compressive tests were repeated 2 times and the measurements had scatter of approximately 5% in stress and 3% in failure strain (Siegkas et al. [75]).

It is well known that metallic alloys display a symmetric response in tension and compression, and it is also accepted that porous metals may display a tension/compression asymmetry, due to the details of the plastic deformation mechanisms induced by the pores; however, the asymmetry observed in Figure 5.1(a) is too large to be due to the plasticity only, considering the small porosity of only 5%. This indicates that the observed tension/compression asymmetry may be due to damage mechanisms activated in tension but not in compression.

5.2.2.2 Stiffness-sensing uniaxial tests

To further investigate the differences in the compressive and tensile responses of the titanium, this was tested, in both tension and compression, using a special test protocol, aimed at measuring the material stiffness as a function of the imposed macroscopic strain. Selected specimens of the material were tested, in both tension and compression, using a special test protocol, aimed at measuring the material stiffness as a function of the imposed strain. This involved super-imposing to the monotonic loading of the specimen a series of N

unloading/reloading cycles of strain amplitude chosen to ensure that loading and unloading occurred at the same strain rate. The corresponding measured responses were identical to those obtained by simple monotonic loading, apart from the presence of the unloading/reloading cycles.

Figure 5.1(b) presents the response of the Titanium under sensing tension, in terms of true stress versus true strain histories. For T3 approximately 300 unloading/reloading cycles of strain amplitude of 0.0004 were performed whereas in T4 approximately 60 unloading/reloading cycles were performed at a higher strain amplitude of 0.002. It was observed that at these number of cycles and amplitude strains the titanium exhibit same behaviour as the monotonic loading (Figure 5.1(b)), indicating that the mechanical response is scarcely affected by the cyclic loading imposed in the tests. The specimens in tension fracture at a strain of order 0.10 in a brittle fashion, by propagation of crack perpendicular to the loading direction.

Figure 5.1(c) presents the response of the Titanium under sensing compression, in terms of true stress versus true strain histories. For both C3 and C4 approximately 50 unloading/reloading cycles of strain amplitude of 0.004 were performed. As in sensing tension it was observed that at these number of loading/unloading cycles and at this amplitude strain the titanium exhibit same behaviour as the monotonic loading (see Figure 5.1(c)). In sensing compression the test was terminated at a total strain of 0.2.

5.2.2.3 Monotonic three-point bending

Three point bending tests on notched specimens were performed to measure the plane-strain fracture toughness, K_{IC} of the material. Specimen dimensions were chosen according to [209] with thickness, $B = 4\text{ mm}$, span, $S = 40\text{ mm}$, width, $W = 8\text{ mm}$ and crack length $a = 3.6\text{ mm}$. The force was measured by a resistive load cell, while the deflection was measured by a laser extensometer. The test was recorded by a digital camera in order to measure crack evolution via digital image analysis. The fracture toughness, K_{IC} was calculated by

$$K_{IC} = \frac{F S}{B W^{3/2}} f(\alpha / W) \quad (5.1)$$

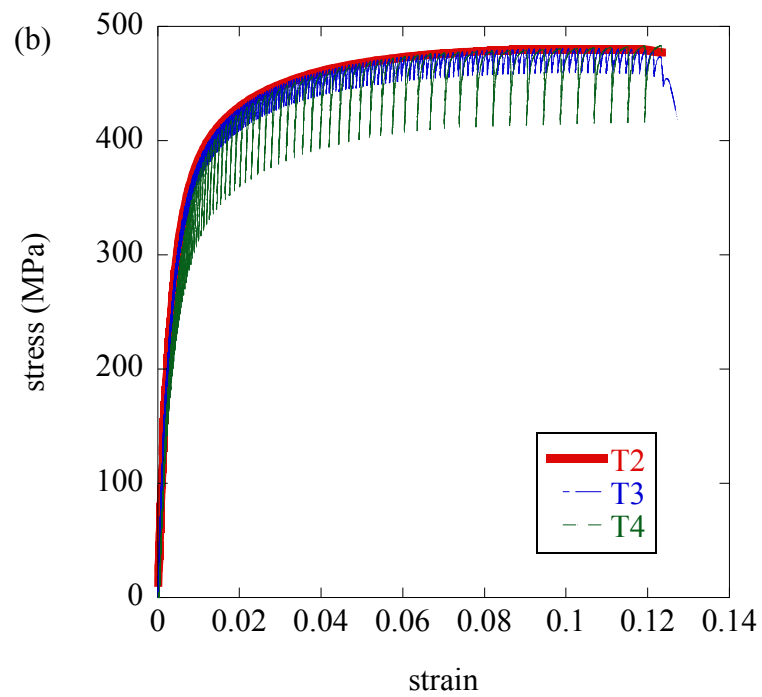
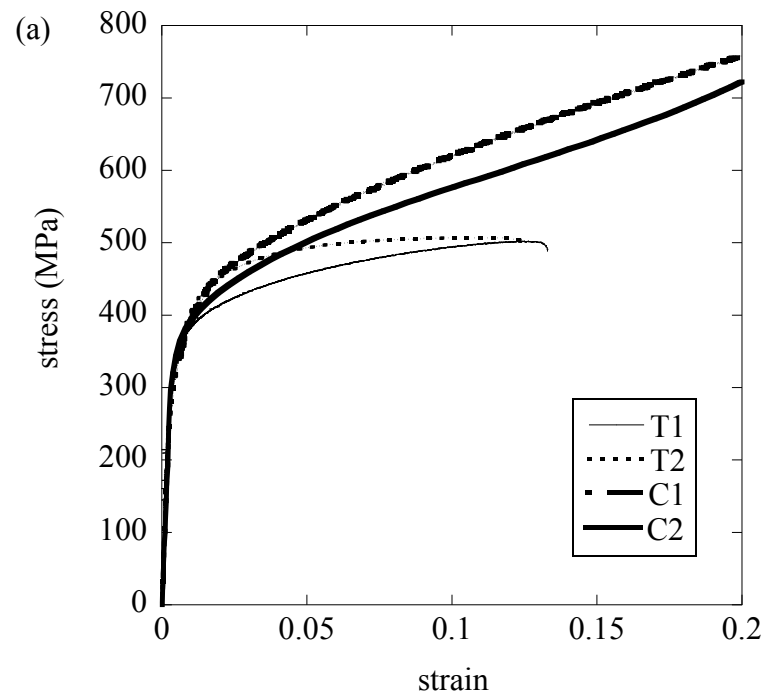
Where F is the force and $f(\alpha / W)$ is a geometric parameter and equal to 0.45.

Figure 5.1(d) presents the three-point bending response of the Titanium, in terms of force versus deflection histories. Two monotonic three-point bending loading tests were performed (B1 and B2). The peak force is approximately in the range of 1100 N and at failure the deflection is in the order of 1.3 mm. The scatter in terms of peak force is 16% and in terms of deflection at failure is 8%.

5.2.2.4 Stiffness-sensing three-point bending

Selected three point bending specimens (B3 and B4) were tested using a special test protocol, aimed at measuring the material stiffness as a function of the imposed deflection. This involved super-imposing to the monotonic loading of the specimen a series of N unloading/reloading cycles of deflection amplitude chosen to ensure that loading and unloading occurred at the same strain rate. The corresponding measured responses were similar to those obtained by simple monotonic three-point bending loading, apart from the presence of the unloading/reloading cycles.

Figure 5.1(d) presents the response of the Titanium under sensing three point bending, in terms of force versus deflection histories. The sensing three-point bending tests (B3 and B4) were repeated 2 times. For B3 approximately 35 unloading/reloading cycles of deflection amplitude of 0.0036 were performed whereas in B4 approximately 28 unloading/reloading cycles were performed at a higher deflection amplitude of 0.0048. It was observed that at these number of cycles and amplitude deflections the titanium exhibit similar behaviour as the monotonic loading (see Figure 5.1(d)). The scatter in terms of peak force is approximately 20% and in terms of failure at deflection is approximately 12%.



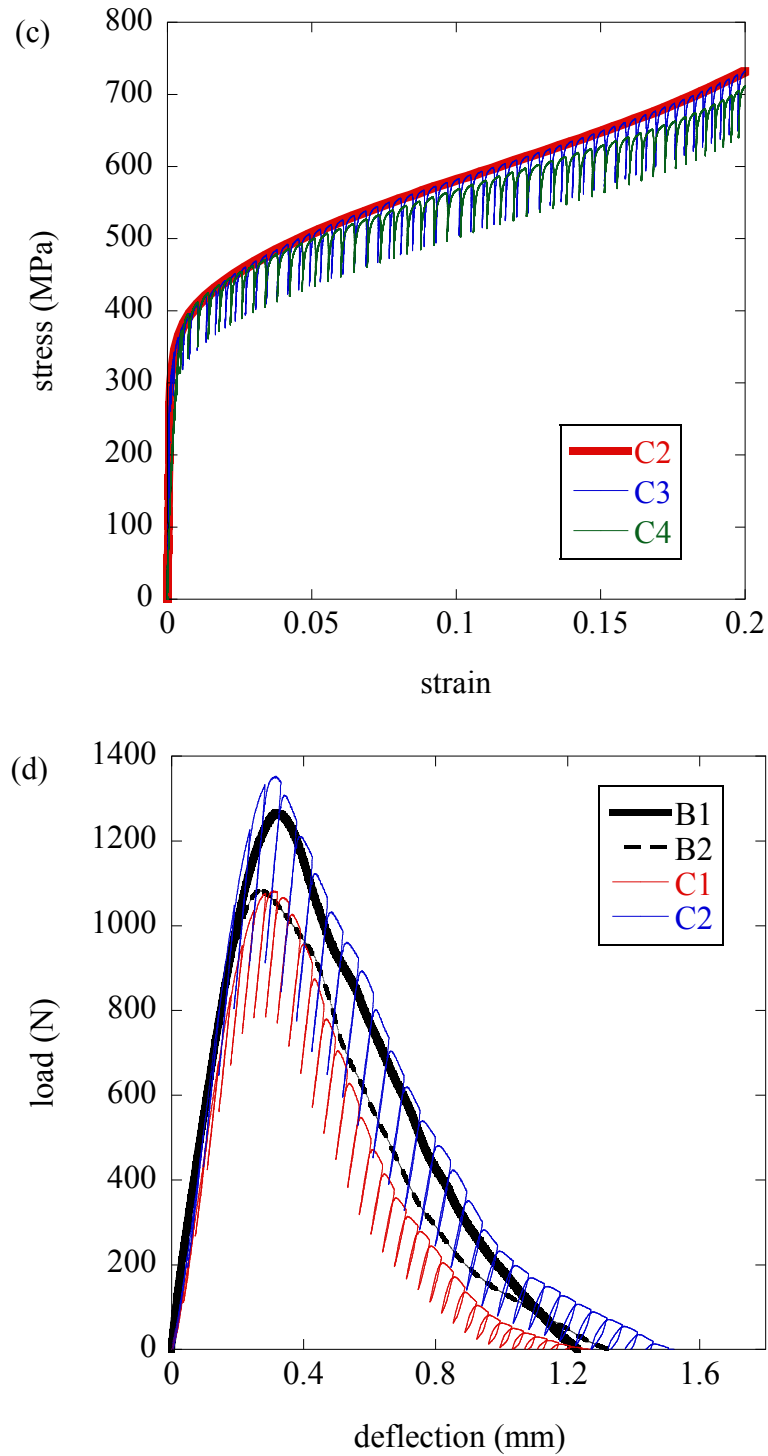


Figure 5.1 (a) Monotonic loading for tension and compression. (c) Monotonic and cyclic tensile response (d) Monotonic and cyclic compressive response. (d) Three-point bending response of monotonic and cyclic loading.

