



Master's Dissertation in Mechanical Engineering on:

**Multi-Scale Analysis of Martensitic Transformation
Based on Second-Order Homogenisation**

Author:

João Araújo Marques da Silva

Supervisor:

Igor André Rodrigues Lopes

Co-Supervisors:

Miguel Vieira de Carvalho

Rui Pedro Cardoso Coelho

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Computational Multi-Scale
Modeling of Solids and Structures

*To my parents
and my sister.*

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*"If you're going to try, go all the way.
Otherwise, don't even start."*

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João Araújo Marques da Silva

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Multi-Scale Analysis of Martensitic Transformation Based on Second Order Homogenisation

Over the last decades, high-strength advanced steels (AHSSs), often exhibiting unparalleled mechanical properties, have been in continuous development. Recently, one particular mechanism that has become increasingly present in such materials is the so-called transformation induced plasticity (TRIP) effect, which, through the progressive transformation of a fraction of retained metastable austenite into martensite during deformation, grants these materials both high strength and good ductility. Evidently, these phenomena entail notably complex interactions at the microstructural level and attempting to predict the macroscopic constitutive behaviour of these materials demands detailed attention to such micro-scale phenomena.

Multi-scale models based on computational homogenisation establish a direct link between the material response and the underlying microstructure. A fully coupled implicit continuum, micro-mechanical based scheme, embedded in a computational multi-scale analysis framework, is used to model both crystal slip plasticity and martensitic transformation. In addition, two different types of multi-scale formulations, both derived from the method of multi-scale virtual power, are addressed in this work: *(i)* the standard first-order homogenisation approach; and *(ii)* the second-order homogenisation-based scheme where the macro-scale is modelled as a second-order continuum, while the micro-scale is still described by classical first-order continuum mechanics.

In this work, the influence of different macroscopic deformations on the homogenised martensitic transformation and its consequent impact on the macroscopic behaviour is assessed by means of several distinct displacement-driven analyses under the standard first-order homogenisation scheme performed with the elasto-crystal plasticity constitutive models with and without martensitic transformation. In first-order models, the homogenised response converges for increasing RVE sizes, thus a convergence analysis is also carried out and the adequate RVE size is determined. To correctly evaluate the extent to which first-order homogenisation may fail to accurately predict the transformation phenomena, several decoupled micro-scale analyses are performed with both homogenisation schemes, and, in the case of the second-order scheme, with different RVE lengths. An adequate range of first and second gradients of the macroscopic displacements are selected. Comparing the obtained results, it is shown that, while the second-order homogenisation approach may lead to a better prediction of the martensitic transformation at the micro-scale, it is also clearly dependent on the magnitude of the macroscopic strain (as well as on the RVE length and second gradient of the macroscopic displacements - albeit to a much lesser extent). Based on these observations, a numerical framework, descriptive of the observed differences between both homogenisation schemes and based on these three dominant factors is proposed in order to quantitatively estimate the relevance of second-order homogenisation. By per-

forming this study with both constitutive models, very specific deviations can be linked with the martensitic transformation phenomena.

Keywords: Multi-scale modelling, Finite element method, Second-order computational homogenisation, Transformation-induced plasticity, Mechanically-induced martensitic transformation.

Análise Multi-Escala da Transformação Martensítica Baseada em Homogeneização Computacional de Segunda Ordem

Nas últimas décadas, os aços avançados de elevada resistência (AHSS) têm sido alvo de constante desenvolvimento. Mais recentemente, um mecanismo em particular tem-se vindo a tornar cada vez mais presente nestes materiais: a designada plasticidade induzida por transformação, que consiste na contínua transformação de uma fração de austenite metaestável retida em martensite ao longo da deformação, conferindo a estes materiais propriedades ímpares como, por exemplo, elevada resistência e boa ductilidade. Naturalmente, estes tipo de mecanismos acarretam interações particularmente complexas ao nível microestrutural e qualquer esforço no sentido de prever o seu comportamento macroscópico deve implicar uma especial atenção a estes fenómenos à micro-escala.

Os modelos multi-escala baseados em homogeneização computacional estabelecem uma relação direta entre a resposta do material e a microestrutura subjacente. Um esquema micro-mecânico, assente na consideração de um meio contínuo e completamente acoplado, integrado numa abordagem de análise multi-escala computacional, é usado para modelar a plasticidade por deslizamento cristalino e a transformação martensítica. Além disso, duas formulações multi-escala são abordadas neste trabalho: (i) a formulação convencional de homogeneização de primeira ordem; e (ii) uma estratégia de homogeneização de segunda ordem em que o domínio macroscópico é modelado como um meio contínuo de segunda ordem, enquanto que a micro-escala continua a ser descrita pela mecânica clássica dos meios contínuos de primeira ordem.

Neste trabalho, a influência de diferentes deformações macroscópicas na medida homogeneizada da transformação martensítica e o seu consequente impacto no comportamento macroscópico do material é avaliada através de diferentes análises de deslocamento prescrito. Estas foram realizadas com a formulação convencional de homogeneização de primeira ordem e admitindo os modelos constitutivos de elasticidade e plasticidade cristalina, com e sem transformação martensítica. Em modelos de primeira ordem, a resposta homogeneizada converge com o aumento do tamanho do Elemento de Volume Representativo (EVR), logo, um estudo de convergência é, também, realizado no sentido de determinar o tamanho de EVR mínimo. De forma a corretamente avaliar em que medida é que a homogeneização de primeira ordem pode levar a uma previsão imprecisa do fenómeno de transformação, são ainda executadas várias análises à micro-escala com ambas as formulações de homogeneização computacional e, no caso da abordagem de segunda ordem, com distintos comprimentos do EVR. Neste sentido, foi, também, selecionada uma gama adequada de primeiro e segundo gradientes dos deslocamentos macroscópicos. Por comparação dos resultados, verifica-se que, enquanto a homogeneização de segunda-ordem pode efetivamente permitir uma melhor caracterização da transformação martensítica à micro-escala, esta é, também, claramente dependente da magnitude das deformações macroscópicas (bem como

do comprimento do EVR e do segundo gradiente dos deslocamentos, embora em muito menor grau). Com base nestas observações, é proposto um modelo numérico, representativo das diferenças observadas entre ambos os esquemas de homogeneização e baseado nestes três fatores preponderantes, com o objetivo de estimar, de uma forma quantitativa, a relevância da formulação de homogeneização de segunda ordem. Este estudo é realizado com base em ambos os modelos constitutivos, permitindo, assim, a associação de desvios específicos ao fenómeno da transformação martensítica.

Palavras-chave: Modelação multi-escala, Método dos elementos finitos, Homogeneização computacional de segunda ordem, Plasticidade induzida por transformação, Transformação martensítica promovida por solicitação mecânica.

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General notation

a	Scalar
$\mathbf{a}$	Vector
A	Second-order tensor
$\mathbf{a}, \mathbf{A}$	Fourth-order tensor
$\mathbf{a}, \mathbf{A}$	Finite elements array (vector, tensor)
$\mathcal{A}$	Space, set or body
$\mathfrak{A}$	Constitutive functional

Acronyms

2D	Bidimensional
3D	Tridimensional
BCC	Body-centered cubic
CM2S	Computational Multi-Scale Modeling of Solids and Structures
CMSA	Coupled Multi-Scale Analysis
CMT	Continuum Mechanics and Thermodynamics
FCC	Face-centered cubic
FE	Finite Element
FEM	Finite Element Method
Links	Large Strain Implicit Non-Linear Finite Element Analysis of Solid Linking Scales
MT	Martensitic Transformation
MSM	Multi-Scale Models
RVE	Representative Volume Element
TRIP	Transformation-induced plasticity

Indices

$(\cdot)^{(e)}$	Element entity (within the Finite Element Method framework)
$(\cdot)^g$	Global entity (within the Finite Element Method framework); $(\cdot)$ expressed in relation to the global
$^h(\cdot)$	Finite element interpolation of $(\cdot)$
$(\cdot)_{iso}$	Isochoric component of $(\cdot)$
$^{Lin}(\cdot)$	Linear boundary model related entity
$(\cdot)_p$	Plasticity related entity

$(\cdot)_n$	Associated with instant t_n
$\text{Per}(\cdot)$	Periodic boundary model related entity
$(\cdot)_t$	Associated with instant t
$\text{Tay}(\cdot)$	Taylor model related entity
$\text{Uni}(\cdot)$	Uniform boundary traction model related entity
$(\cdot)_{vol}$	Volumetric component of $(\cdot)$
$(\cdot)^\alpha$	$(\cdot)$ of a slip system α
$(\cdot)_\mu$	Microscopic $(\cdot)$
$(\dot{\cdot})$	Incremental constitutive function for $(\cdot)$
$(\cdot)_0$	Associated with the initial configuration

Operators

$\mathbf{A}(\cdot)$	Finite element assembly
$\det(\cdot)$	Determinant of $(\cdot)$
$\text{div}_{\mathbf{p}}(\cdot)$	Material divergence of $(\cdot)$
$\text{div}_{\mathbf{x}}(\cdot)$	Spatial divergence of $(\cdot)$
$\ln(\cdot)$	Natural logarithm of $(\cdot)$
$\text{skew}(\cdot)$	Skew-symmetric part of $(\cdot)$
$\text{sym}(\cdot)$	Symmetric part of $(\cdot)$
$\text{tr}(\cdot)$	Trace of $(\cdot)$
$\nabla_{\mathbf{p}}(\cdot)$	Material gradient of $(\cdot)$
$\nabla_{\mathbf{x}}(\cdot)$	Spatial gradient of $(\cdot)$
$\partial(\cdot)$	Boundary domain of $(\cdot)$
$\frac{\partial(\cdot)}{\partial a}$	Derivative of $(\cdot)$ with respect to a
$(\dot{\cdot})$	Material first order time derivative of $(\cdot)$
$(\ddot{\cdot})$	Material second order time derivative of $(\cdot)$
$(\cdot)^T$	Transpose of $(\cdot)$
$\mathbf{a} \cdot \mathbf{b}$	Single contraction of two generic vectors $\mathbf{a}$ and $\mathbf{b}$
$\mathbf{A} \cdot \mathbf{b}$	Single contraction of a generic tensor $\mathbf{A}$ and a generic vector $\mathbf{b}$
$\mathbf{A} \cdot \mathbf{B}$	Single contraction of two generic tensors $\mathbf{A}$ and $\mathbf{B}$
$\mathbf{a} \times \mathbf{b}$	Cross product of generic vector $\mathbf{a}$ by vector $\mathbf{b}$
$\mathbf{a} \otimes \mathbf{b}$	Tensor product of generic vectors $\mathbf{a}$ and $\mathbf{b}$
$\mathbf{A} : \mathbf{B}$	Double contraction of two generic tensors $\mathbf{A}$ and $\mathbf{B}$
$\mathbf{A} \vdots \mathbf{B}$	Triple contraction of two generic tensors $\mathbf{A}$ and $\mathbf{B}$