5.2.3 Data processing

5.2.3.1 Stiffness-sensing tests

An in house algorithm was developed in MATLAB to calculate the Young's modulus degradation as a function of strain. A low pass filter was incorporated to improve the strain signal which was experimentally measured via two strain gauges attached. The common part of the local reloading and unloading Modulus was calculated and the result was shown in Figure 4.5 for specimens T4 and C4. Similar approach was implemented to measure the stiffness of the specimens under stiffness-sensing three-point bending (see Figure 5.2). In compression, the stiffness is insensitive to strain until the imposed strain exceeds the value 0.1, after which closure of the small pores results in a slight material stiffening. In tension the modulus decreases monotonically with strains when these exceed a value of approximately 0.003. Such reduction is a consequence of both pore cavitation and nucleation and growth of micro-cracks, also observed in *in-situ* tests. In addition, in order to shed light on the microscopic mechanisms of deformation and fracture of the material, optical microscopy was conducted as shown in Figure 4.4.in Section 4.2.2. The sensing tests together with the optical microscopy study, proved our initial assumption that in tension and compression, titanium exhibits different behaviour. Hence by the in-situ tests as well as the sensing tension and compression tests we calibrate the undamaged response with the compressive measured response.

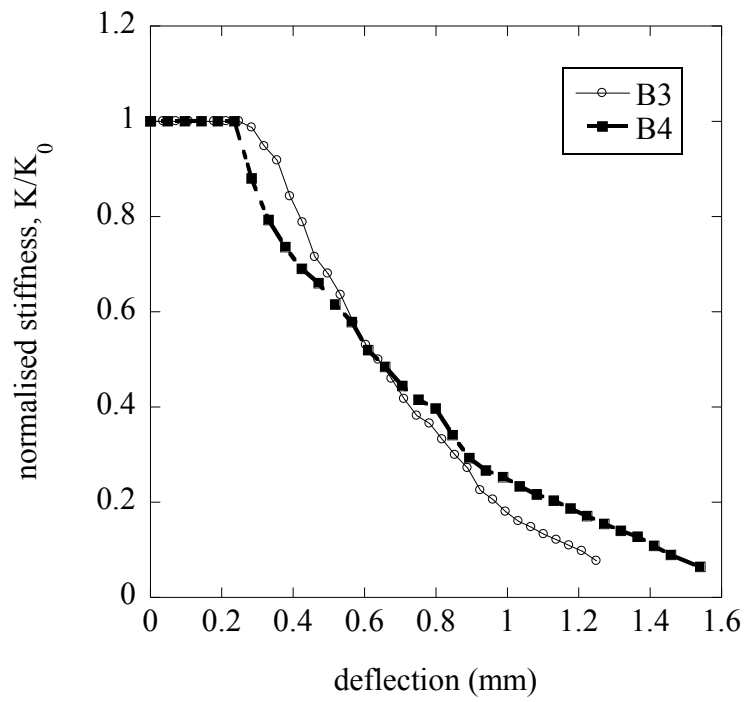


Figure 5.2 Percentage decrease of experimental stiffness as a function of deflection.

5.2.3.2 Video processing

An in house algorithm was developed to calculate crack length as a function of the applied deflection. The video analysis environment was implemented in MATLAB. An analysis over recorded videos during the three-point bending tests is employed. The crack length is recorded using a digital camera, producing .avi type video data. The video stream consists of continuous stream of recorded images called frames. Consequently the method for video analysis was applied for every frame. The video analysis checks for a number of consecutive frames that the pixel is cracked (colour is black) and after that declares corresponding pixel as a cracked pixel.

The crack length is calculated using a method that determines a number of sequential pixels that belong to the cracked segment which is progressively formed. The algorithm starts from an initial cracked pixel and moves iteratively to the next one. Horizontal or vertical movement is permitted according to a decision algorithm. This algorithm was not able to capture crack evolution when the crack occurred at isolated fragments i.e. when it was not continuous. Consequently the algorithm stopped and an amount of the cracked segment was lost.

For the cases where the crack was not continuous a second algorithm was employed based on the cracked area. For every frame the algorithm detects all the cracked pixels and sums their cracked area. For every frame the summed cracked area creates fictitious triangles where their heights represent the crack length.

Figure 5.2 shows the percentage decrease of the stiffness of titanium as a function to the crack length. For both B3 and B4 the stiffness remains constant up to approximately 0.2 mm deflection and decreases almost exponentially therefore after. B3 has a higher crack length because the crack evolution is curved.

In Figure 5.3(a) the crack length as a function of deflection history is plotted. For B2 and B4 specimens the cracks were observed to be straight. For B1 and B3 the cracks were observed to be curved. Linear elastic FE models with pre-existing cracks were performed to determine the crack length as a function of deflection. Details of the simulations are shown in APPENDIX A

(Section 5.6). The linear elastic FE models were able to predict the crack length versus deflection history as shown in Figure 5.3(b).

In Figure 5.4 the plain-strain fracture toughness, K_{IC} is plotted as a function of crack length for the specimens which had straight cracks only. For B2 the initial fracture toughness was $K_{IC} = 33.4 \text{ MPa m}^{1/2}$ whereas for B4 it was $K_{IC} = 37.5 \text{ MPa m}^{1/2}$.

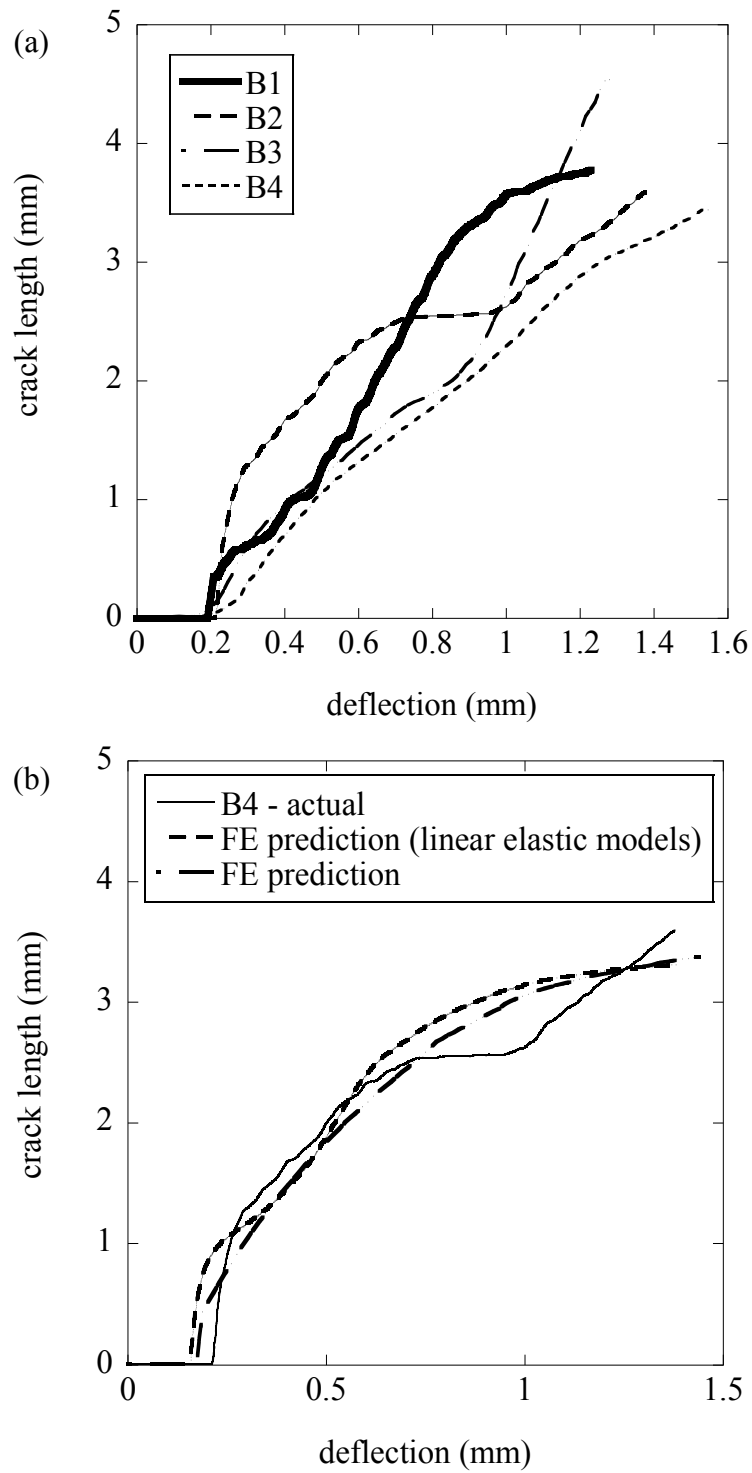


Figure 5.3 (a) Crack length as a function of deflection for the different types of loading for the three-point bending test. (b) Measured and predicted crack length versus deflection history for B4.

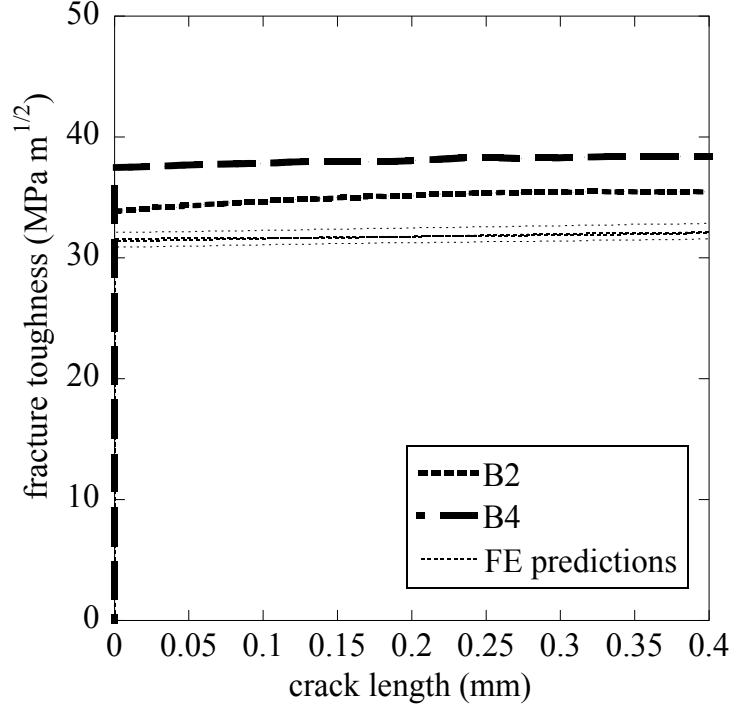


Figure 5.4 Measured and predicted fracture toughness as a function of crack length (Experiments and FE simulations with straight cracks only are shown).

5.3 Analytical model

An analytical model was developed to mimic the tensile experiments. In order to mimic the tensile experiment, only the gauge section (2mm x 2mm x 4mm) of the tensile specimen was modelled. The gauge section consists of N_s slices loaded in tension with heterogeneous random fracture properties. Every slice comprises a number of elements which undergo the same strain (parallel model). A bilinear damage law was assumed for every element within a slice. Damage initiation strain, intermediate strain and failure strain vary for every element within each slice according to

$$\begin{aligned}
 \varepsilon_o(r_i) &= \varepsilon_o^{\min} + r_i(\varepsilon_o^{\max} - \varepsilon_o^{\min}) \\
 \varepsilon_{\text{int}}(r_i) &= \varepsilon_{\text{int}}^{\min} + r_i(\varepsilon_{\text{int}}^{\max} - \varepsilon_{\text{int}}^{\min}) \\
 \varepsilon_f(r_i) &= \varepsilon_f^{\min} + r_i(\varepsilon_f^{\max} - \varepsilon_f^{\min})
 \end{aligned} \tag{5.2}$$

where, r_i denote uniformly distributed, uncorrelated random numbers in the interval [0,1]. The damage at intermediate strain was fixed at 0.14. Thus each element has a unique stress-strain

curve based on the damage parameters assigned to that element. The homogenised response of each slice undergoes the same stress. In other words this may be considered as a series model consisting of N_s slices where each element is now a slice and is the homogenised response of N_p parallel elements. Thus, again, each slice possesses a varying damaged stress-strain characteristic which is the result of the parallel response of N_p elements according to the parallel model. Hence, the series–parallel model is effectively the series model with the parallel model applied as a sub–step to each slice. Illustration of the model is shown in Figure 5.5.

The aim of the analytical model is to determine the length scale and the fracture properties variation range at the local level. The analytical investigation was performed in three stages; a series model, a parallel model and then a series–parallel model representing the actual specimen.

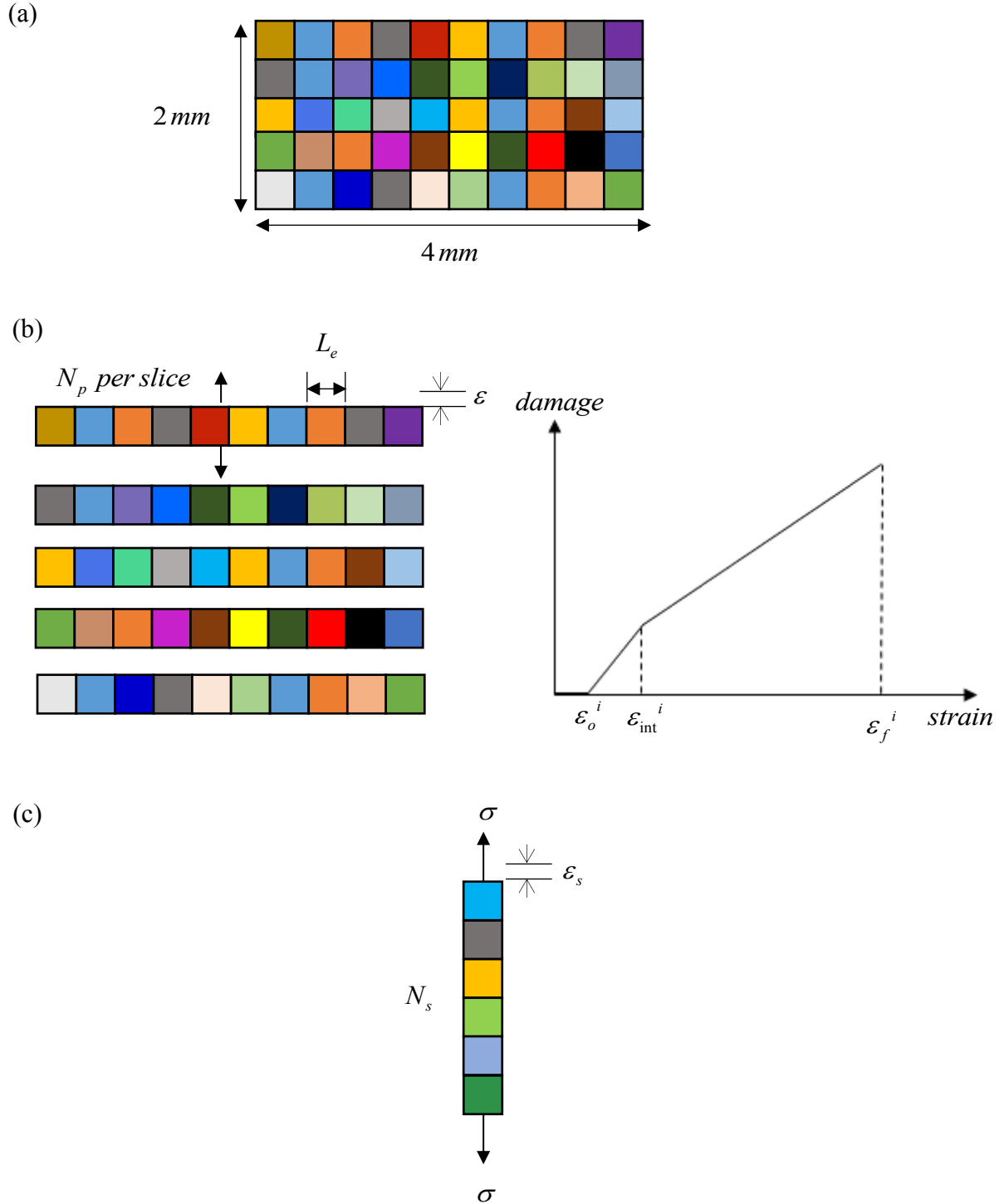


Figure 5.5 (a) Schematic illustration of a planar view of the tensile specimen (gauge section). (b) Schematic illustration of the parallel model (random bilinear damage profiles were assumed for all elements within a slice) (c) Schematic illustration of the series model (each slice is the homogenised response of a parallel model).

5.3.1 Analysis of a series model

A series model consisting of N_s elements each possessing varying damaged stress-strain responses, σ_i , was shown in Figure 5.5(c). The undamaged response of the material, σ_u is calibrated according to the measured compressive response of the titanium shown in Figure 5.1(a). The damage coefficient for element i at a strain ε_i is given by:

$$d_i(\sigma) = 1 - \frac{\sigma}{\sigma_u(\varepsilon_i)} \quad (5.3)$$

Figure 5.6(a) shows the stress-strain profile for an undamaged material as well as the damaged profiles for the N_s elements that constitute the series model; for clarity, only 2 elements are shown. It should be noted that for a given level of stress in the model, σ , that not all of the elements may be damaged; some may possess a deterministic response which is equivalent to $d_i = 0$ for these elements. A key value of stress in the model is the min-max stress, σ_{mm} , which is the maximum stress of the weakest element in the chain of elements; this is equivalent to the weakest link theory which defines the overall global response of the model. The σ_{mm} separates the two regimes of response, the loading phase where strain in the weakest link, w , is less than that corresponding to σ_{mm} , i.e. $\varepsilon_{i=w} \leq \varepsilon_{mm}$, and the unloading phase for strains after this point and up until the fracture strain, ε_{max} , i.e. $\varepsilon_{mm} < \varepsilon_{i=w} \leq \varepsilon_{max}$. In this context, unloading refers to the fact that there is decreasing stress in the series model with increasing applied strain. These two phases are shown in Figure 5.6(a).

During the loading and subsequent unloading phases, the level of stress, σ , supported by the element chain is given by the weakest link or element in the model. The global strain, ε_s , is related to the element strains by virtue of the true strain addition law:

$$\varepsilon_s = \ln \left[\frac{1}{N_s} \sum_{i=1}^{N_s} \exp(\varepsilon_i) \right] \quad (5.4)$$

For the loading phase, the strain in damaged element i is that corresponding to $\sigma_i = \sigma$

$$\varepsilon_i = \varepsilon(\sigma_i = \sigma) \quad (5.5)$$

Substituting Eq. (5.4) into Eq. (5.3), we have

$$\varepsilon_s = \ln \left[\frac{1}{N_s} \sum_{i=1}^{N_s} \exp(\varepsilon(\sigma_i = \sigma)) \right] \quad (5.6)$$

The global damaged unloading modulus, E_s , is given by,

$$E_s = \left[\sum_{i=1}^{N_s} \frac{\varphi_i}{E_i(\sigma_i)} \right]^{-1} \quad (5.7)$$

where φ_i is the strain fraction of the element i :

$$\varphi_i = \frac{\exp(\varepsilon_i)}{\sum_{i=1}^{N_s} \exp(\varepsilon_i)} \quad (5.8)$$

and E_i is the damaged modulus of element i :

$$E_i(\sigma_i) = E_0(1 - d_i(\sigma_i)) \quad (5.9)$$

Substituting Eq. (5.7) and Eq. (5.8) into Eq. (5.6), we have for the global unloading modulus

$$E_s = \left[\sum_{i=1}^{N_s} \frac{\exp(\varepsilon_i)}{E_0 \left(\sum_{i=1}^{N_s} \exp(\varepsilon_i) \right) (1 - d_i(\sigma_i))} \right]^{-1} \quad (5.10)$$

However, once the stress in the model reaches σ_{mm} , the strains in the damaged elements obey different laws from this point onwards in what is now the unloading phase, Figure 5.6(b). For the weakest element, the strain is as before:

$$\varepsilon_i = \varepsilon(\sigma_i = \sigma), \quad i = w \quad (5.11)$$

For the remaining $N_s - 1$ elements, they now start to unload elastically, since their corresponding maximum stresses have not been reached. Thus the strain for element i is equal to the strain at σ_{mm} minus an elastic unloading component:

$$\varepsilon_i = \varepsilon(\sigma_i = \sigma_{mm}) - \frac{\sigma_{mm} - \sigma}{E_i} \quad i \neq w \quad (5.12)$$

or, substituting for the damaged modulus from Eq. (5.8) based on stress at σ_{mm} ,

$$\varepsilon_i = \varepsilon(\sigma_i = \sigma_{mm}) - \frac{\sigma_{mm} - \sigma}{E_o(1-d_i(\sigma_{mm}))} \quad i \neq w \quad (5.13)$$

Thus, as a global strain formula, we have

$$\varepsilon_s = \ln \left[\frac{1}{N} \left[\exp(\varepsilon_{i=w}(\sigma)) + \sum_{i \neq w}^N \exp \left(\varepsilon(\sigma_i = \sigma_{mm}) - \frac{\sigma_{mm} - \sigma}{E_o(1-d_i(\sigma_{mm}))} \right) \right] \right] \quad (5.14)$$

A similar construction for the global modulus yields:

$$E_s = \left[\frac{\exp(\varepsilon_{i=w})}{E_o \left(\sum_{i=1}^N \exp(\varepsilon_i) \right) (1-d_{i=w}(\sigma_{i=w}))} + \sum_{i \neq w}^N \frac{\exp(\varepsilon_i)}{E_o \left(\sum_{i=1}^N \exp(\varepsilon_i) \right) (1-d_i(\sigma_{mm}))} \right]^{-1} \quad (5.15)$$

This means that only the weakest element has a decreasing damaged modulus with increasing strain since the remaining elements have a constant modulus which was determined by the element damages at σ_{mm} .