$\|(\cdot)\|$ Euclidean norm of a generic vector or tensor

Variables

a, b, c	Lattice parameters
$A^{\alpha\beta}$	Coplanarity Matrix
A	Generic tensor field
$\mathbf{a}$	Consistent spatial tangent modulus
$\mathbf{A}$	Consistent material tangent modulus
b	Body forces vector per unit deformed volume
b_0	Body forces vector per unit reference volume
B	Left Cauchy-Green strain tensor
$\mathcal{B}$	Generic continuum body
C	Right Cauchy-Green strain tensor
D	Stretching tensor
$\mathbf{D}^e$	Anisotropic elasticity tensor
e	Specific internal energy
E^e	Green-Lagrange elastic strain tensor
$E^{(m)}$	Lagrangian strain tensor of order m
E^2	Green-Lagrange strain tensor
$\mathcal{E}$	Three-dimensional Euclidean space
F	Deformation gradient
F^e	Elastic deformation gradient
F^p	Plastic deformation gradient
F^{tr}	Transformation deformation gradient
$\mathbf{f}_{int}$	Internal nodal force vector (within the finite element framework)
$\mathbf{f}_{ext}$	External nodal force vector (within the finite element framework)
$\mathfrak{F}$	Constitutive functional for the Cauchy stress tensor
$\mathfrak{G}$	Constitutive functional for the specific free energy
g	Spatial divergence of temperature field
$\mathbf{G}$	Second gradient of the displacements
$h^{\alpha\beta}$	Matrix of hardening coefficients
$\mathfrak{H}$	Constitutive functional for the specific entropy
I	Second-order identity tensor
$\mathfrak{J}$	Constitutive functional for the heat flux

J	Determinant of the deformation gradient
l	Typical length of the micro-constituents
L	Length of the macroscopic body
l_{RVE}	Length of the RVE
$\mathbf{L}$	Spatial velocity gradient
$\mathcal{L}$	Generic surface of a continuum
K	Hardening parameter
$\mathbf{K}_T$	Global tangent stiffness matrix
m	Hardening exponent
$\mathcal{K}$	Set of kinematically admissible displacements
$\mathcal{K}^*$	Set of minimally constrained kinematically admissible displacements
$\tilde{\mathcal{K}}$	Set of displacement fluctuations
$\tilde{\mathcal{K}}^*$	Set of minimally constrained displacement fluctuations
$\mathbf{m}$	Slip plane unit normal vector
$\mathbf{M}$	Schmid tensor
n_{dof}	Number of spatial dimensions
n_{elem}	Number of elements within a generic finite element mesh
n_{gaussp}	Number of considered Gauss points
n_{nodes}	Number of nodes of a generic finite element
n_{poin}	Number of points within a generic finite element mesh
n_{slip}	Number of slip systems
$\mathbf{n}$	Generic unit normal vector to a surface in the deformed configuration
$\mathbf{n}_0$	Generic unit normal vector to a surface in the reference configuration
$\mathbf{N}$	Interpolation matrix
$\mathbf{o}$	Origin of a generic lattice
$\mathcal{O}$	The orthogonal group
$\mathcal{O}^+$	The rotation (proper orthogonal) group
p	Hydrostatic pressure
$\mathbf{p}$	Position of a generic particle in the reference configuration
$\mathbf{P}$	First Piola-Kirchhoff stress tensor
q	Latent hardening ratio
$\mathbf{q}$	Position of the center of rotation in a rigid rotation; heat flux
$\mathbf{Q}$	Higher-order stress tensor
r	Density of heat production

$\mathbf{r}$	Position of a generic lattice point
$\mathbf{R}$	Generic rotation tensor
$\mathbf{r}$	Global finite element residual force vector
s	Specific entropy; quantitative measure of differences between the responses of first and second-order
S	Standard Error of the Regression
S_k	Weighted standard Error of the Regression
s_{RVE}	Size of the RVE
$\mathbf{s}$	Unit vector in the slip direction
$\mathbf{S}$	Second Piola-Kirchhoff stress tensor
$\mathbf{t}$	Cauchy stress vector; surface traction
$\mathbf{t}_0^*$	True Reference surface traction
$\mathbf{t}_0$	Reference surface traction
$\mathbf{u}$	Displacement vector field
$\bar{\mathbf{u}}$	Prescribed boundary displacement field
$\tilde{\mathbf{u}}$	Displacement fluctuation field
$\mathbf{U}$	Right stretch tensor
$\mathbf{u}$	Global finite element vector of nodal displacements
v	Volume in the deformed configuration
v_0	Volume in the reference configuration
$\mathbf{v}$	Velocity vector field
$\mathbf{V}$	Left stretch tensor
$\mathcal{V}$	Space of admissible virtual displacements
$\mathcal{V}^*$	Space of minimally constrained admissible virtual displacements
w_i	Weight associated with Gauss point i
$\mathbf{W}$	Spin tensor
$\mathbf{x}$	Position of a generic particle in the deformed configuration
α	Contraction/expansion ratio; Generic slip system
α, β, γ	Angles between the lattice parameters
α_k	Generic internal variable (can be a scalar, vectorial or tensorial quantity)
$\boldsymbol{\alpha}$	Generic set of internal variables
δ_{ij}	Kronecker delta
ϵ_p	Plasticity associated rate-sensitivity parameter
ϵ_{tr}	Transformation associated rate-sensitivity parameter
$\boldsymbol{\epsilon}$	Infinitesimal strain tensor

$\boldsymbol{\eta}$	Virtual displacement vector field
η	Global finite element vector of virtual nodal displacements
θ	Temperature; polar angle
μ_p	Plasticity associated viscosity parameter
μ_{tr}	Transformation associated viscosity parameter
$\boldsymbol{\xi}_i$	Natural coordinate vector; natural coordinates of Gauss point i
ρ	Mass per unit volume
σ_{vm}	Equivalent Cauchy stress (or equivalent von Mises stress)
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\sigma}^*$	Prescribed stress state
τ	Schmid resolved shear stress
τ_y	Critical resolved resolved shear stress
$\boldsymbol{\tau}$	Kirchhoff stress tensor
Φ	Yield function
φ	Deformation mapping function; motion
ψ	Specific free energy
Ω	Domain of a generic continuum body in the reference configuration

1

Introduction

Over the last decades, industrial applications such as the automotive and aerospace fields, where structural analysis and the development of novel materials and structures are of the utmost importance, have become tremendously reliant on computational tools. Notably, advanced heterogeneous materials, which encompass an intricate arrangement of multiple constituent phases at the microscopic level, and the tools increasingly present in their development have been the subject of intense research within industrial and scientific circles. These materials are often capable of offering improved properties, inconceivable in conventional materials, allowing them to be integrated into components and structures with unparalleled mechanical performances. A class of materials that falls into this picture is known as advanced high-strength steels (AHSSs), such as *Transformation-induced plasticity* (TRIP) steels. These feature the continued transformation of a fraction of retained metastable austenite into martensite during deformation and consequently exhibit exceptional strength to ductility ratios, making them particularly attractive for the automotive industry, for impact related components, for example, due to their high energy absorption.

Generally, these materials display extremely complex microstructural phenomena that dictate the overall macroscopic behaviour and, while modelling these physical features is paramount for the accurate prediction of the materials' mechanical behaviour, it can prove to be a quite difficult task. Indeed, experimental procedures may be rather expensive for most engineering applications, therefore, when possible, the adoption of predictive numerical models is usually favoured. However, due to the aforementioned degree of complexity, common phenomenological approaches devised for the characterisation of these materials' behaviour rely on an extensive number of parameters, while still not necessarily considering all relevant micro-scale phenomena and, therefore, possibly leading to rather coarse macroscopic results. For this reason, the growing interest and adoption of *multi-scale* modelling approaches, which link the large-scale material behaviour to its underlying microstructure, is easily understood. Under such framework, the macroscopic stress and strain states at each macro-integration point are computed from the averaging (also known as *homogeni-*

sation) of its corresponding microscopic counterparts over a *Representative Volume Element* (RVE), obtained from the solution of the microscopic equilibrium problem. The RVE is a sample of the material's microstructure that contains all relevant microscopic details, whose behaviour is usually modelled by continuum constitutive models (since, at the micro-scale, matter may still be regarded as continuous).

Within the scope of *numerically homogenised multi-scale models*, the focus is often set on first-order computational homogenisation, where the deformation quantity transferred from the macro to the micro-scale depends exclusively on the first gradient of the macroscopic displacement field. Thus, most models are founded on the assumption of uniformity of the macroscopic strain and stress field distributions in the RVE, that is, in the infinitesimal neighbourhood of any given macroscopic point. As a result, the standard first-order homogenisation scheme only allows the micro-scale representation of linear deformation modes and the computed response is valid provided the *scale separation principle* is satisfied (in other words, as long as the length of the RVE is significantly smaller than the macro-scale deformation wavelength). However, in certain circumstances, such as macroscopic deformations involving high curvatures, for example, said assumption cannot be made and the first-order approach becomes inadequate for an accurate prediction of the material mechanical behaviour. In this context, the second-order homogenisation based approach emerges as a more complete alternative, increasing the range of applicability of multi-scale models. Briefly, the second-order homogenisation scheme involves also passing the second gradient of the displacements from the macro to the micro-scale, along with the first-order strain measure. As a result, contrarily to the standard first-order homogenisation scheme, which solely allows the prescription of linear deformation modes at the micro-scale, second-order homogenisation includes quadratic deformation modes in the microscopic equilibrium problem, which may be paramount when phenomena such as phase transformation, for instance, are present and are relevant for the prediction of the overall structural behaviour.

1.1 Main Goal

The main purpose of this work is to systematically study the effect of the RVE employed to model polycrystalline austenitic steels undergoing mechanically-induced martensitic transformation on the response obtained at the structural level. To do so, the conducted analyses consider both the standard first-order homogenisation scheme and its expansion, based on second-order homogenisation. The latter introduces the length of the RVE as a measure of the material characteristic length.

Firstly, a set of different displacement-driven coupled multi-scale analyses (CMSA) are performed considering exclusively elasticity followed by crystal slip plasticity and using first-order homogenisation with Taylor's boundary condition, which enables algorithmic simplifications that strongly improve the computational performance. Thereafter, similar studies are conducted, but, in this instance, including the possibility of mechanically-induced

martensitic transformation in the constitutive model, coupled with the formerly admitted plasticity mechanism. Comparing these results allows us to briefly assess how different macroscopic deformations distinctly promote the activation and progress of the martensitic transformation and its impact on the macroscopic behaviour. Simultaneously, due to the aforementioned favourable computational setting, this stage is also adequate for the determination of the minimum RVE size. That being said, a convergence exercise is also performed for both sets of analyses (i.e., without and with martensitic transformation), from which the RVE size that meets our pre-established tolerance parameters is established and allows to capture sufficiently accurate macroscopic deformation histories.

Then, with the aforementioned macroscopic deformation histories collected from selected macro-integration points of each analysis, we progress to the decoupled micro-scale analyses associated with each of those selected material points. Here, the second-order homogenisation scheme is adopted and the analyses are repeated with distinct RVE lengths, whose results are thus compared with those obtained from first-order homogenisation. With the computed results, we evaluate the relative importance of the macroscopic deformation gradients and RVE length in the development of martensitic transformation at the micro-scale. For this reason, an adequate range of first and second deformation modes is carefully chosen. Lastly, and in line with this final assessment of the importance of second-order homogenisation on the accurate prediction of martensitic transformation, a numerical framework developed to quantitatively estimate the relevance of second-order homogenisation and the associated RVE length is presented.

1.2 Brief Literature Review

In this Section, we present a brief review of the main topics relevant to this dissertation and to which we will aim our attention in the following Chapters. Several references are highlighted with the purpose of detailing all crucial advancements and contributions that constructed the state-of-the-art of these subjects. These also offer a more comprehensive description of particular issues, should the reader be interested in a more thorough discussion.

1.2.1 Multi-Scale Models Based on Computational Homogenisation

Within the scope of multi-scale models, different variants can be defined (Matous et al., 2017): (i) *concurrent methods*, in which there is no separation of scales and, thus, different parts of a problem's domain are modeled with distinct scales (Lloberas-Valls et al., 2012a,b); (ii) *hierarchical methods*, where the micro and macroscopic length scales are sufficiently separate and, therefore, both scales are hierarchically coupled in the same portion of the domain (Feyel and Chaboche, 2000; Kouznetsova et al., 2001); and (iii) *hybrid methods*, which link both scales through a hybrid coupling scheme (Miehe and Bayreuther, 2007; Plews and Duarte, 2015). In this dissertation, we focus on hierarchical computational

homogenisation-based multi-scale models.

A crucial notion consistently present in multi-scale modelling theories concerns the concept of a Representative Volume Element, which is built upon the scale separation principle, firstly introduced by Hashin (1983). Simply put, the scale separation principle establishes that the size of the RVE may be smaller than the macroscopic continuum domain, but has to be much larger than its microscopic constituents that carry the relevant micro-heterogeneities. This is critical so that it embodies a statistically representative sample of the infinitesimal neighbourhood of its respective material point and leads to reliable homogenised results. The convergence of the homogenised results with respect to increasing RVE sizes and distinct boundary conditions is studied by Terada et al. (2000) and a numerical framework for the quantitative assessment of the RVE size is proposed by Kanit et al. (2003). On this basis, the continuum mechanics theory becomes conveniently applicable at the micro-scale. A collection of some definitions of RVE found throughout relevant literature can be found in Gitman et al. (2007).

While the biggest advantage of multi-scale RVE-based modelling techniques is their flexibility and wide range of applications, their development was mostly promoted by the increasingly well-established acceptance of composite materials and the intrinsic need to characterise their mechanical behaviour. Indeed, most of the work related to homogenisation in the prediction of heterogeneous materials' response and, as such, the development of multi-scale models based on computational homogenisation over RVEs trace back to early efforts in determining the homogenised elastic properties of composite materials. Guedes and Kikuchi (1990), for instance, proposed a framework for the numerical estimation of the macroscopic elastic properties of composite structures through finite element analyses of RVEs based on an asymptotic homogenisation procedure and subsequent introduction of these properties in the macroscopic finite element model. Here, the fundamental principles of state-of-the-art multi-scale modelling based on computational homogenisation are obvious. Smit et al. (1998) introduced a coupled multi-scale finite element model, where the macroscopic stresses at each macro-integration point are obtained by the microscopic equilibrium of its corresponding unique discretised RVE, which, in turn, is subjected to the macroscopic deformation history collected from the point to which it is attached, under periodic boundary conditions.

Besides coupled micro-macro schemes (CMSA), homogenisation-based multi-scale models may also be used to perform micro-mechanical studies, otherwise known as decoupled multi-scale schemes. Since CMSA entail an high computational cost, the decoupled approach may be favourable for many practical problems - assess or improve existing constitutive models, calibrate parameters or develop new laws. This may be achieved by studying a single point from the macroscopic level, in which case a unique RVE is considered. Watanabe and Terada (2010) study and compare both coupled and decoupled multi-scale schemes.

In this dissertation, two distinct classes of multi-scale formulations based on computational homogenisation are considered: (i) the standard first-order homogenisation scheme;

and (ii) a standard (or *partial*) second-order homogenisation scheme, where the macro-scale is modelled as a second-order continuum, whereas the micro-scale formulation is based on classical first-order continuum mechanics. It should be noted that a *fully* second-order homogenisation scheme, where the micro-scale is described by a second-order continuum theory as well, and consequently allows the capture of size effects associated with the size of the micro-constituents, also exists. Lesicar (2015) and Lesicar et al. (2017) introduce a fully second-order homogenisation-based framework for small strains. A variationally consistent fully second-order homogenisation-based multi-scale model for solids undergoing large (finite) strains is presented by Rodrigues Lopes (2019).

First-Order Computational Homogenisation

Most of the contributions to the study of multi-scale models are based on first-order computational homogenisation, whereby the deformation state information transferred from the macro to the micro-scale solely depends on the first gradient of the macroscopic displacements' field. de Souza Neto and Feijóo (2006, 2010) presented a complete variational foundation for multi-scale constitutive theories based on computational homogenisation. Recently, a continuation of this work was proposed by Blanco et al. (2016a), where the *Principle of Multi-Scale Virtual Power* is introduced as an extension of the *Hill-Mandel Principle*.

Second-Order Computational Homogenisation

The concept of second-order computational homogenisation, which, in addition to the first-order strain measure, also includes the second gradient of the macroscopic displacements in the exchange of information between the macro and microscopic scales, was firstly introduced by Kouznetsova et al. (2002), Kouznetsova (2002) and Kouznetsova et al. (2004). Specifically, regarding the standard second-order homogenisation scheme, with which we are concerned in this dissertation, the micro-scale is modelled by means of the first-order continuum mechanics theory, while the macro-scale is regarded as a second-order continuum. The upside of this approach is that a second-order constitutive law is produced at the macroscopic level without having to formulate its underlying equations, as it naturally arises from the homogenisation technique, and standard first-order constitutive laws may be used at the RVE level. Other advantages include: (i) the relaxation of the scale separation principle, due to the assumption of a linear variation of the macro-deformation in the RVE - in a first-order approach, the RVE must be sufficiently small so that the macroscopic deformation can be considered constant within it; and (ii) the inclusion of the effect of quadratic deformation modes, such as bending and torsion.

Irrespective of the aforementioned advantages, second-order homogenisation is far from a subject of profound research. In addition to Kouznetsova's formulation, Luscher (2010) proposed a formulation where the micro-constraints are obtained through orthogonality conditions. This author also points out that in a standard second-order homogenisation

scheme, the imposed microscopic constraints lead to a constant body force in the RVE. Blanco et al. (2016b) presented a second-order multi-scale formulation based on the Principle of Multi-scale Virtual Power which also accounts for inertia and body forces at both scales. In Rodrigues Lopes (2019) this subject is studied to greater detail, not only presenting a detailed comparison of the standard second-order computational models reported in relevant literature, but also proposing an alternative formulation derived from the *Method of Multi-Scale Virtual Power*, by modifying the definition of the homogenised second gradient.

1.2.2 TRIP Effect in the Development of Advanced High-Strength Steels

Mostly motivated by the automotive industry's permanent search for safer and lighter structural components, intensive research is constantly dedicated to developments around advanced high-strength steels. Generally, AHSSs exhibit intricate and carefully balanced microstructures, where features such as multiple phases, metastable austenite (and its possibly resulting mechanically-induced transformation phenomena and twinning effects), complex dislocation substructures and broad variety of interfaces can be responsible for their favourable properties. While this class of materials has been present for some decades, recent developments have been marked by what some refer to as 3rd generation Advanced High Strength Steels, which, in general, exhibit dual-phase microstructures with a retained metastable austenite phase that, in turn, provides the TRIP effect during deformation (Liu et al., 2018). This effect results in an improved strain-hardening behaviour and, therefore, high tensile strength and good ductility when compared to previous AHSS's generations and, especially, to conventional martensitic steels, which, albeit of high strength, exhibit low ductility due to a lack of microstructural strain-hardening and damage resistance mechanisms (Kwon et al., 2013). As a result, these steels can be cold formed to complex geometries and still exhibit ductility suitable for the impact performance of crash-prone components.

In general, two significant mechanisms occur during the deformation-induced martensitic transformation: (i) the elastoplastic accommodation in both product and parent phases of the shape strain sustained during phase transformation, also known as *Greenwood-Johnson mechanism* (Greenwood et al., 1965); and (ii) the preferable orientation (and consequent favoured transformation) of martensite variants with respect to the applied stresses, or *Magee mechanism* (Magee and Paxton, 1966). Indeed, the formation of martensite induces increased dislocations in both phases (Jacques et al., 2001) - due to differences in the crystalline structures between austenite and martensite, the martensitic transformation is inevitably accompanied by a volumetric expansion, which is then accommodated through the generation and propagation of dislocations (Fahr, 1971). Furthermore, the austenite phase possesses different mechanical properties than those from the martensitic product, which leads to a stress/strain partition between the two phases (Wang et al., 2015). Jacques et al. (2001) states that these two mechanisms constitute the major underlying agents behind the enticing mechanical properties resulting from the TRIP effect.

In particular, the extent of the transformation and its results are intimately related to the mechanical stability of the retained austenitic phase. A proper understanding of the factors that influence the austenite's stability is crucial to the development of AHSSs that rely on the TRIP effect. In terms of the chemical composition, for instance, an increase in the stability of austenite (and consequent inhibition of the martensitic transformation promoted by either thermal quenching or mechanical deformation) can be achieved by the addition of elements such as Carbon¹ (C) and Manganese (Mn) (Andrews, 1965; Fahr, 1971). In addition, grain size refinement also leads to a more stable austenite phase (Jimenez-Melero et al., 2007). Indeed, a reduced grain size leads to increased interface density and interfacial energy (which constitutes a phenomenon commonly referred to as *Hall-Petch strengthening* that relates the reduction of the average grain size with an higher material strength), which, in turn, increases the strain energy barrier that must be met for the occurrence of martensite nucleation (Wang and Van Der Zwaag, 2001). Thus, in those circumstances, a larger external mechanical driving force would be required for the initiation of martensitic transformation. While most studies support that the TRIP effect is indeed suppressed by smaller grain sizes, the precisely contrary behaviour has also been documented. Wang et al. (2015) and Matsuoka et al. (2013) report the non-effective or even decreasing role of grain refinement on austenite's mechanical stability. Lastly, other factors, such as austenite's morphology (Xiong et al., 2013), for instance, also influence the stability of retained austenite.

1.2.3 Modelling of Slip Plasticity and Martensitic Transformation

The link between the plastic flow observed in the plastic domain of the deformation of solid metallic materials with the underlying crystallographic slip mechanism was firstly presented in the early works of Taylor and Elam (1923, 1925) and Taylor (1938) and the continuum-based constitutive equations that establish the associated single crystal elastoplastic behaviour were firstly formulated by Mandel (1965) and Hill (1966). These were later adapted to finite strains by Rice (1971), Hill and Rice (1972), Asaro and Rice (1977) and Asaro (1983a,b).

Regarding the martensitic transformation phenomenon, Patel and Cohen (1953) observed that mechanical loadings directly impact the transformation's onset temperature and proposed a criterion (restricted to uniaxial stress states and small strains) based on the mechanical contribution to the total thermodynamical driving force. They justified this behaviour, referred to as *stress-assisted transformation*, with the work done between the applied stresses and the transformation displacements. Furthermore, Olson and Cohen (1972) found that, in certain temperature ranges, a distinct mechanism, known as *strain-induced transformation* may be involved, in which case the transformation begins at stresses higher than the austenite (parent-phase) yield stress. They suggested that the slip activity in the austenite, and resulting shear band intersections, leads to martensite nucleation. In Ol-

¹ In fact, the meta-stabilization (or retaining) of the austenite at room temperature is attained by carbon enrichment during specific thermomechanical treatments, namely, intercritical annealing (Jacques, 2004).

son and Azrin (1978) these findings are compiled: at lower temperatures, stress-assisted transformation is dominant, and, as a result, transformation begins at stresses lower than the yield stress, while, at higher temperatures, strain-induced transformation prevails, and transformation is observed for stress values above the austenite yield stress. This contrast is easily explained by the intrinsic thermodynamical instability of the austenite phase at lower temperatures, particularly at room temperature, and its increasing stability for higher temperatures (hence the class of TRIP materials known as *metastable*² austenitic stainless steels). Still on this subject, the works of Wechsler (1953) and Bowles and Mackenzie (1954) proved to be quite compelling and established what came to be known as *Phenomenological Theory of Martensitic Crystallography* (PTMC³). As suggested by its name, PTMC does not account for the underlying mechanisms associated with phase transformation, but rather aims to predict the observed crystallographic features, namely orientation relationships, habit planes and overall shape deformations of the formed martensitic structures. Although the theories presented in the two aforementioned works were devised independently and followed distinct formulations, they were later proved to be equivalent (Christian, 1956). Decades later, the work of Ball and James (1987) lead to a polished version of the PTMC theory, having shown that precisely the same predictions can be derived from the assumption that the transformation results in a fine mixture of phases minimising the material's total free energy.