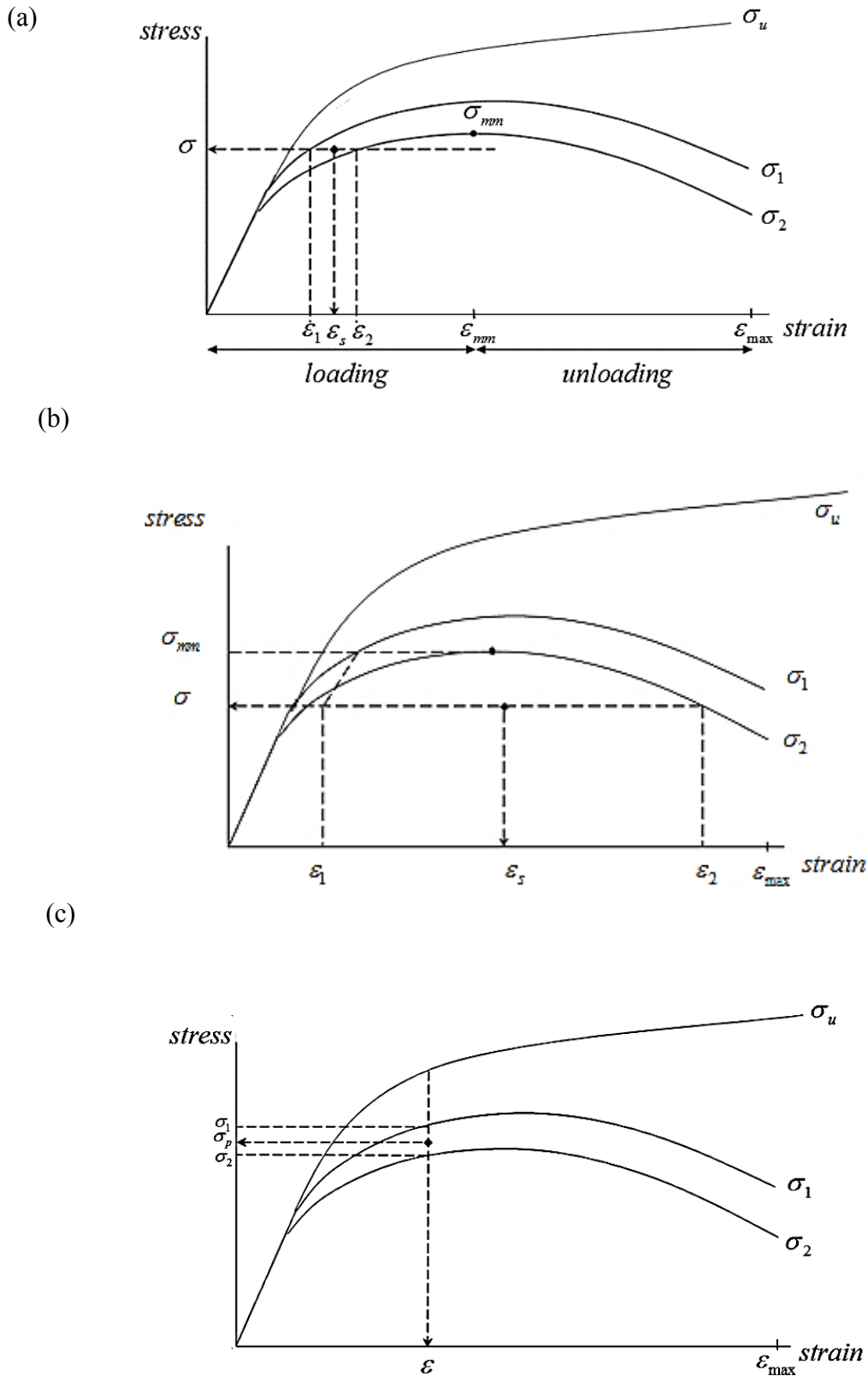


Figure 5.6 (a) Response during loading phase for the series model. (b) Response during unloading phase for the series model (c) Response for the parallel model.

5.3.2 Analysis of a parallel model

A parallel model consisting of N_p elements each possessing varying damaged stress-strain responses is discussed below. In a similar manner as before, Figure 5.6(c) shows the stress-strain profile for an undamaged material as well as the damaged profiles for 2 elements under same strain. The constituent equations are simpler than for the series model since there is only one loading regime. The stress in element i is given by

$$\sigma_i(\varepsilon) = \sigma_u(1 - d_i(\varepsilon)) \quad (5.16)$$

where, again $d_i = 0$, if the element is as yet undamaged for the given level of applied strain.

The global stress, σ_p , in the model is given by the sum of the element stresses:

$$\sigma_p(\varepsilon) = \frac{1}{N_p} \sum_{i=1}^{N_p} \sigma_i(\varepsilon) \quad (5.17)$$

By substituting Eq. (5.15) into Eq. (5.16), we have

$$\sigma_p(\varepsilon) = \frac{1}{N_p} \sum_{i=1}^{N_p} \sigma_u(1 - d_i(\varepsilon)) \quad (5.18)$$

The global unloading modulus is given by the analogous expression:

$$E_p(\varepsilon) = \frac{1}{N_p} \sum_{i=1}^{N_p} E_o(1 - d_i(\varepsilon)) \quad (5.19)$$

5.3.3 Analytical results

Bi-linear damage profiles were assumed for all elements within a slice of the model. The undamaged response of the material, σ_u is calibrated according to the measured compressive response of the titanium shown in Figure 5.1(a). A parametric study was performed to investigate the influence of the randomisation ranges of both the damage initiation, the intermediate strain and fracture strains within the material. These damage parameters ranges were then inferred from correlation of the parametric study with the experimental tensile stress–strain profiles shown in Figure 5.1(a). The ranges that were found to correlate best with tensile experiments are

$$\begin{aligned}\varepsilon_0 &= 0.001 - 0.002 \\ \varepsilon_{\text{int}} &= 0.01 - 0.03 \\ \varepsilon_f &= 0.57 - 0.64.\end{aligned}\tag{5.20}$$

For further information on the choice of the strain ranges, see APPENDIX B (Section 5.6). A further examination was made to determine the N_s required to accurately represent the gauge section of the tensile specimen. Number of series elements ranging from $N_s = 3 - 20$ were examined and the effect on the average response based on 10 realisations is shown in Figure 5.7(a). By increasing the number of series elements it was observed that the average failure strain decreased, whereas the average response always correlated with the tensile experiments. For every element in the combined model we calculated the fracture energy per unit area, G_f , which is given by:

$$G_f = \int_0^{\bar{u}_f^{pl}} \sigma_y d\bar{u}^{pl}\tag{5.21}$$

The consequent variation of the fracture energy per unit area, G_f , was determined from the varying damaged stress–strain profiles for the elements in the model. This was achieved by employing a trapezoidal rule numerical integration scheme. Cumulative distributions for the fracture energy, G_f are shown in Figure 5.7(b) and Table 4.

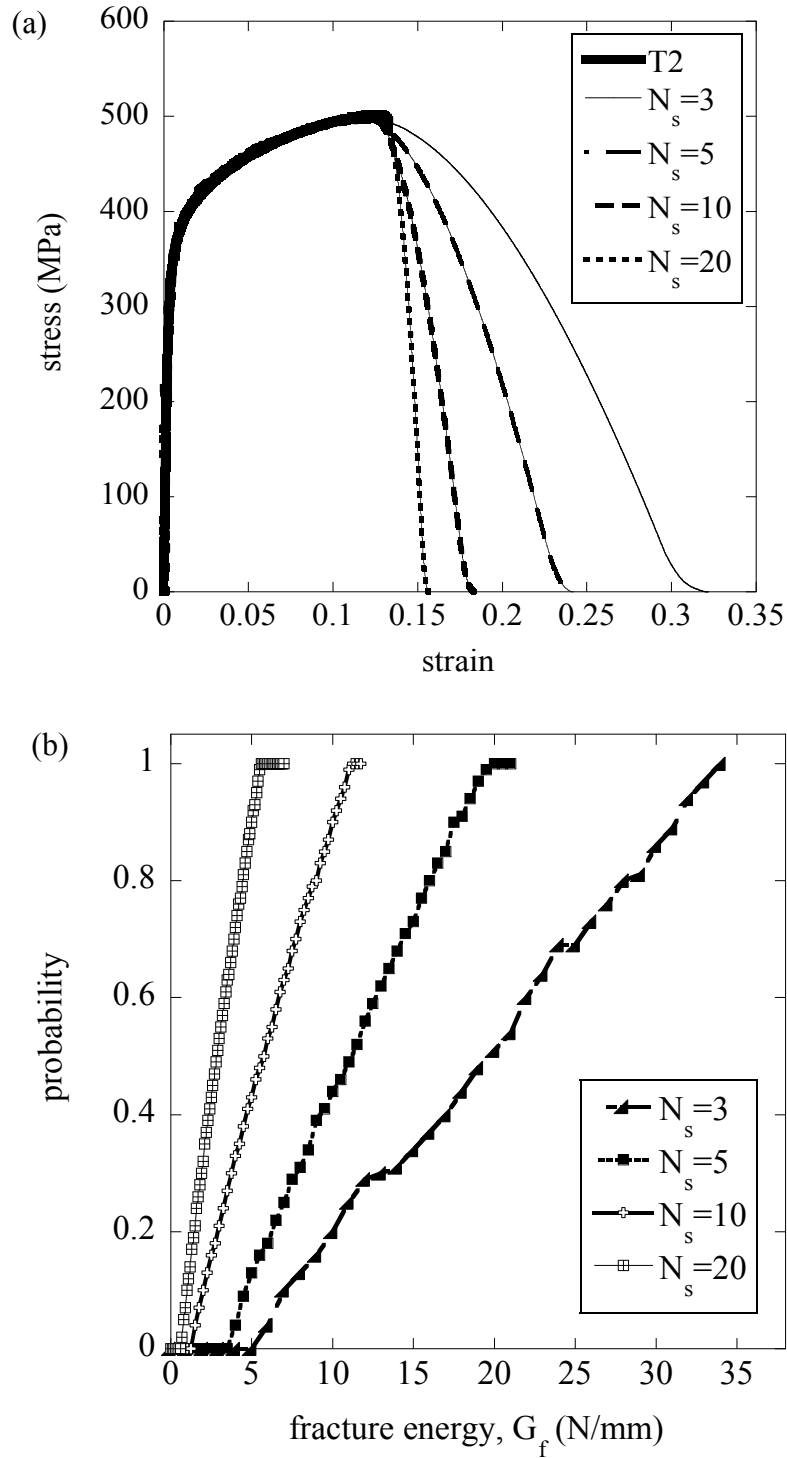


Figure 5.7 (a) Effect of N_s on the stress-strain response. (b) Cumulative distribution functions of fracture energy, G_f as a function of N_s . The variation of damage initiation strain, intermediate strain and failure strain are $\varepsilon_0 = 0.001-0.002$, $\varepsilon_{int} = 0.01-0.03$ and $\varepsilon_f = 0.57-0.64$ respectively.

N_s	L_e (mm)	$G_{f,\min}$ (N/mm)	$G_{f,\max}$ (N/mm)
3	0.67	5.03	33.50
5	0.4	3.00	20.00
10	0.2	1.50	10.00
20	0.1	0.08	5.00

Table 4 Summary of the results for the analytical model.

The choice of N_s was achieved by comparing the scatter in stress values across multiples simulations. Over 10 repeated simulations the mean predicted stress-strain profiles correlated almost perfectly (see Figure 5.8) with the tensile experimental data for $N_s = 10$ and $N_s = 20$. The scatter was found to be 5% from experiments (see Figure 5.1(a)), and for the analytical model it was observed that for $N_s = 10$ the scatter was also 5%, whereas for $N_s = 20$ the scatter was less than 1%. Hence in order to mimic the experimental testing results we conclude that the length scale of heterogeneity of the gauge section must be $L_e = 0.2 \text{ mm}$ ($N_s = 10$).