To this day, the PTMC still remains the most accepted predictive theory of martensite crystallography and many of the more recently proposed constitutive models for the overall behaviour of materials that exhibit mechanically-induced martensitic transformation still rely on its fundamentals to predict the transformation's crystallographic features. Indeed, in recent decades, this has been a topic of some discussion and, as a result, many constitutive models, encompassing a wide variety of approaches, may be found in the literature: phenomenological models, which postulate the existence of internal variables, micro-mechanical approaches and, more recently, computational homogenisation approaches. However, in general, many of these are formulated under the assumption of small strains, which may not be adequate for the modelling of the large local deformations generally involved in the martensitic transformation mechanism. de Bortoli (2017) tackled this issue and proposed a micro-mechanical based constitutive model, installed within a computational multi-scale analysis framework. More recently, Vieira de Carvalho et al. (in submission) built upon Bortoli's work and developed an implicit fully coupled model for crystal plasticity and martensitic transformation in large strains.

² In short, a metastable phase is simply a kinetically trapped phase with positive free energy above the equilibrium state (Sun et al., 2016).

³ Also referred to as the Phenomenological Theory of Martensitic Transformations (PTMT) in the relevant literature.

1.3 Outline

In this Section, a general outline of the contents of the remaining Chapters of this document is presented.

Chapter 2

A detailed review of the fundamental concepts of the classical first-order description of continuum mechanics is here presented and followed by the discussion of some features central to the application of the finite element method in large-strain continuum mechanics problems. Finally, the main ingredients of the second-order continuum mechanics' theory are also briefly exposed.

Chapter 3

Firstly, the distinction between coupled and decoupled multi-scale schemes is explained and the concept of Representative Volume Element is discussed. Then, the general framework of first-order computational homogenisation, based on the Method of Multi-Scale Virtual Power, is formulated and the corresponding micro-scale constraints are also presented. Thereafter, again following the Method of Multi-Scale Virtual Power, the standard second-order homogenisation-based model is presented, along with the appropriate micro-scale boundary conditions. Lastly, the computational program **Links** used for the numerical analyses in this dissertation is introduced and an outline of the plan regarding those analyses is also schematically presented.

Chapter 4

Initially, we touch on some basic concepts regarding crystalline materials, before presenting the anisotropic single crystal plasticity constitutive model, formulated under the assumption of finite strains and used to model the austenite slip flow. Then, we allude to important physical aspects associated with martensitic transformations, with particular focus being directed to the Phenomenological Theory of Martensitic Crystallography and Patel and Cohen's transformation criteria. The large-scale mechanically-induced martensitic transformation constitutive model is subsequently presented and a short discussion on plastic slip and on some of the important considerations involved in its computational treatment concludes this Chapter.

Chapter 5

Here, several displacement-driven coupled multi-scale analyses based on first-order computational homogenisation are performed and the development of the martensite phase and its consequent impact on the macroscopic material behaviour are assessed. Firstly, these analyses only admit elasticity followed by slip plasticity and are carried out under several

RVE sizes, so that, simultaneously, we may examine the convergence of the macroscopic homogenised results with increasing RVE sizes. The minimum RVE size that meets the pre-established statistical parameters is then adopted and the initial analyses are repeated with the fully coupled plasticity and martensitic transformation constitutive model. The obtained results are compared with those from the initial set of simulations and concluding remarks on the overall nature of martensitic transformation are ultimately presented.

Chapter 6

Decoupled micro-scale analyses based on the standard second-order homogenisation scheme are performed at selected macro-integration points under several RVE lengths and the results are compared to those initially obtained from the first-order homogenisation approach (Chapter 5). The influence of the second gradient of the macroscopic displacements and of the length of the RVE on the response at the micro-scale is discussed, considering both the exclusively-plastic and the coupled constitutive model. Lastly, a quantitative framework for the assessment of the importance of the adoption of the second-order homogenisation with respect to the respective first and second gradients of the displacements is proposed.

Chapter 7

The main conclusions from this work are presented and suggestions for future work related to the topics discussed in this dissertation are also made.

2

Continuum Mechanics, Thermodynamics and Finite Element Method

Before addressing Multi-Scale Models, there are some key concepts that one must first be familiar with. To accurately depict any solid's behaviour under an arbitrary thermomechanical loading, its underlying physical relations need to be understood. Solid materials are very complex systems formed by molecules of atoms and subatomic particles. Thus, in principle, it might seem that the best approach to study a material's response to a thermomechanical loading would be to predict that of its atoms. Conceptually, this approach may seem feasible; however, these theories do not provide a practical model for ordinary engineering applications. At the complete opposite end of the spectrum lies *Continuum Mechanics and Thermodynamics* (CMT). CMT is a general subject and, just as its name implies, deals with the mechanics of the continua, establishing a coherent framework for the prediction of continuum bodies behaviour, in which the details of the atomic structure and interatomic interaction are not considered. In other words, this approach treats bodies as continuous distributions of matter that can be repeatedly subdivided into infinitesimal elements without losing the properties of the bulk material. Except for some particular phenomena, CMT actually provides the basis for most theories regarding solids' mechanical behaviour. In fact, as long as the length of the body is sufficiently larger than that of its atomic structure, the continuum assumption remains valid. Given the geometrical complexity and the non-linearity of their constitutive relations, most solid mechanics problems are generally difficult to solve analytically. Therefore, numerical approximations, typically through the *Finite Element Method* (FEM), are often employed.

In this Chapter, fundamental concepts of the Continuum Mechanics theory and the application of the Finite Element Method for the solution of a *quasi-static initial boundary value problem* are presented. The textbook of [de Souza Neto et al. \(2008\)](#) served as the primary reference for the writing of this Chapter. Nevertheless, other works, such as [Bonet](#)

and Wood (2008) and Tadmor et al. (2011), were also consulted and are recommended if the reader desires a more thorough description of these topics. Additionally, tensor calculus provides the mathematical framework for the formulation of the CMT theory. Although an in-depth understanding of these mathematical concepts is not necessarily required to follow the ensuing sections, it is still somewhat recommended. That being said, any of the references above also provide a good, clear revision if one desires to become more familiar with tensor calculus and its notation.

2.1 Kinematics of Deformation

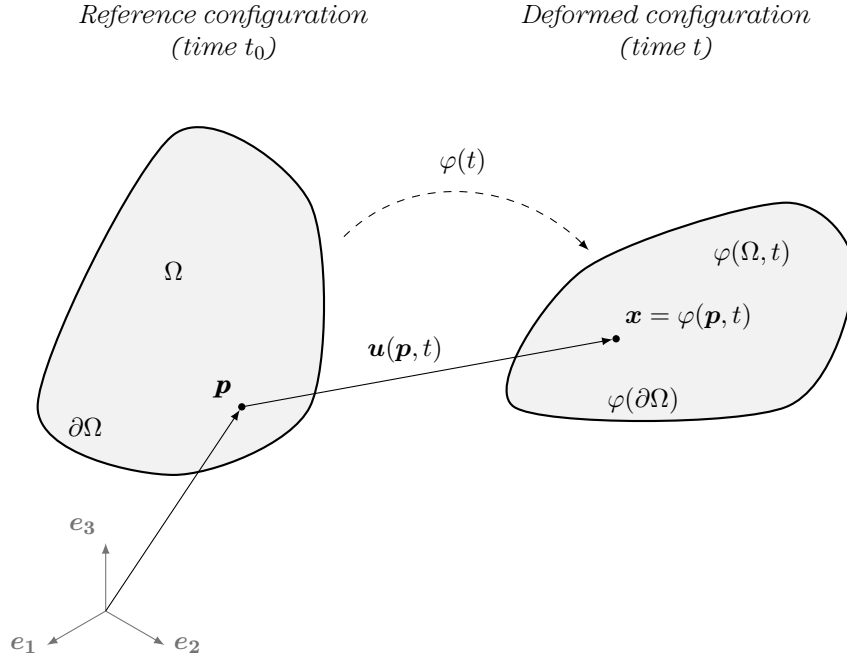
As previously stated, CMT is a general subject, and, as such, it must apply to a wide range of problems. Therefore, contrary to what is typically observed in theories such as strength of materials and linear elasticity, the number of assumptions and restrictions must be minimal. One crucial aspect of CMT is that it is applicable regardless of the strain magnitude, i.e., it can deal with strains of arbitrarily large magnitude (usually called *finite strains*, as opposed to *infinitesimal strains* typically assumed in theories like the mentioned above). For this reason, an accurate description of deformation and motion is fundamental to finite deformation analysis.

The *kinematics of deformation* provides the tools required for measuring all possible deformations a body might undergo. For now, this description is established purely from geometrical and spatial points of view. The relation between deformation and the corresponding loads and stresses will be the subject of forthcoming sections.

2.1.1 Deformation Mapping Function

Upon deformation, a continuum body may assume an infinite number of geometrical configurations. Therefore, it is appropriate to establish one of them as the *reference configuration*, to which any other observable configuration shall be compared in order to assess the corresponding deformation. In this sense, it is common practice to assign the unloaded, initial configuration as the reference one. Consider a general continuum body $\mathcal{B}$, in its reference configuration, occupying a region Ω of the three-dimensional ($\mathbb{R}^3$) Euclidean space $\mathcal{E}$ with a regular boundary $\partial\Omega$. Moreover, let $\mathbf{p}$ denote the position (in the reference configuration) of an arbitrary particle of the body, such that $\mathbf{p} \in \Omega$. Contrary to what has been initially regarded as *particle*, it now refers to an infinitesimal volume of the body, as in a point in a geometrical space, rather than an actual constitutive entity of a material, i.e., an atom or subatomic particle. According to this description, it becomes clear that particles cannot be formed, nor can they perish. Thus, at any given configuration, each particle can be discriminated by its coordinates in the reference configuration, $\mathbf{p}$, much like a label, distinguishing it from all others.

The deformation of $\mathcal{B}$ is expressed using a time-dependent, smooth one-to-one *deformation mapping function* φ , which maps every particle's position in the reference config-

Figure 2.1: Deformation of a continuum body $\mathcal{B}$.

uration to its new coordinates in the deformed configuration (see Figure 2.1). Therefore, in the deformed configuration, at any given instant t , the continuum body now occupies the region given by $\varphi(\Omega, t)$, delimited by the boundary $\varphi(\partial\Omega)$. Considering $\mathbf{x}$ as the position of a given particle $\mathbf{p}$ after deformation, we may write that,

$$\mathbf{x} = \varphi(\mathbf{p}, t). \quad (2.1.1)$$

The displacement vector field $\mathbf{u}(\mathbf{p}, t)$ is given by the difference between the positions of the particle $\mathbf{p}$ between the deformed and reference configurations. Thus, recalling equation (2.1.1), $\mathbf{u}$ can be written in terms of φ as:

$$\mathbf{u}(\mathbf{p}, t) = \varphi(\mathbf{p}, t) - \mathbf{p}. \quad (2.1.2)$$

Taking into account equations (2.1.1) and (2.1.2), the position of any given particle, whose original, undeformed position is known, at the deformed configuration can now be written as:

$$\mathbf{x} = \mathbf{p} + \mathbf{u}(\mathbf{p}, t). \quad (2.1.3)$$

Deformation implies a change in shape from the initial to the final (deformed) configuration. However, it is worth noting that, although motion may be associated with deformation, it does not necessarily imply its existence and may, in turn, be solely associated with a rigid-body displacement, in which the distance between any two particles is preserved. Thus, a generic particle's motion can be accomplished through deformation of the continuum, rigid-body displacement or a combination of both. Before addressing deformation per se, we shall, first, see rigid-body displacements, which are discussed below:

1. *Rigid Translation*: The displacement vector $\mathbf{u}(\mathbf{p}, t)$ is constant through space, i.e., independent of $\mathbf{p}$, such that:

$$\mathbf{x}(\mathbf{p}, t) = \mathbf{p} + \mathbf{u}(t); \quad (2.1.4)$$

2. *Rigid Rotation*: Rotation of the continuum $\mathcal{B}$ around a fixed point $\mathbf{q}$ given by a second-order rotational tensor $\mathbf{R}$:

$$\mathbf{x}(\mathbf{p}, t) = \mathbf{q} + \mathbf{R}(t)(\mathbf{p} - \mathbf{q}); \quad (2.1.5)$$

3. *Combination of Rigid Translation and Rotation*: Combination of the two displacement mechanisms expressed above:

$$\mathbf{x}(\mathbf{p}, t) = \varphi(\mathbf{q}, t) + \mathbf{R}(t)(\mathbf{p} - \mathbf{q}). \quad (2.1.6)$$

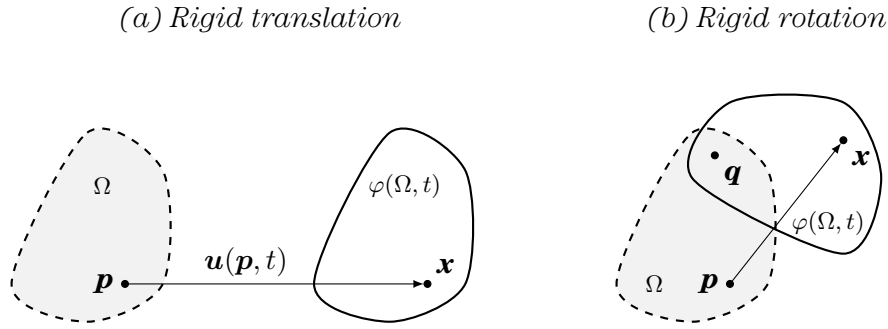


Figure 2.2: Rigid translation (a) and rigid rotation (b) of a continuum body $\mathcal{B}$.

These mechanisms imply that the configuration observed at a given time instant t_1 might be entirely different from the observed at a future one, t_2 , in what constitutes the notion of *motion*. For this reason, the deformed configuration is often referred to as the *current configuration*. Naturally, as $\mathcal{B}$ moves through space and time, so do its particles. The velocity of a particle $\mathbf{p}$ then comes as the derivative of its *current* position $\mathbf{x}$ in order to time t and might be expressed by:

$$\dot{\mathbf{x}}(\mathbf{p}, t) = \frac{\partial \mathbf{x}(\mathbf{p}, t)}{\partial t} = \frac{\partial \varphi(\mathbf{p}, t)}{\partial t}. \quad (2.1.7)$$

Furthermore, since a one-to-one deformation function is assumed, thus ensuring the previously stated condition that particles are not destroyed nor created, a particle $\mathbf{p}$ cannot be mapped into two different positions at a generic time t . It must, therefore, admit an inverse function, allowing an arbitrary particle to be identified by its position at any given time. We may then write that,

$$\mathbf{p} = \varphi^{-1}(\mathbf{x}, t) = \mathbf{x} - \mathbf{u}(\varphi^{-1}(\mathbf{x}, t), t), \quad (2.1.8)$$

where φ^{-1} is called *reference map* or, alternatively, inverse mapping function. Using this function, one may still define the concept of *spatial velocity*, given by:

$$\mathbf{v}(\mathbf{x}, t) = \dot{\mathbf{x}}(\varphi^{-1}(\mathbf{x}, t), t), \quad (2.1.9)$$

and that defines the velocity of the material particle positioned at $\mathbf{x}$ at time t . At first glance, the difference between spatial velocity $\mathbf{v}$ and particle velocity $\dot{\mathbf{x}}$ (see equation 2.1.7) might seem insignificant or even non-existent; however, these quantities constitute very different concepts related to entirely different frames of reference, which are the coordinate systems with respect to which a configuration is described. These differences are discussed next.

2.1.2 Material and Spatial Field Descriptions

In finite deformation analysis, the concept of *frame of reference* plays a pivotal role in the mathematical description of the deformation of a continuous body. Relevant quantities, such as velocity (be it spatial or of the particle), can be defined in terms of either initial (reference) or current (deformed) configurations. If the former is admitted, a *material* (or *Lagrangian*) description is adopted, whereas, with the latter, a *spatial* (or *Eulerian*) description is assumed. Thus, the coordinates of a given particle $\mathbf{p}$ in the reference configuration might be referred to as *material coordinates*, while the coordinates of a spatial position $\mathbf{x}$ may be addressed, quite evidently, as *spatial coordinates*.

In the material description, the continuous body's motion is described with respect to the initial undeformed configuration. General time-dependent material fields (scalar, vectorial or tensorial) are defined over the continuum's domain in its reference configuration, Ω . That being said, the particle velocity $\dot{\mathbf{x}}$ is an example of a material quantity since, just as its name suggests, it represents a vectorial field whose sole argument (besides time t) is $\mathbf{p}$ (see equation 2.1.7). On the other hand, a spatial description alludes to the behaviour at a specific fixed point in space (spatial position), represented by $\mathbf{x}$. Note that, while $\mathbf{x}$ was previously used to denote the current position of a particle $\mathbf{p}$, it is now being employed to define a point in space, free of any connection with $\mathcal{B}$. Although mathematically, the quantity remains the same, the actual meaning may differ according to the context and description being exercised. Spatial descriptions involve fields defined over $\varphi(\Omega)$ and dependent on time, t , and spatial position, $\mathbf{x}$. Under these circumstances, it becomes clear that, in contrast with $\dot{\mathbf{x}}$, $\mathbf{v}$ defines a spatial quantity. In short, through the material (or Lagrangian) frame of reference, the observer follows one particular particle (fixed material point) of the body $\mathcal{B}$ as it deforms and its corresponding variables, whereas, with the spatial (or Eulerian) frame of reference, the observer is concerned with the evolution of those same variables in a fixed point in space.

In the context of solid mechanics, a material description is the most adequate option, given the fact that a reference configuration can be readily defined. In contrast, in fluid mechanics, a spatial description might be the most prudent approach. Nevertheless, throughout the remainder of this Chapter, in an attempt to keep itself as self-contained as possible,

both material and spatial entities will be considered.

2.1.3 Deformation Gradient

The deformation mapping function, φ , presented earlier may describe how particles move through space and is an essential quantity for the description of motion, but it does not provide information regarding the particles' shape change. In fact, to accurately measure this concept, it is necessary to characterize the deformation in a particle's infinitesimal neighbourhood. Thus, a new definition must be introduced in order for a careful mathematical representation of deformation to be achieved.

The *deformation gradient*, $\mathbf{F}$, is a crucial quantity in finite deformation analysis and, as a second-order tensor, allows the mapping of vectors from the reference to the spatial configuration and vice-versa, just as also previously verified with φ . This link relates to the concepts of *push forward* and *pull back*, which stem from the bridge between the material and spatial configurations. We will come back to this subject later on.

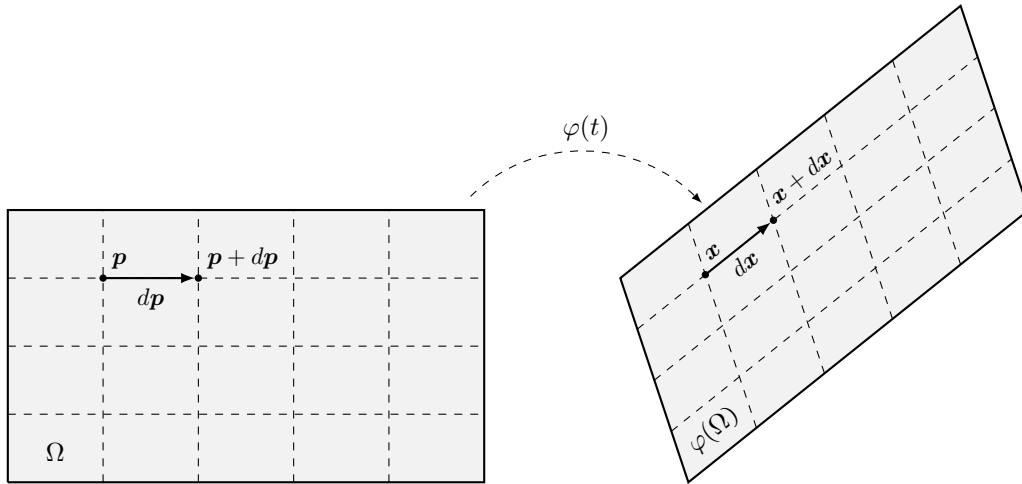


Figure 2.3: Deformation gradient: positions of two neighbouring particles before and after deformation.

Considering two neighbouring material particles, $\mathbf{p}$ and $\mathbf{p} + d\mathbf{p}$, of a generic continuum body $\mathcal{B}$, after motion, the particles are located at $\mathbf{x}$ and $\mathbf{x} + d\mathbf{x}$, respectively (see Figure 2.3). The deformation gradient tensor enables the relative spatial position of two neighbouring particles after deformation (current configuration) to be expressed in terms of their relative material position before deformation (reference configuration). Thus, we may write,

$$d\mathbf{x} = \mathbf{F}d\mathbf{p}. \quad (2.1.10)$$

The Cartesian components of the deformation gradient $\mathbf{F}$ are given by:

$$F_{ij} = \frac{\partial x_i}{\partial p_j}. \quad (2.1.11)$$

Returning, now, to the concepts of push forward and pull back, introduced above, one might say that the spatial vector $d\mathbf{x}$ is the push forward equivalent of the material vector $d\mathbf{p}$. On the contrary, $d\mathbf{p}$ can be regarded as the pull back equivalent of its spatial counterpart, $d\mathbf{x}$, a relation that can be expressed as:

$$d\mathbf{p} = \mathbf{F}^{-1}d\mathbf{x}. \quad (2.1.12)$$

Using the concept of deformation mapping function, equation (2.1.10) may be rewritten as:

$$\mathbf{F}(\mathbf{p}, t) = \frac{\partial \mathbf{x}}{\partial \mathbf{p}} = \nabla_{\mathbf{p}}[\varphi(\mathbf{p}, t)], \quad (2.1.13)$$

in which $\nabla_{\mathbf{p}}$ represents the material gradient operator of a generic tensorial quantity with respect to $\mathbf{p}$ for a fixed time t .

Taking into account expression (2.1.3), the deformation gradient becomes:

$$\mathbf{F}(\mathbf{p}, t) = \mathbf{I} + \nabla_{\mathbf{p}}[\mathbf{u}(\mathbf{p}, t)], \quad (2.1.14)$$

where $\mathbf{I}$ denotes the second-order identity tensor.

Since, besides time t , the argument of the deformation gradient $\mathbf{F}$ established in the previous equations is the material particle $\mathbf{p}$, it is clear that a material description has been adopted. Nevertheless, a spatial description might too be considered:

$$\mathbf{F}(\mathbf{x}, t) = \nabla_{\mathbf{x}}[\varphi^{-1}(\mathbf{x}, t)], \quad (2.1.15)$$

where $\nabla_{\mathbf{x}}$ is the spatial gradient operator, which, analogous with its material equivalent seen in equations (2.1.13) and (2.1.14), is given by:

$$\nabla_{\mathbf{x}}(\cdot) = \frac{\partial(\cdot)}{\partial \mathbf{x}}. \quad (2.1.16)$$

In the particular event of $\mathbf{F}$ applied to $\mathcal{B}$ being uniform, i.e., independent of $\mathbf{p}$, the deformation is called *homogeneous*. In these circumstances, the deformation mapping function may be written as:

$$\varphi(\mathbf{p}, t) = \varphi(\mathbf{q}, t) + \mathbf{F}(\mathbf{p} - \mathbf{q}), \quad (2.1.17)$$

for all points $\mathbf{p}, \mathbf{q} \in \mathcal{B}$. The resemblance between equations (2.1.6) and (2.1.17) is manifestly clear - in short, rigid-body motions constitute homogeneous deformations.