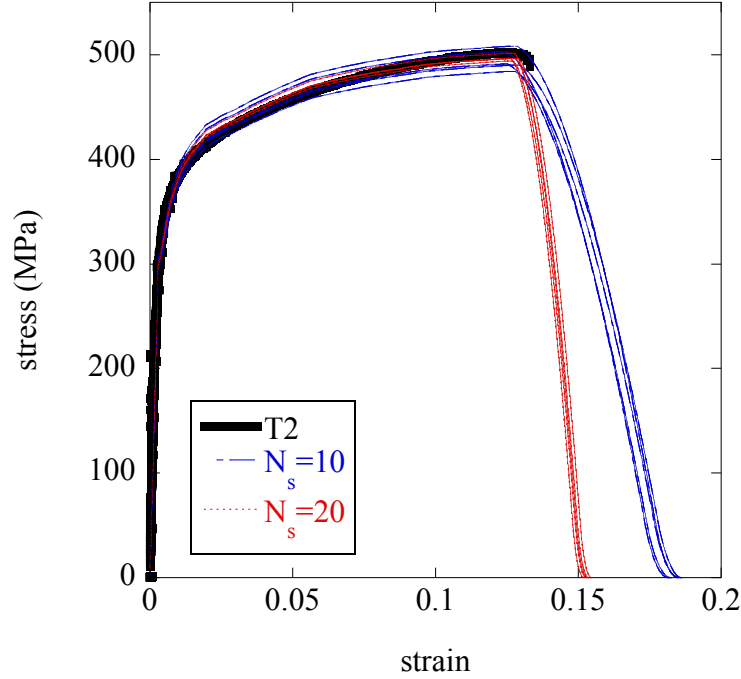


Figure 5.8 Scatter of stress-strain response for $N_s = 10$ and $N_s = 20$. Repeated simulations have been plotted for each N_s . The variation of damage initiation strain, intermediate strain and failure strain are $\varepsilon_0 = 0.001 - 0.002$, $\varepsilon_{\text{int}} = 0.01 - 0.03$ and $\varepsilon_f = 0.57 - 0.64$ respectively.

5.4 Finite Element Simulations

In this section we present the details of the numerical FE simulations. The Monte Carlo method was employed and repeated FE simulations on different realisations of random fields of material properties were examined. Every simulation is performed in ABAQUS Standard. Two different tests are modelled, a three-point bending and a uniaxial tension. While the elastic and the plastic response of titanium are modelled as homogeneous, the failure parameters i.e. strain at which ductile fracture initiates, as well as that corresponding to final fracture are randomised according to a uniform distribution spatially in the domain.

5.4.1 Constitutive model

Elasticity of this solid was modelled as linear isotropic, with $E = 100 \text{ GPa}$ and $\nu = 0.1$ as measured. We model the plastic behaviour of the material with J_2 plasticity. The plastic response is calibrated according to the measured compressive response of the titanium, shown in Figure 5.1(a). The onset and evolution of failure is modelled using a continuum ductile

damage model. The chosen damage model allows specifying an equivalent plastic strain at initiation of damage and the subsequent damage evolution as a function of the applied equivalent plastic displacement of the element.

The damage initiation strain is specified as a function of stress triaxiality η , defined as the ratio of hydrostatic to deviatoric (equivalent von Mises) stress, $\eta = \sigma_H / \sigma_{VM}$. At triaxiality $\eta \geq 1/3$ the damage initiation strain is taken as independent of triaxiality and is varied according to a uniform distribution function between $\bar{\varepsilon}_{PL} = 0.0009 - 0.00019$ (these values are found from the analytical model). At triaxiality $\eta = 0$ (pure shear), the equivalent plastic strain at damage initiation is taken as the equivalent von Mises plastic strain corresponding to a maximum tensile principal strain resulting in a variation of $\bar{\varepsilon}_{PL} = 0.001 - 0.002$. A linear interpolation is used to calculate the damage initiation strain at triaxiality $0 < \eta < 1/3$. In presence of compressive hydrostatic stress, and for $\eta \leq -1/3$, the damage initiation strain is arbitrarily set to a relatively large constant value ($\bar{\varepsilon}_{PL} = 0.2$), in line with the fact that no damage or appreciable stiffness degradation was measured for the material in compression at applied strains less than 0.2. A linear interpolation is used to determine the damage initiation strain in the range $-1/3 < \eta < 0$.

The damage evolution is characterised by the progressive degradation of the material modulus and ranges between 0 and 1. In order to define damage evolution, ABAQUS requires the damage variable as a function of plastic displacement. The analytical results are in terms of strain, thus the plastic displacement was obtained from the plastic strain by multiplying by the element size L_e of the finite elements employed. The intermediate strain and fracture strain varied according to a uniform distribution function between $\varepsilon_{int} = 0.01 - 0.03$ and $\varepsilon_f = 0.57 - 0.64$ (values obtained from the analytical model).

5.4.2 FE simulations for the 3PB

5.4.2.1 Boundary conditions

Prismatic beams of thickness, $B = 4 \text{ mm}$, span, $S = 40 \text{ mm}$, width, $W = 8 \text{ mm}$ and crack length $\alpha = 3.6 \text{ mm}$ were loaded in three-point bending by rigid fully constrained analytical surfaces of radius $R = 3 \text{ mm}$ to mimic the experimental boundary conditions. Rigid fully constrained analytical surfaces were created to support the model and a rigid surface pushing downward on the centre of the upper surface of the body was defined; this was achieved by specifying a vertical displacement on the rigid surface ($u_2 = -1.5 \text{ mm}$). The contact between the beam and the analytical surfaces were modelled by using a surface-to-surface algorithm of frictionless tangential behaviour. Further boundary conditions applied were to the tip of the notch to prevent lateral movements ($u_1 = u_3 = 0$) as well as to points A and A' (see Figure 5.9) to prevent transverse movement ($u_3 = 0$).

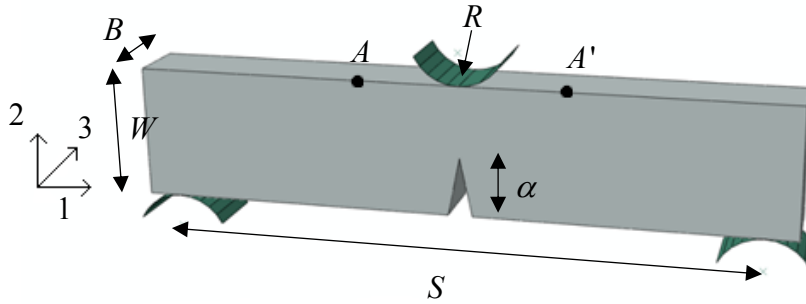


Figure 5.9 Dimensions of the beam.

5.4.2.2 3PB deterministic simulations

The beam was meshed using fully integrated eight-node brick linear elements (C3D8). Preliminary sets of simulations were conducted to determine numerical convergence of the three point bending (Figure 5.10). The mean fracture energy values inferred from the analytical model were employed, for each element size. Five different element sizes were considered which correspond to the element sizes that were investigated in the analytical model (see Table 4). What is observed is that by decreasing the element size (G_f decreases as well) the three-point bending response becomes weaker.

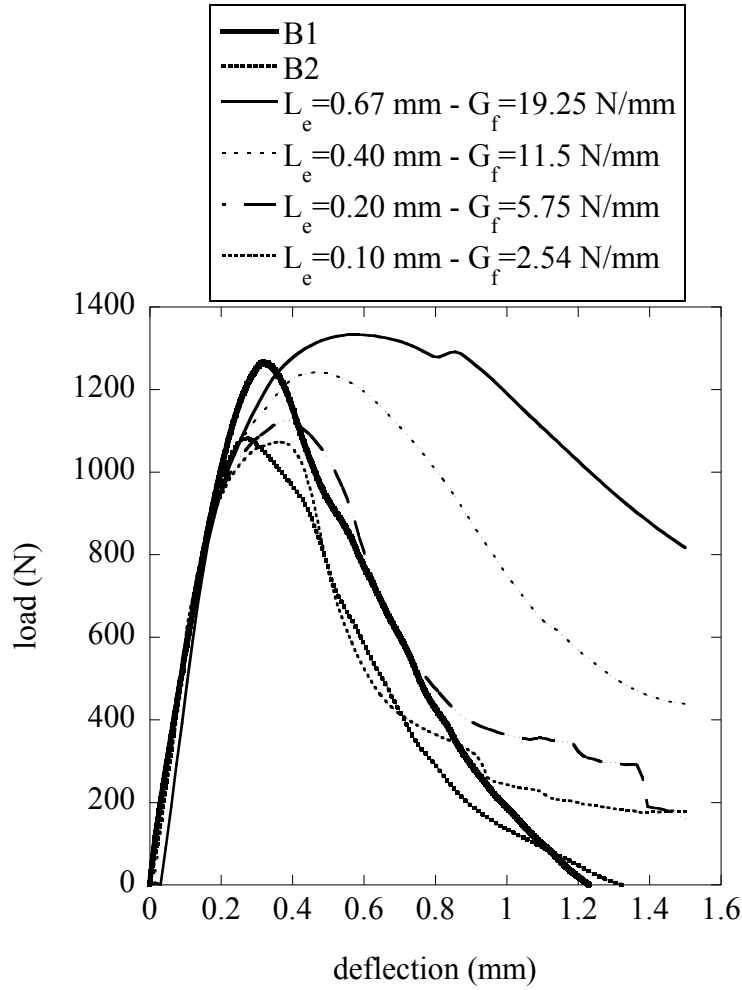


Figure 5.10 Effect of L_e on the deterministic FE simulations.

5.4.2.3 3PB Monte Carlo FE simulations

FE predictions are compared to experimental results in Figure 5.11. The variation of damage initiation strain, intermediate strain and fracture strain are given by (5.20). Linear brick elements (C3D8) were used. Monte Carlo FE simulations were performed for two different element sizes i.e. $L_e = 0.2\text{ mm}$ and $L_e = 0.1\text{ mm}$; for both element sizes 10 realisations were conducted and the scatter is in the order of 4%. Simulations with homogeneous properties were also conducted; the mean values inferred from the simulations with heterogeneous properties were employed for each element size. The peak force of the FE simulations with homogeneous properties was found to be 1120 N and 1070 N for $L_e = 0.2\text{ mm}$ and $L_e = 0.1\text{ mm}$ respectively. FE simulations with random heterogeneous fracture properties were found to be below that of the FE simulations with homogeneous properties. The mean values of the peak force were

found to be 1040 N and 1010 N for $L_e = 0.2$ mm and $L_e = 0.1$ mm respectively. In addition the simulations with homogeneous properties could not predict cracks that are curved whereas simulations with random heterogeneous fracture properties can predict both straight and curved cracks. In Figure 5.12(a) we show photographs of the tested beams at deflection of 1 mm whereas in Figure 5.12(b) we show photographs of the finite element model for four different realisations for same deflection as the experiments. In conclusion, the choice of $L_e = 0.2$ mm provide results which are very close to the experiments.

5.4.3 Monte Carlo FE predictions of fracture toughness K_{IC}

Predictions are compared to experiments in Figure 5.4. Five realisations are shown for the FE simulations that developed straight cracks. The element size, $L_e = 0.2$ mm was employed. Fracture toughness was calculated using Eq. (5.1). The crack length versus deflection was calculated using the predicted stiffness versus deflection curve found by the combination of linear elastic FE simulations with pre-existing cracks which are discussed in the APPENDIX A, in Section 5.6. Hence the initial mean fracture toughness of the FE simulations was found to be $K_{IC} = 31.1 \text{ MPa m}^{1/2}$ and the scatter of the results are less than 7%. The experimental fracture toughness was found to be slightly above that found by the Monte Carlo FE simulations.

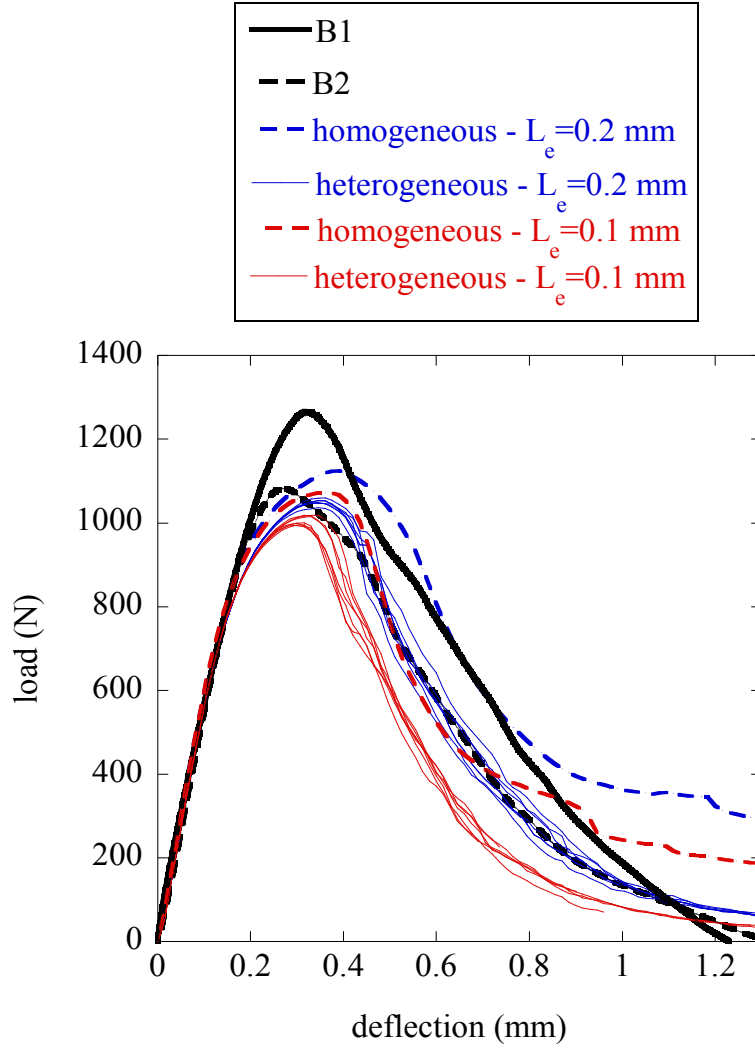


Figure 5.11 Three-point bending repeated FE simulations for the stochastic case for $L_e = 0.2\text{ mm}$ and $L_e = 0.1\text{ mm}$. The variation of damage initiation strain, intermediate strain and failure strain are $\varepsilon_0 = 0.001 - 0.002$, $\varepsilon_{\text{int}} = 0.01 - 0.03$ and $\varepsilon_f = 0.57 - 0.64$ respectively.

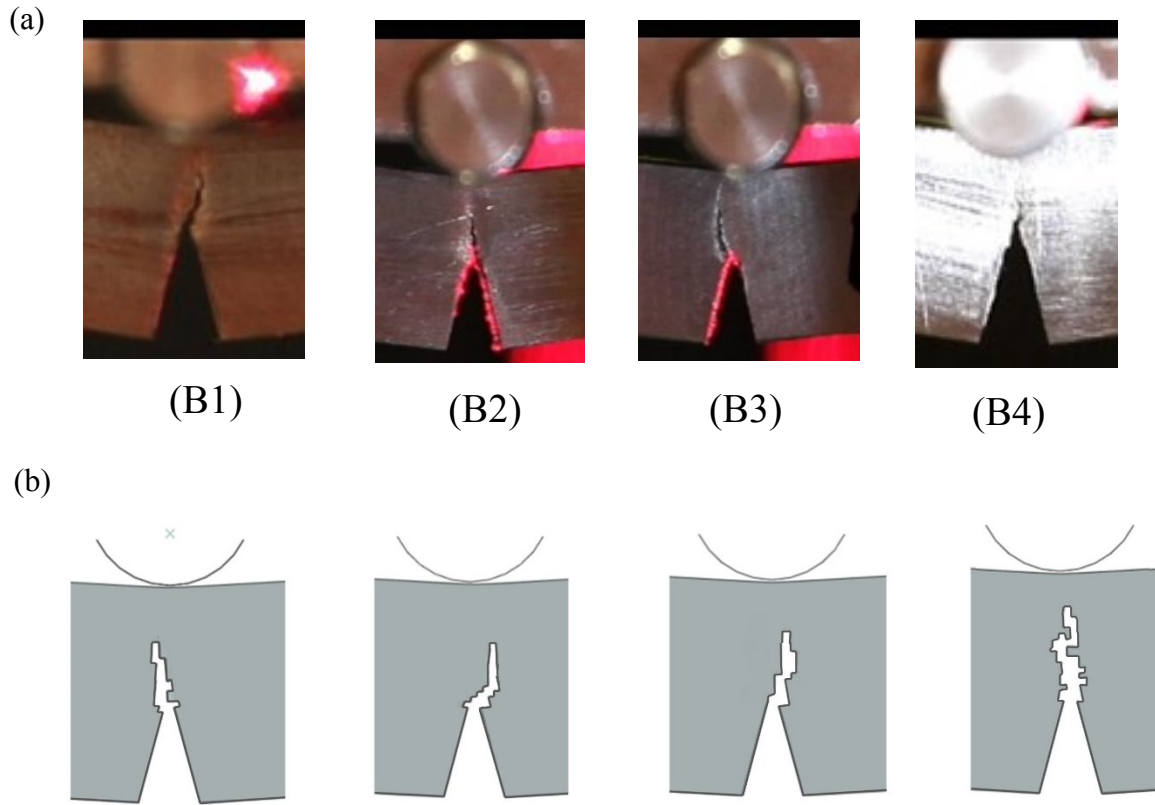


Figure 5.12 (a) Crack evolution for the three-point bending experiments at deflection equal to 1 mm.(b) Crack evolution for the three-point bending FE simulations at deflection equal to 1 mm.

5.4.4 Monte Carlo FE simulations for uniaxial tension

In order to validate the analytical model a uniaxial tension was modelled in ABAQUS. Elastic and plastic properties were taken from Figure 5.1(a). The plastic response was calibrated with the experimental compressive response. Random heterogeneous fracture properties were assigned to each element. Bilinear damage profiles were assumed. Damage initiation strain, the intermediate strain and failure strain are varied according to Eq. (5.20).

A rectangular of dimensions $2\text{mm} \times 2\text{mm} \times 4\text{mm}$ was modelled in order to mimic the gauge section of the tensile experiment. One of the faces of the cubic SVE has normal displacements constrained, while the opposite face is subject to linearly ramped normal displacements, such to induce axial tensile strain. The lateral faces are constrained to remain planar and the normal

displacements on opposite lateral faces are forced to be equal and opposite; these constraints are imposed via the constraint equation. tool of ABAQUS CAE, making use of dummy nodes.

The rectangular was meshed using linear brick elements (C3D8). Two element sizes were employed $L_e = 0.2\text{mm}$ and $L_e = 0.1\text{mm}$. Monte Carlo FE simulations were performed based on 10 different realisations. The output of the Monte Carlo simulations is shown in Figure 5.13. For $L_e = 0.2\text{mm}$ the scatter was found to be 5% whereas for $L_e = 0.1\text{mm}$ the scatter is less than 1%. Similar scatter was obtained from the analytical model (see Figure 5.8).

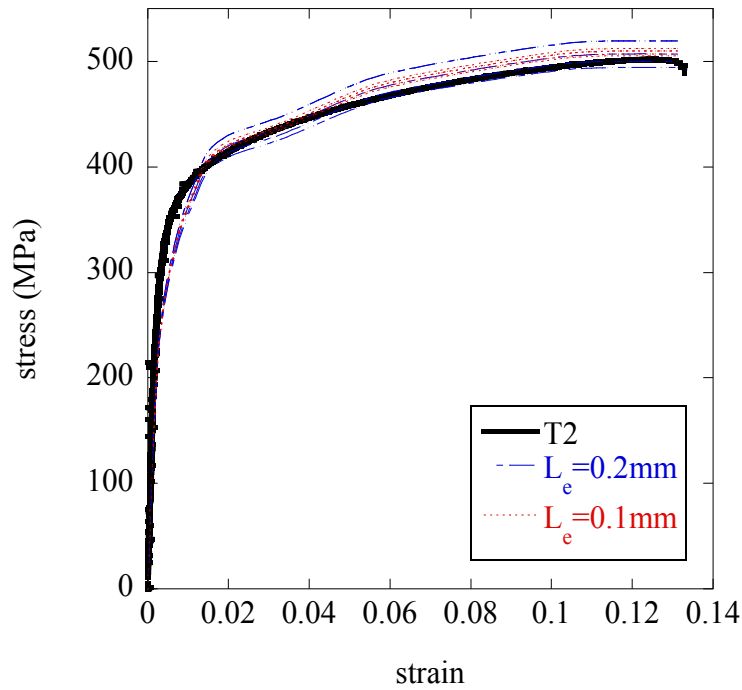


Figure 5.13 Tensile repeated FE simulations for the stochastic case for $L_e = 0.2\text{mm}$ and $L_e = 0.1\text{mm}$. Damage initiation strain, intermediate strain and fracture strain vary according to a uniform distribution functions; $\varepsilon_0 = 0.001-0.002$, $\varepsilon_{\text{int}} = 0.01-0.03$ and $\varepsilon_f = 0.57-0.64$ respectively.

5.5 Concluding Remarks

Experimental, analytical and numerical analyses were conducted for a sintered titanium solid. The aim of the chapter was to predict fracture toughness from a uniaxial tension and compression. Uniaxial tension, compression and three point bending experiments were performed to investigate the mechanical behaviour of the titanium solid. An analytical model was developed to mimic the tensile experiment of titanium by employing a heterogeneous approach where the gauge section comprises of elements with random fracture material properties. The analytical model determined the length scale of heterogeneity and the range of variation of the fracture properties at that scale. Monte Carlo FE simulations were then performed to model the three-point bending response of the titanium and predictions were compared to experiments. The main conclusions of this chapter are the following:

- New stiffness-sensing test protocols are presented to inform stochastic analytical models and FE simulations and to aid interpretation of three-point bending tests on notched beams, as well as measuring material cohesion.
- Comparing the predictions of a stochastic analytical model to experiments we determined the range of variation of the fracture properties at the local level as well as the length scale of heterogeneity.
- Stochastic FE simulations were conducted, using a uniform finite element mesh of size equal to that determined from uniaxial tests and the analytical model; these predict correctly the fracture toughness of the material.
- Stochastic modelling, unlike deterministic modelling, predicts realistic crack paths and the correct mechanical response.
- Fracture toughness and strength are different expressions of a single physical property, the cohesion of the material, and the relation between strength and toughness is established by the details of microstructural heterogeneity.