2.1.4 Isochoric and Volumetric Split of the Deformation Gradient

Any deformation can be locally split into a purely *volumetric* deformation, $\mathbf{F}_{vol}$, followed by a volume preserving (*isochoric*) deformation, $\mathbf{F}_{iso}$, or, alternatively, as an isochoric de-

formation followed by a purely volumetric one. Hence, the deformation gradient $\mathbf{F}$ may be decomposed as:

$$\mathbf{F} = \mathbf{F}_{iso}\mathbf{F}_{vol} = \mathbf{F}_{vol}\mathbf{F}_{iso}. \quad (2.1.18)$$

In order to further explore the notions of isochoric and volumetric deformation, we shall first consider the determinant of the deformation gradient,

$$J = \det(\mathbf{F}), \quad (2.1.19)$$

which represents the volume change of a particle:

$$J = \frac{dv}{dv_0}, \quad (2.1.20)$$

where dv and dv_0 are, respectively, the local current and initial volumes. Having established this, it becomes quite clear that if volume is preserved after the deformation, then J must be equal to 1. Moreover, it is essential to realize that the gradient's determinant must always satisfy $J > 0$. Naturally, $J = 0$ would mean that, at any given moment, the infinitesimal volume collapses, which is physically impossible (particles cannot perish). In light of this, two types of deformation can be defined:

1. *Isochoric deformation:* As already stated, an isochoric deformation consists of a volume-preserving deformation; therefore, only shape change is observable. In this case, $J = 1$. The deformation gradient related to an isochoric deformation is denoted as $\mathbf{F}_{iso}$.
2. *Volumetric deformation:* A volumetric deformation consists of a uniform contraction/expansion in all directions. Considering l as the final distance (along an arbitrary direction) between two neighbouring particles and l_0 as the corresponding undeformed (reference) quantity, we may define $\alpha = l/l_0$ as the contraction/expansion ratio and, therefore, $dv = \alpha^3 dv_0$. Thus, according to equation (2.1.20), we may write that $J = \alpha^3$. The volumetric deformation gradient promptly comes as:

$$\mathbf{F}_{vol} = \alpha \mathbf{I}. \quad (2.1.21)$$

Note that $\det(\mathbf{F}_{vol}) = (J^{1/3})^3 \cdot \det(\mathbf{I}) = J$, which implies that, as expected, the volume changes (measured by the quantity J) associated with the volumetric component of the deformation gradient, $\mathbf{F}_{vol}$, and the deformation gradient $\mathbf{F}$ itself are the same.

In turn, taking to account equations (2.1.18) and (2.1.21), the purely volumetric deformation gradient can too be expressed as a function of $\mathbf{F}$:

$$\mathbf{F}_{iso} = J^{-1/3} \mathbf{F}. \quad (2.1.22)$$

2.1.5 Polar Decomposition of the Deformation Gradient

Similarly to the idea illustrated in the previous Section, the deformation gradient might also be deconstructed into *shape-change*¹ and *pure rotation* components. While the notion that $\mathbf{F}$ provides a measure for the neighbourhood's deformation is true, it is not entirely accurate. Indeed, rotation does not play a role in the deformation process. Therefore, it might be useful to separate $\mathbf{F}$ into its rotation and shape-change parts. Conveniently, according to the *polar decomposition theorem* (valid for any tensor $\mathbf{F}$ with positive determinant²), the deformation gradient tensor can be uniquely expressed as:

$$\mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{V} \mathbf{R}, \quad (2.1.23)$$

in what constitutes the right and left polar decompositions of $\mathbf{F}$ and where the proper-orthogonal tensor $\mathbf{R}$ denotes the local rotation tensor and $\mathbf{U}$ and $\mathbf{V}$ are symmetric positive-definite tensors called, respectively, right and left stretch tensors. Recalling that, as proper-orthogonal tensor, $\mathbf{R}$ is a tensor with unitary determinant and whose inverse is equal to its transpose, i.e., $\mathbf{R} \mathbf{R}^T = \mathbf{R}^T \mathbf{R} = \mathbf{I}$, then, in line with the relation established in equation (2.1.23), the right and left stretch tensors are related by the rotation tensor as:

$$\mathbf{V} = \mathbf{R} \mathbf{U} \mathbf{R}^T. \quad (2.1.24)$$

Given their symmetry, the stretch tensors $\mathbf{U}$ and $\mathbf{V}$ may be expressed via the spectral decomposition as follows:

$$\mathbf{U} = \sum_{i=1}^3 \lambda_i \mathbf{l}_i \otimes \mathbf{l}_i, \quad (2.1.25)$$

$$\mathbf{V} = \sum_{i=1}^3 \lambda_i \mathbf{e}_i \otimes \mathbf{e}_i, \quad (2.1.26)$$

in which $\lambda_1, \lambda_2, \lambda_3$ denote the eigenvalues shared by both stretch tensors, i.e., the *principal stretches*, while $\mathbf{l}_i$ and $\mathbf{e}_i$ are the unit eigenvectors of the right and left stretch tensors, respectively, and define the Lagrangian and Eulerian *principal directions*, which are related by the rotation tensor through:

$$\mathbf{l}_i = \mathbf{R} \mathbf{e}_i. \quad (2.1.27)$$

To better illustrate the significance of the polar decomposition of $\mathbf{F}$, see Figure 2.4. Assuming the right polar decomposition is considered, the neighbourhood of $\mathbf{p}$ is firstly

¹ Changes in the shape of the neighbourhood of a given particle include *stretching* (length changes) and *shearing* (angle changes).

² Actually, any second-order tensor (with positive determinant) can be expressed as the product of an orthogonal tensor with a symmetric tensor, which is to say that the polar decomposition theorem is true for any second-order tensor; however, in this text, we are only concerned with its application in the two-point deformation gradient $\mathbf{F}$.

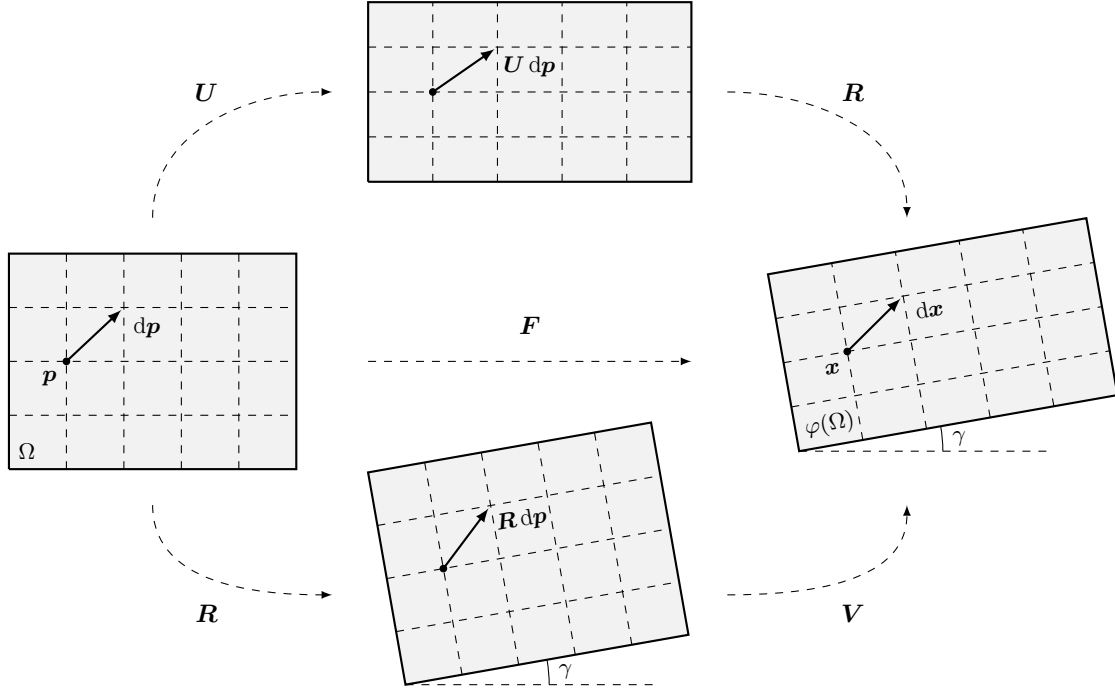


Figure 2.4: Left and right polar decompositions of $\mathbf{F}$ as two-step sequences involving arbitrary stretching with a superimposed rigid rotation of angle γ .

subjected to shape change, by means of the stretch tensor $\mathbf{U}$, and then rotated, so that $\mathbf{F}d\mathbf{p} = \mathbf{R}(\mathbf{U}d\mathbf{p})$. Contrarily, for the left decomposition, the neighbourhood is first rotated and only then shaped into its deformed (final) configuration. In this case, $\mathbf{F}d\mathbf{p} = \mathbf{V}(\mathbf{R}d\mathbf{p})$. In any case, the mapping $d\mathbf{x} = \mathbf{F}d\mathbf{p}$ is split into two sequential steps. In summary, it must be understood that $\mathbf{U}$ acts on a vector in the reference configuration; $\mathbf{V}$, in turn, acts on a vector in the current configuration. Therefore, the right stretch tensor is a material quantity, whereas the left stretch tensor is a spatial quantity.

2.1.6 Strain Measures

In search of an accurate description of the deformation phenomenon, multiple tensors have been proposed in previous sections. In Section 2.1.5, in particular, it was demonstrated how pure rotations could be separated from pure stretches by applying the polar decomposition of the deformation gradient. In this context, two tensors, in particular, have been established for the characterization of a particle's neighbourhood shape change: the right and left stretch tensors, $\mathbf{U}$ and $\mathbf{V}$, respectively. However, these tensors' components are irrational functions of $\mathbf{F}$ and, as a result, might be difficult to obtain. Therefore, it is usually inconvenient to work with these quantities. Indeed, the right and left *Cauchy-Green* strain tensors arise as much more appealing options for defining strain measures. Considering $\mathbf{C}$ and $\mathbf{B}$ as the right and left Cauchy-Green strain tensors, respectively, these can be uniquely

expressed as functions of the the deformation gradient as follows:

$$\mathbf{C} = \mathbf{F}^T \mathbf{F}, \quad (2.1.28)$$

$$\mathbf{B} = \mathbf{F} \mathbf{F}^T. \quad (2.1.29)$$

Additionally, the Cauchy-Green strain tensor can also be written in terms of the polar decomposition's right and left stretch tensors as:

$$\mathbf{U} = \sqrt{\mathbf{C}} = \sqrt{\mathbf{F}^T \mathbf{F}}, \quad (2.1.30)$$

$$\mathbf{V} = \sqrt{\mathbf{B}} = \sqrt{\mathbf{F} \mathbf{F}^T}. \quad (2.1.31)$$

According [Tadmor et al. \(2011\)](#), the most convenient quantity for solids analysis is $\mathbf{C}$. In order to better comprehend the usefulness of the right Cauchy-Green tensor, let us first establish, by recalling equation (2.1.10), the following deduction:

$$\begin{aligned} \|\mathrm{d}\mathbf{x}\|^2 &= \mathrm{d}\mathbf{x} \cdot \mathrm{d}\mathbf{x} \\ &= \mathbf{F} \mathrm{d}\mathbf{p} \cdot \mathbf{F} \mathrm{d}\mathbf{p} \\ &= \mathbf{C} \mathrm{d}\mathbf{p} \cdot \mathrm{d}\mathbf{p} \\ &= (\mathbf{I} + 2\mathbf{E}^{(2)}) \mathrm{d}\mathbf{p} \cdot \mathrm{d}\mathbf{p} \end{aligned} \quad (2.1.32)$$

where $\mathbf{E}^{(2)}$ is the *Green-Lagrange* strain tensor, which can be expressed as a function the the right Cauchy-Green tensor:

$$\mathbf{E}^{(2)} = \frac{1}{2}(\mathbf{C} - \mathbf{I}). \quad (2.1.33)$$

Despite the momentary focus on this particular strain measure, it must be emphasised that the presented Green-Lagrange strain tensor is, by no means, the only adequate way to evaluate strain. It is merely one of many strain tensors that make up the *Lagrangian strain tensors* family, typically represented by $\mathbf{E}^{(m)}$. The adoption of a particular strain measure is, to some extent, arbitrary and usually dictated by its mathematical and physical convenience in respect to the the phenomenon in question. The Lagrangian strain tensors family is based on the Lagrangian triad $\{\mathbf{l}_1, \mathbf{l}_2, \mathbf{l}_3\}$, which means its tensors measure strains along the principal Lagrangian directions, hence its name. That being said, a relation between the generic Lagrangian strain tensor and the right stretch tensor can be found and is written as:

$$\mathbf{E}^{(m)} = \begin{cases} \frac{1}{m}(\mathbf{U}^m - \mathbf{I}) & , m \neq 0 \\ \ln(\mathbf{U}) & , m = 0 \end{cases} \quad (2.1.34)$$

where m is a real number and $\ln(\cdot)$ stands for the tensor logarithm of $(\cdot)$. Using equation (2.1.34), the Green-Lagrange strain tensor can be swiftly determined by imposing $m=2$.