5.6 APPENDICES

APPENDIX A

The FE linear elastic model is presented discussed. Prismatic beams of thickness, $B = 4\text{ mm}$, span, $S = 40\text{ mm}$, width, $W = 8\text{ mm}$ and initial crack length $\alpha = 3.6\text{ mm}$ were loaded in in three-point bending by rigid fully constrained analytical surfaces of radius $R = 3\text{ mm}$ as shown in Fig. A1. Eight linear elastic FE models ($E = 100\text{ GPa}$ and $\nu = 0.1$) with pre-existing crack lengths ranging from $\Delta\alpha = 0 - 3.5\text{ mm}$ were conducted and load-deflection curves were recorded in order to determine the stiffness as a function of total crack length. Preliminary sets of simulations were conducted to determine numerical convergence of the three point bending. The beam was meshed using fully integrated eight-node brick linear elements (C3D8) and an element size, $L_e = 0.4\text{ mm}$. Rigid fully constrained analytical surfaces were created to support the model and a rigid surface pushing downward on the centre of the upper surface of the body was defined; this was achieved by specifying a vertical displacement on the rigid surface ($u_2 = -3.5\text{ mm}$). The contact between the beam and the analytical surfaces were modelled by using a surface-to-surface algorithm of frictionless tangential behaviour. Further boundary conditions applied were to the tip of the notch to prevent lateral movements ($u_1 = u_3 = 0$) as well as to points A and A' (see Fig. A1) to prevent transverse movement ($u_3 = 0$).

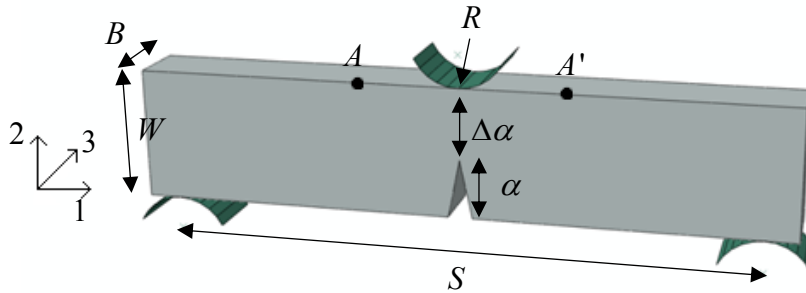


Figure A.1 Boundary conditions for the linear FE models.

In Fig. A.2 stiffness of titanium versus crack length history is shown for the eight linear FE models with pre-existing crack lengths. The experiment, B4 (straight crack) is compared to the FE linear elastic models. Experimental and numerical results agree very well. Based on this graph we can predict the crack length as a function of deflection and the fracture toughness as a function of crack length for the titanium.

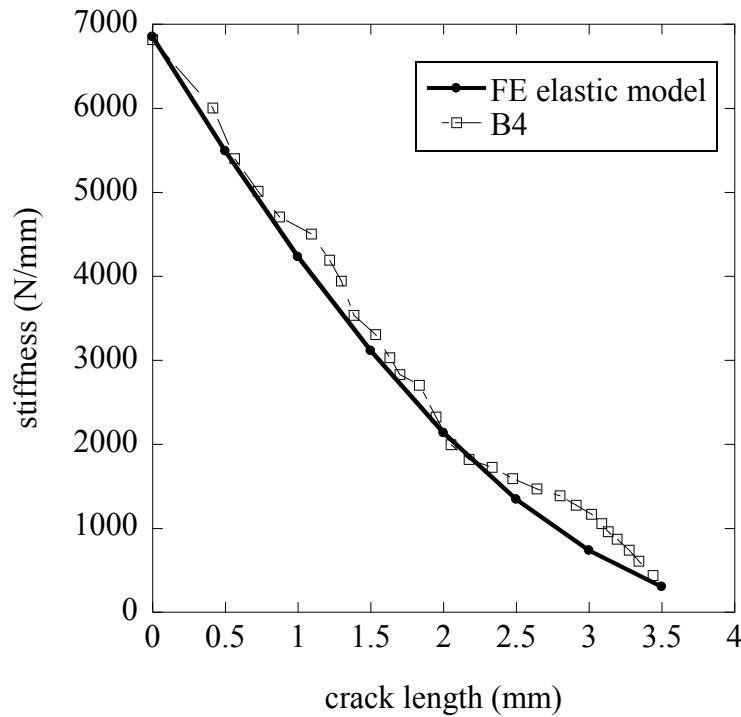


Figure A.2 Stiffness as a function of crack length for the experimental test C2 and for linear elastic FE models with pre-existing crack lengths.

APPENDIX B

To determine the strain ranges for the analytical model two different effects were investigated; the effect of the scatter range and the effect of the mean of the strains, defined as $(\varepsilon^{\min} + \varepsilon^{\max})/2$. To determine the effect of the scatter range, four different scenarios were examined, while the average values of damage initiation strain, intermediate strain and failure strain were held constant, $\varepsilon_0^{ave} = 0.0015$, $\varepsilon_{int}^{ave} = 0.0150$, $e_f^{ave} = 0.36$ respectively. The effect of increasing $\Delta\varepsilon/\varepsilon^{ave}$ of each strain, parametrically from 0.67 to 1.1 is shown in Figure B.1. The biggest effect on the macroscopic response is observed when increasing the range of the intermediate strain, whereas smaller effects were observed for the damage initiation strain as well as for the failure strain. For each curve ten realisation were conducted and average values are plotted. The parameters employed are summarised in Table B.1.

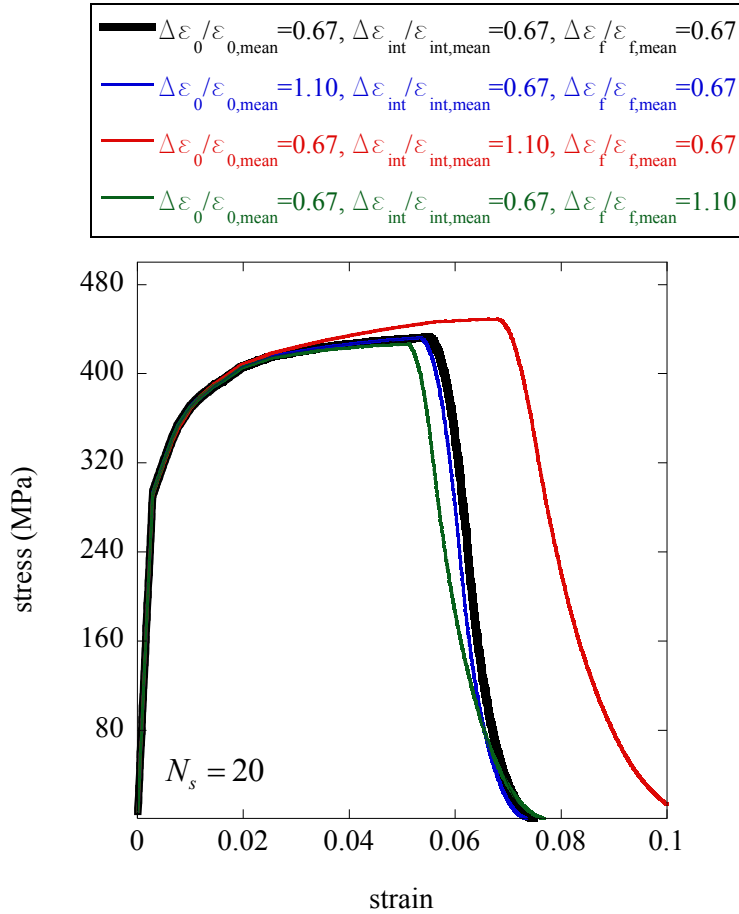


Figure B.1 Effect of increasing the range of variation in strains. The average strains are $\varepsilon_0^{ave} = 0.0015$, $\varepsilon_{int}^{ave} = 0.0150$, $e_f^{ave} = 0.36$.

	Scenario 1	Scenario 2	Scenario 3	Scenario 4
$\varepsilon_0^{\min}$	0.0010	0.0007	0.0010	0.0010
$\varepsilon_0^{\max}$	0.0020	0.0023	0.0020	0.0020
ε_0^{ave}	0.0015	0.0015	0.0015	0.0015
$\Delta\varepsilon_0 / \varepsilon_0^{ave}$	0.6667	1.1000	0.6667	0.6667
$\varepsilon_{int}^{\min}$	0.0100	0.0100	0.0068	0.0100
$\varepsilon_{int}^{\max}$	0.0200	0.0200	0.0233	0.0200
ε_{int}^{ave}	0.0150	0.0150	0.0150	0.0150
$\Delta\varepsilon_{int} / \varepsilon_{int}^{ave}$	0.6667	0.6667	1.1000	0.6667
$\varepsilon_f^{\min}$	0.2400	0.2400	0.2400	0.1620
$\varepsilon_f^{\max}$	0.4800	0.4800	0.4800	0.5580
ε_f^{ave}	0.3600	0.3600	0.3600	0.3600
$\Delta\varepsilon_f / \varepsilon_f^{ave}$	0.6666	0.6666	0.6666	1.1000

Table B.1 Parameters employed for Figure B.1.

To determine the effect of the mean of the strains on the macroscopic response, again four scenarios were examined, while the scatter range of damage initiation strain, intermediate strain and failure strain were held constant, $\Delta\varepsilon_0 / \varepsilon_0^{ave} = \Delta\varepsilon_{int} / \varepsilon_{int}^{ave} = \Delta\varepsilon_f / \varepsilon_f^{ave} = 0.67$ respectively. The effect of increasing the mean value of each strain, parametrically from 1 to 3 is shown in Figure B.2. The biggest effect on the macroscopic response is observed when increasing the mean value of the failure strain, which increases the macroscopic failure strain by approximately 3 times. A smaller effect was observed when increasing the mean intermediate strain and minimal effect when changing the mean damage initiation strain. For each curve ten realisations were conducted and average values are plotted. The parameters employed are summarised in Table B.2.

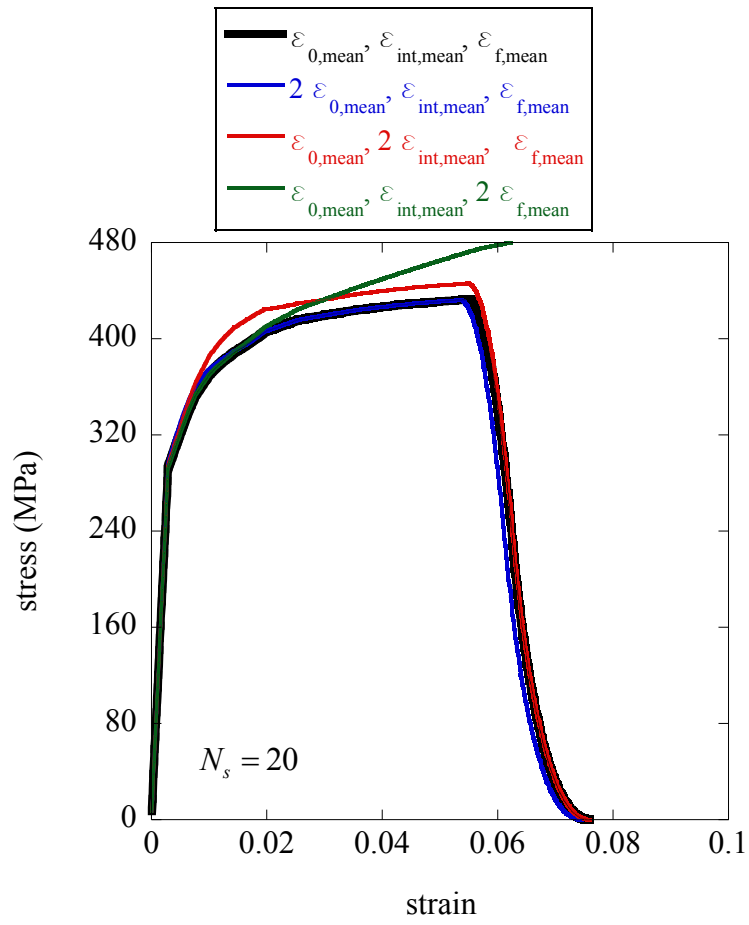


Figure B.2 Effect of increasing the average values of strains. The scatter range is fixed, $\Delta\varepsilon_0 / \varepsilon_0^{\text{ave}} = \Delta\varepsilon_{\text{int}} / \varepsilon_{\text{int}}^{\text{ave}} = \Delta\varepsilon_f / \varepsilon_f^{\text{ave}} = 0.67$.