Alternatively, we can also define strain tensors expressed in terms of the left stretch tensor:

$$\boldsymbol{\varepsilon}^{(m)} = \begin{cases} \frac{1}{m}(\mathbf{V}^m - \mathbf{I}) & , m \neq 0 \\ \ln(\mathbf{V}) & , m = 0 \end{cases} \quad (2.1.35)$$

where $\boldsymbol{\varepsilon}^{(m)}$ denotes the *Eulerian strain tensors* family, which, analogous to Lagrangian strain tensors, are based on the Eulerian triad $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. Similarly to equation (2.1.24), the Lagrangian and Eulerian strain tensors can also be related through the rotation tensor $\mathbf{R}$ by:

$$\boldsymbol{\varepsilon}^{(m)} = \mathbf{R} \mathbf{E}^{(m)} \mathbf{R}^T. \quad (2.1.36)$$

2.1.7 Spatial Velocity Gradient

The spatial velocity $\mathbf{v}$ was defined in equation (2.1.9). The *spatial velocity gradient* results from deriving $\mathbf{v}$ with respect to a given spatial position $\mathbf{x}$:

$$\mathbf{L} = \nabla_{\mathbf{x}}(\mathbf{v}). \quad (2.1.37)$$

Applying the chain rule, one arrives at:

$$\mathbf{L} = \frac{\partial}{\partial t} \left(\frac{\partial \varphi}{\partial \mathbf{p}} \right) \frac{\partial \mathbf{p}}{\partial \mathbf{x}} = \dot{\mathbf{F}} \mathbf{F}^{-1}. \quad (2.1.38)$$

Two relevant tensors can be obtained by splitting $\mathbf{L}$ into its symmetric and skew components. The symmetric part, $\mathbf{D}$, is called *rate of deformation tensor* or, alternatively, *stretching tensor*, whereas the skew part, $\mathbf{W}$, is referred to as the *spin tensor*. Let $\mathbf{A}$ denote a generic second-order tensor - in general, its symmetric and skew components can be respectively expressed as:

$$\text{sym}(\mathbf{A}) = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T), \quad (2.1.39)$$

$$\text{skew}(\mathbf{A}) = \frac{1}{2}(\mathbf{A} - \mathbf{A}^T), \quad (2.1.40)$$

and, accordingly, the symmetric and skew parts of $\mathbf{L}$ may be expressed as:

$$\mathbf{D} = \text{sym}(\mathbf{L}) \quad , \quad \mathbf{W} = \text{skew}(\mathbf{L}) \quad (2.1.41)$$

To fully grasp the physical meaning behind the tensors $\mathbf{D}$ and $\mathbf{W}$, consider an arbitrary body $\mathcal{B}$ undergoing a motion with uniform velocity gradient (i.e., $\mathbf{L}$ independent of $\mathbf{x}$). For such circumstances, the velocity field is:

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{v}(\mathbf{q}, t) + \mathbf{L}(t)(\mathbf{x} - \mathbf{q}). \quad (2.1.42)$$

If the decomposition of $\mathbf{L}$ into its symmetric and skew components is assumed, the velocity field can be then split and the expression (2.1.42) subsequently written as follows:

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{v}^R(\mathbf{x}, t) + \mathbf{v}^S(\mathbf{x}, t), \quad (2.1.43)$$

where $\mathbf{v}^R$ and $\mathbf{v}^S$ can be related with tensors $\mathbf{D}$ and $\mathbf{W}$:

$$\mathbf{v}^R(\mathbf{x}, t) = \mathbf{v}(\mathbf{q}, t) + \mathbf{W}(t)(\mathbf{x} - \mathbf{q}), \quad (2.1.44)$$

$$\mathbf{v}^S(\mathbf{x}, t) = \mathbf{D}(t)(\mathbf{x} - \mathbf{q}). \quad (2.1.45)$$

As it happens, a motion whose spatial velocity field admits the representation established in equation (2.1.44) implies a rigid motion, therefore, $\mathbf{v}^R$ can be identified as *rigid velocity*. Thus, $\mathbf{v}^S$, which is related with the rate of deformation tensor $\mathbf{D}$, provides the only contribution to deformation. As a consequence, it may be referred to as *straining velocity*. Note that if a general motion is considered and $\mathbf{L}$ ceases to be uniform, the decomposition presented above remains valid in the local sense, i.e., in the infinitesimal neighbourhood of $\mathbf{x}$.

2.1.8 Infinitesimal Strain Tensor

As a final remark, it might be relevant to establish the bridge between the CMT theory presented so far and the *infinitesimal strain tensor* associated with small displacements and frequently addressed in introductory engineering courses. Small or infinitesimal deformations are deformations with a sufficiently small displacement gradient $\nabla_{\mathbf{p}}(\mathbf{u})$, which leads to significant simplifications regarding the whole corresponding description of deformation kinematics.

Considering the definition of the deformation gradient established in the equation (2.1.14), the expressions (2.1.28) and (2.1.29) may be rewritten in terms of the displacement gradient as follows:

$$\mathbf{C} = \mathbf{I} + \nabla_{\mathbf{p}}(\mathbf{u}) + [\nabla_{\mathbf{p}}(\mathbf{u})]^T + [\nabla_{\mathbf{p}}(\mathbf{u})]^T \cdot \nabla_{\mathbf{p}}(\mathbf{u}), \quad (2.1.46)$$

$$\mathbf{B} = \mathbf{I} + \nabla_{\mathbf{p}}(\mathbf{u}) + [\nabla_{\mathbf{p}}(\mathbf{u})]^T + \nabla_{\mathbf{p}}(\mathbf{u}) \cdot [\nabla_{\mathbf{p}}(\mathbf{u})]^T. \quad (2.1.47)$$

Since, in this case, the displacement gradient is small, the second order terms in $\nabla_{\mathbf{p}}(\mathbf{u})$ of the expressions above can be neglected and, as a result, the following statement can be made:

$$\mathbf{C} \approx \mathbf{B} \approx \mathbf{I} + \nabla_{\mathbf{p}}(\mathbf{u}) + [\nabla_{\mathbf{p}}(\mathbf{u})]^T. \quad (2.1.48)$$

Combining the expression above with the definitions of the Lagrange strain tensor and its Eulerian counterpart previously presented, it is too verified, to the same order of approx-

imation³, that, regardless of m :

$$\boldsymbol{\varepsilon} \approx \mathbf{E}^{(m)} \approx \boldsymbol{\varepsilon}^{(m)}, \quad (2.1.49)$$

where the infinitesimal strain tensor $\boldsymbol{\varepsilon}$ is a linear functional of the displacement vector field $\mathbf{u}$:

$$\boldsymbol{\varepsilon} = \nabla_p^s(\mathbf{u}), \quad (2.1.50)$$

with $\nabla^s(\cdot)$ as the symmetric gradient of $(\cdot)$:

$$\nabla^s(\cdot) = \frac{1}{2}[\nabla(\cdot) + \nabla(\cdot)^T]. \quad (2.1.51)$$

2.2 Forces and Stresses

The previous Section was dedicated to the mathematical analysis of the tools necessary for the measurement of all possible deformations a body may undergo. It should be noted that, thus far, no reference has been made to *forces* or how they translate into *stresses* and deformations. Therefore, it is now imperative that, before we attempt to understand the physical and constitutive laws that reign over a material's behaviour, we define ways of measuring stress. Generally speaking, two main types of forces can be identified:

1. *Body Forces*: Forces exerted on the interior of the body (such as gravitational and magnetic forces). Body forces are usually expressed per unit of mass (or volume).
2. *Surface Forces*: Surface forces include boundary forces, which consist of forces applied to the boundary of the body (such as those resulting from the interaction with its neighbourhood) and forces that arise from internal interactions between adjacent parts of a body. In any case, the dimension is force per unit area.

Throughout this Section, different ways of quantifying stresses will be presented. Similarly to strain measures, stress measures can also be defined in the current or initial body configurations. That being said, both the material and spatial configurations will continue being explored.

2.2.1 Cauchy Stress Vector

A fundamental step in the description of surface forces is the understanding of Cauchy's axiom, which allows for the definition of the *Cauchy stress vector*. In light of this, consider a body $\mathcal{B}$ in an arbitrarily deformed configuration (see Figure 2.5). In it, two oriented surfaces of the body ($\mathcal{L}$ and $\mathcal{T}$) can be observed. A unit vector at a point $\mathbf{x}$, $\mathbf{n}$, normal to the two mentioned surfaces is also represented. Note that $\mathbf{x}$ does not necessarily belong to the

³ It must be emphasized that by performing this simplification, we incur an error of second-order in $\nabla_p(\mathbf{u})$, which is small, given the fact that small displacements are assumed.

surface of the body. Cauchy's axiom states: "At $\mathbf{x}$, the force per unit infinitesimal area (surrounding the particle) exerted across the surface $\mathcal{L}$ by the material on the side of $\mathcal{L}$ into which $\mathbf{n}$ is pointing, upon the material on the other side of $\mathcal{L}$, depends on $\mathcal{L}$ only, through its normal $\mathbf{n}$ " (de Souza Neto et al., 2008). In other words, the forces exerted across surfaces that share the same normal vector at an arbitrary spatial position $\mathbf{x}$ (such as $\mathcal{L}$ and $\mathcal{T}$) are the same, provided that the continuum is in equilibrium. This force is called the Cauchy stress vector and will hereafter be denoted by $\mathbf{t}(\mathbf{n}, \mathbf{x}, t)$.

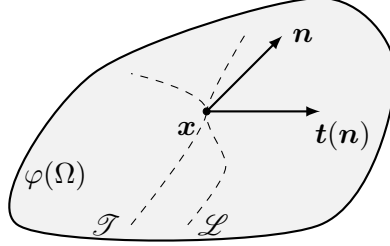


Figure 2.5: Schematic representation of the Cauchy Stress Vector at time t and its dependence on the normal vector to the surfaces $\mathcal{L}$ and $\mathcal{T}$ at a point $\mathbf{x}$.