	Scenario 1	Scenario 2	Scenario 3	Scenario 4
$\varepsilon_0^{\min}$	0.0010	0.0030	0.0010	0.0010
$\varepsilon_0^{\max}$	0.0020	0.0060	0.0020	0.0020
ε_0^{ave}	0.0015	0.0045	0.0015	0.0015
$\Delta\varepsilon_0 / \varepsilon_0^{ave}$	0.6667	0.6667	0.6667	0.6667
$\varepsilon_{int}^{\min}$	0.0100	0.0100	0.0300	0.0100
$\varepsilon_{int}^{\max}$	0.0200	0.0200	0.0600	0.0200
ε_{int}^{ave}	0.0150	0.0150	0.0450	0.0150
$\Delta\varepsilon_{int} / \varepsilon_{int}^{ave}$	0.6667	0.6667	0.6667	0.6667
$\varepsilon_f^{\min}$	0.2400	0.2400	0.2400	0.7000
$\varepsilon_f^{\max}$	0.4800	0.4800	0.4800	1.4000
ε_f^{ave}	0.3600	0.3600	0.3600	1.0800
$\Delta\varepsilon_f / \varepsilon_f^{ave}$	0.6666	0.6666	0.6666	0.6667

Table B.2 Parameters employed for Figure B.2.

CHAPTER 6

CONCLUSION AND FUTURE WORK

In contrast to the multiscale numerical modelling, in order to predict the mechanical response of engineering materials, we propose that it may not be mandatory to simulate the microstructural details at all length scales, as this is a very challenging task. Hence to perform accurate predictions of the deformation and fracture responses of solid materials, it is necessary to account for material heterogeneity. In the thesis we adopted simple computationally inexpensive models, whose calibration requires easily measurable quantities and probability density distributions, of a number of different physical parameters. The aim was to develop constitute models that can predict the macroscopic response of materials when heterogeneity exists at the small-scale. The chapters covered different types of materials and their conclusions, as well as future research is proposed for each chapter individually.

Elasto-plastic solid (Chapter 2)

Monte Carlo FE simulations were conducted to investigate the effects of microscopic variations in elastic modulus, yield strength and hardening modulus of heterogeneous elasto-plastic solids. Random SVEs were generated and the macroscopic multiaxial stress-strain behavior was examined. Material properties were varied in each element according to random fields of uniform probability density functions. Each element was taken as linear elastic with J_2 plasticity (constant hardening modulus and isotropic hardening was assumed). The size of the SVE size was determined and the sensitivity of the macroscopic to the mesh density was explored. Predictions were compared to analytical Voigt/Reuss bounds representing upper and lower bounds. The main conclusions of the study were as follows:

- By a microscopic variation of the Young's Modulus the macroscopic response of heterogeneous elasto-plastic solid was softer than of the homogeneous with the same mean elastic modulus. The reduction in stiffness was found to be proportional to the degree of variation.
- By a microscopic variation of the yield stress it was found that the heterogeneous elasto-plastic solid had a weaker response than the homogeneous with the same mean yield stress. The reduction in yield strength was found to be proportional to the degree of variation.
- The onset of yield in the heterogeneous elasto-plastic solid occurred at stresses which were significantly lower than the proof stress; the higher the degree of heterogeneity, the lower was the stress to cause first yield.
- Tension/compression asymmetry was observed due to strain localisation by shear banding and necking instability during the uniaxial tension simulations with either microscopic variation of stiffness or yield stress. The strain at which necking occurred increases with the degree of heterogeneity, suggesting that material ductility must be related to such degree.
- Such heterogeneous approach can capture size effects in the response, in line with experimental observations.
- A heterogeneous elasto-plastic solid, comprising of homogeneous elastic heterogeneous and heterogeneous plastically incompressible elements with isotropic hardening, exhibits a macroscopic response which is plastically compressible, pressure-sensitive and was characterised by non-isotropic hardening.

The current approach was an attempt to describe the macroscopic behavior of elasto-plastic heterogeneous solids with random material properties. The approach neglected many physical mechanisms of such materials such as strain gradient plasticity or damage mechanisms. The method can be extended into modelling bi-phase composite materials, comprising of two strong phases, and should be compared to readily available experimental measurements such as those reported in [46]. Predictions of size effects, shear bands and the multiaxial behavior of such materials should be investigated. The model can be refined to account for anisotropic elasticity and plasticity as well as for damage mechanisms. Better probability density functions should be assumed for the spatial variation of material properties.

Low porous solids (Chapter 3)

Monte Carlo FE simulations were performed and the multiaxial elasto-plastic response of solids with high relative density, in the range 0.70-0.99 was examined. The material was treated as a two-phase composite consisting of an incompressible elasto-plastic solid and voids. The voids were modelled as plastically compressible solids of negligible stiffness and strength, but included a strain-locking behavior at high strains to simulate self-contact of the pore. The RVE was determined as well as a mesh convergence study was employed. Predictions of the simulations were compared to previously published numerical studies, in which the geometrical details of the pores were explicitly modelled, as a random array of identical spherical voids. The main conclusions were the following:

- The micromechanical approach was more computational efficient than the previous numerical study conducted by Fritzen et al. [61] and is able to predict the response of ductile solids with relative density in the range of 0.70-0.99.
- Predictions of the current approach were nearly identical to those of the more detailed studies implemented by Fritzen et al., in which geometrical details were explicitly modelled. Much less degrees of freedom were used than that in [61]. Hence it was concluded that the details of the pore size and shape distribution have a minor effect on the response of low porous ductile solids with relative densities in the range of 0.70-0.99, whereas the prominent effect is the overall relative density.
- The onset of yield is symmetric for uniaxial tension and compression, however at higher strains an asymmetry is observed; this was mainly due to the different macroscopic hardening displayed by the material in uniaxial tension and compression.

- Scaling laws could be predicted for the Young's modulus and yield strength of the porous solids.

Future work should focus on modelling low porous elasto-plastic solids, by employing this approach, and compare predictions with experimental measurements. In the current approach the constitutive model did not account for damage mechanisms in the material; the tension/compression asymmetry was only due to the details of plastic deformation induced by the pores. By considering also for the damage mechanisms, the behaviour of such materials at high strains should be modelled and compared to experiments. In addition, there is a lack of experimental data on the multiaxial behaviour of low porous ductile solids, so it is proposed to perform experiments in order to compare with predictions.

Titanium foam (Chapter 4)

The mechanical behavior of sintered Titanium cellular solids with intermediate relative densities, in the range 0.35-0.48 were examined. Two algorithms were developed to construct representative microstructures of sintered Titanium foams; Algorithm I correctly represents the overall relative density of the foams; Algorithm II also models the distribution of pore size within the microstructure and capture the pore shape. Monte Carlo FE simulations on SVEs were performed and the size of the RVE was determined. The predictions were found in good agreement with measurements and were compared to the results of FE analyses reported in [75] for the same materials. A damage model was used to represent stiffness degradation of the parent material of the cellular solids and was calibrated exclusively against the available uniaxial stress versus strain response of the parent material, rather than obtained via a curve-fitting exercise. The main conclusions from this study are the following:

- The proposed modelling approach was computationally inexpensive compared to similar approaches for the same material, and is able to capture the stress versus strain responses of sintered Titanium foams in compression, tension and shear up to large strains, as well as the dependence of these responses upon relative density. The models are calibrated using exclusively measured data.
- It was found that the response of the foams analysed is scarcely size-dependent as long as the specimen volume contains at least 50 pores.

- Comparisons with the predictions reported in [75] showed that it is not necessary to capture all geometrical details of the foam microstructure (such as pore shape) in order to obtain accurate predictions.
- Our approach did not explicitly model the self-contact of the cell walls but introduced the effect of such self-contact by assigning a non-linear, plastically compressible response to the pores; such approach proved effective.
- Algorithms I and II yield similar, effective predictions of the response of the foams examined, if Algorithm I is appropriately calibrated. Algorithm I is more computationally effective than Algorithm II.

Future research should focus on modelling the high strain rate response of such materials using the same technique, where experimental data is readily available in [189]. In addition to generalize the current approach similar types of foams should be studied and experiments as well as numerical simulations should be performed. It would be interesting to model the behavior of polyurethane syntactic foams by employing the current approach due to existing experimental measurements reported in [45]. Syntactic foams are composites materials, comprised of two phases; the parent material and hollow brittle particles. When the composite is loaded in tension it was observed that cracks propagate perpendicular to the loading direction within the brittle particles whereas when loaded in compression cracks form at the same direction as the loading. Different constitutive model approaches should be employed to model these characteristics. Mechanical behavior at low and high strain rates of such materials should be examined and compared to the existing experimental data.

Solid titanium (Chapter 5)

Experimental, analytical and numerical analysis were conducted for a sintered titanium solid of 5% microporosity. The aim of this chapter was to show that from a uniaxial tension and compression tests we can determine the fracture toughness of the material. Uniaxial tension and compression tests were performed under a special test protocol and the undamaged response was determined. An analytical model was then developed to mimic the tensile experiment of the solid. The model assumed that fracture properties of the gauge section of the tensile specimen comprises of elements with random fracture properties i.e. damage initiation strain and damage evolution. By employing this approach, the length scale of heterogeneity

was determined as well as the range of variation of the fracture properties at that scale. Finally, Monte Carlo FE simulations on notched prismatic beams under three-point bending were performed to predict the fracture toughness of the material and compared to three-point bending experiments. The main conclusions of this chapter were the following:

- New stiffness-sensing test protocols are presented to inform stochastic analytical models and FE simulations and to aid interpretation of three-point bending tests on notched beams, as well as measuring material cohesion.
- Comparing the predictions of a stochastic analytical model to experiments we determined the range of variation of the fracture properties at the local level as well as the length scale of heterogeneity.
- Stochastic FE simulations were conducted, using an uniform finite element mesh of size equal to that determined from uniaxial tests and the analytical model; these predict correctly the fracture toughness of the material.
- Stochastic modelling, unlike deterministic modelling, predicts realistic crack paths and the correct mechanical response.
- Fracture toughness and strength are different expressions of a single physical property, the cohesion of the material, and the relation between strength and toughness is established by the details of microstructural heterogeneity.

Future research should focus on conducting experiments on different prismatic notched beam sizes in three-point bending and investigate whether the method can predict fracture energies as a function of specimen size as well as accurate responses due to these size effects. In addition, to generalize the method similar procedure should be followed for a wide range of engineering materials ranging from brittle to ductile materials.

General

In practice this approach can be employed for any type of material. The microstructure of the material can be reproduced in a non-explicit approach (interconnecting networks of metals, void distributions etc.). The individual phases of the material can be measured by direct measurements such as uniaxial tests. Once the material properties of the individual phases are measured and the microstructure is virtually reproduced, statistical and mesh convergences of the FE model are conducted to determine the necessary finite elements in the simulations. Predictions of the method can be compared to experiments in order to examine the validity of the method.

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