Considering the infinitesimal area da normal to $\mathbf{n}$ in the neighbourhood of spatial point $\mathbf{x}$ and the resultant force $d\mathbf{f}$ exerted on this area, the corresponding Cauchy stress vector $\mathbf{t}$ may be defined as

$$\mathbf{t}(\mathbf{n}, \mathbf{x}, t) = \lim_{da \rightarrow 0} \frac{d\mathbf{f}}{da}. \quad (2.2.1)$$

2.2.2 Cauchy Stress Tensor

Cauchy's theorem establishes that, as a result of the axiom of momentum balance, the Cauchy stress vector relates with the normal vector $\mathbf{n}$ in a linear fashion:

$$\mathbf{t}(\mathbf{n}, \mathbf{x}, t) = \boldsymbol{\sigma}(\mathbf{x}, t) \cdot \mathbf{n}, \quad (2.2.2)$$

where $\boldsymbol{\sigma}(\mathbf{x}, t)$ is the *Cauchy stress tensor* or, alternatively, *true stress tensor*, as it is often referred to. It consists of a second-order spatial tensor, given the fact it refers to the deformed configuration (notice that, besides time t , its only argument is the spatial position $\mathbf{x}$). Furthermore, from the momentum equilibrium, one may also verify that the Cauchy stress tensor is symmetric. Considering an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, each of the components of the Cauchy stress tensor (expressed as σ_{ij}) may be given by:

$$\sigma_{ij} = (\boldsymbol{\sigma} \mathbf{e}_i) \cdot \mathbf{e}_j, \quad (2.2.3)$$

where the term in parenthesis is the force (per unit of area) applied across a surface with normal vector $\mathbf{e}_i$ at the arbitrary point $\mathbf{x}$ and σ_{ij} is the magnitude of the projection of that force along the direction of $\mathbf{e}_j$. Alternatively, considering the concept of the outer product of vectors, expression (2.2.3) may also be written as:

$$\boldsymbol{\sigma} = \sigma_{ij} \mathbf{e}_i \otimes \mathbf{e}_j. \quad (2.2.4)$$

The Cauchy stress tensor components are schematically represented in Figure 2.6. The components acting perpendicularly to the infinitesimal cube faces are the *normal tractions* and correspond to the terms along the diagonal of the stress tensor, whereas each of the remaining components act parallel to their respective face and are called *shear tractions*. It must be noted that, for any point, there is always an orthonormal basis $\{\mathbf{e}_1^*, \mathbf{e}_2^*, \mathbf{e}_3^*\}$ (which defines the *Cauchy principal directions*) for which the shear stress components are null. In this case, the normal stress components are referred to as *Cauchy principal stresses* and correspond to the eigenvalues of the stress tensor $\boldsymbol{\sigma}$.

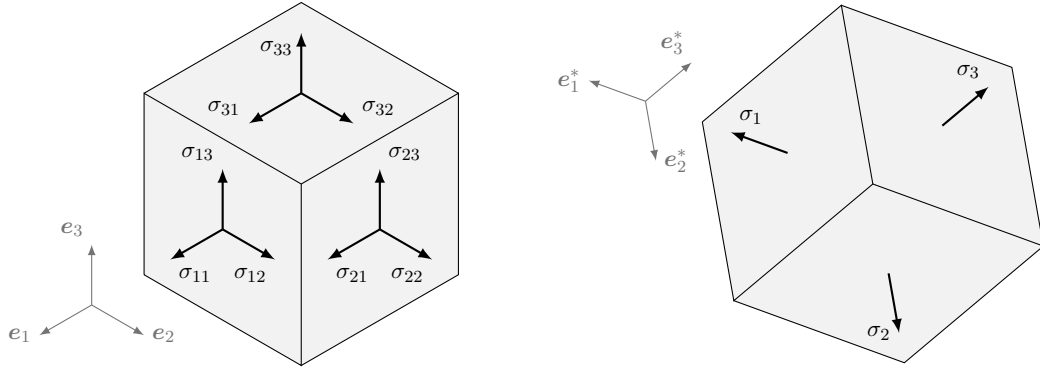


Figure 2.6: Cauchy stress tensor components and principal Cauchy stresses.

Similarly to the deformation gradient, the Cauchy stress tensor can too be split into volume-preserving and purely volumetric components, although, in this case, the decomposition is employed in an additive fashion:

$$\boldsymbol{\sigma} = \mathbf{s} + p\mathbf{I}, \quad (2.2.5)$$

where $\mathbf{s}$ is the *deviatoric stress* (volume-preserving part) and $p\mathbf{I}$ is the *volumetric stress*. Here, p is the *hydrostatic pressure* (or *hydrostatic stress*) and is given by:

$$p = \frac{1}{3} \text{tr}(\boldsymbol{\sigma}). \quad (2.2.6)$$

Note that $\text{tr}(\boldsymbol{\sigma})$ corresponds to the first invariant of the Cauchy stress tensor, I_1 , meaning that p will be the same regardless of the coordinate system used to represent $\boldsymbol{\sigma}$. Following this definition, it may be deduced that $\text{tr}(\mathbf{s}) = \text{tr}(\mathbf{s}) - p \text{tr}(\mathbf{I}) = \text{tr}(\boldsymbol{\sigma}) - 3p = 0$ (traceless tensor); thus, $\mathbf{s}$ only includes information regarding the shear stress, which proves its previously stated volume-preserving nature.

In the closing introductory paragraph of Section 2.2, we stated that different measures of the stress state would be presented according to the adopted configuration. The Cauchy stress vector $\mathbf{t}$ is the force exerted across a surface per unit of infinitesimal deformed area surrounding the particle located at the point of interest $\mathbf{x}$. It is, therefore, a spatial quantity. In contrast, the area itself may be measured in either the deformed or reference configuration. So far, only the Cauchy stress tensor has been introduced. The deformed area was

considered, thus allowing, as shown by equation (2.2.2), the mapping of a spatial vector into another spatial vector. Note that, in this case, the normal vector $\mathbf{n}$ is also a spatial quantity. In the sections that follow, different representations of the stress field will be addressed.

2.2.3 First Piola-Kirchhoff Stress Tensor

The *first Piola-Kirchhoff* stress tensor is the first alternative representation of the stress state, solely established for the purpose of mathematical convenience and does not entail a different physical quantity from the already presented Cauchy stress tensor. That being said, consider the vector $\mathbf{t}_0$ as the force exerted across a given surface per unit reference area containing the infinitesimal neighbourhood of $\mathbf{p}$ (position of the particle in the reference configuration). The normal vector at $\mathbf{p}$ might be entirely different from its current counterpart and will, therefore, be designated as $\mathbf{n}_0$. Analogously, assume da_0 as the infinitesimal area normal to $\mathbf{n}_0$ and da as its spatial equivalent. Admitting that the Cauchy stress vector is known, $\mathbf{t}_0$ may then be obtained by:

$$\mathbf{t}_0 = \frac{da}{da_0} \mathbf{t}. \quad (2.2.7)$$

Using equation (2.2.2), the previous equation may be rewritten in terms of the Cauchy stress tensor as

$$\mathbf{t}_0 = \frac{da}{da_0} \boldsymbol{\sigma} \mathbf{n}, \quad (2.2.8)$$

which, after some algebraic manipulation, leads to

$$\mathbf{t}_0 = J \boldsymbol{\sigma} \mathbf{F}^{-T} \mathbf{n}_0, \quad (2.2.9)$$

where $J = \det(\mathbf{F})$, $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{F}$ is the deformation gradient. Defining the first Piola-Kirchhoff stress tensor as

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^{-T}, \quad (2.2.10)$$

and introducing it in equation (2.2.9), we arrive at a similar version of the expression (2.2.2), given by:

$$\mathbf{t}_0 = \mathbf{P} \mathbf{n}_0. \quad (2.2.11)$$

While the first Piola-Kirchhoff stress tensor seemingly resembles a material entity, we must emphasize that it is not entirely linked to the reference configuration. In fact, although it is associated with the normal vector to the reference area (which in itself comprises a material entity), the stress vector $\mathbf{t}_0$ is derived from a spatial approach, as expression (2.2.7) suggests. Therefore, the first Piola-Kirchhoff stress tensor consists of a two-point tensor, and, contrary to the Cauchy stress tensor, it is not necessarily symmetric.

Alternatively, the first Piola-Kirchhoff stress tensor may also be written in terms of the *Kirchhoff* stress tensor $\boldsymbol{\tau}$:

$$\boldsymbol{P} = \boldsymbol{\tau} \boldsymbol{F}^{-T}. \quad (2.2.12)$$

Comparing the previous expression with equation (2.2.10), we may write

$$\boldsymbol{\tau} = J \boldsymbol{\sigma}. \quad (2.2.13)$$

Note from its relation with the Cauchy stress tensor that $\boldsymbol{\tau}$ is also symmetric.

Kirchhoff's principal stresses, τ_i , are often referenced in the formulation of several constitutive models, and may be directly determined from the principal Cauchy stresses, σ_i , by:

$$\tau_i = J \sigma_i. \quad (2.2.14)$$

2.2.4 Second Piola-Kirchhoff Stress Tensor

Contrary to the first Piola-Kirchhoff stress tensor, the *second Piola-Kirchhoff* stress tensor is a true material entity, in that it is entirely in the reference configuration. This is achieved by pulling the stress vector (or, more specifically, the spatial element of the exerted force) back to its reference configuration (denoted $\boldsymbol{t}_0^*$) as if it were a kinematic quantity. That being said, one may write:

$$\boldsymbol{t}_0^* = \boldsymbol{F}^{-1} \boldsymbol{t}_0, \quad (2.2.15)$$

in which $\boldsymbol{t}_0^*$ expresses the *true reference surface traction*. In other words, the second Piola-Kirchhoff stress tensor, $\boldsymbol{S}$, relates the true reference surface traction with the normal vector to the reference area, $\boldsymbol{n}_0$:

$$\boldsymbol{t}_0^* = \boldsymbol{S} \boldsymbol{n}_0. \quad (2.2.16)$$

Recalling (2.2.11), and considering the former two expressions, we obtain:

$$\boldsymbol{F}^{-1} \boldsymbol{P} \boldsymbol{n}_0 = \boldsymbol{S} \boldsymbol{n}_0. \quad (2.2.17)$$

Combining the definition of $\boldsymbol{P}$ (equation 2.2.10) together with equation (2.2.17), we arrive at the following expression for the second Piola-Kirchhoff stress tensor:

$$\boldsymbol{S} = J \boldsymbol{F}^{-1} \boldsymbol{\sigma} \boldsymbol{F}^{-T}. \quad (2.2.18)$$

Lastly, it is worth noting that, similarly to the Cauchy stress tensor (and, for that matter, contrary to the the first Piola-Kirchhoff stress tensor), $\boldsymbol{S}$ is a symmetric tensor.

2.3 Fundamental Laws of Thermodynamics

To this point, several strain and stress measures have been presented. On their own, these quantities do not provide the required information for the development of a model that accurately predicts a continuum body's behaviour when subjected to a thermomechanical loading. The foundation for such a framework includes a set of universal laws that must be respected and, as a result, place important constraints on the physical processes undergone by matter. What follows is an account of these laws of nature and may be divided into two distinct but complementary parts. First, we will address three fundamental principles in classical mechanics: *conservation of mass* and *balance of linear and angular momentums*. Secondly, the *fundamental laws of thermodynamics* will be discussed. Here, thermodynamics shall not be thought of as the general theory concerning heat flow and energy transfer between material systems. While this definition is still valid, in the scope of continuum mechanics and of this work it may be more appropriate to approach thermodynamics as "the study of the restrictions on the possible properties of matter that follow from the symmetry properties of the fundamental laws of physics" (Callen, 1985). The laws presented throughout this Section are valid for any continuum body.

2.3.1 Conservation of Mass

The principle of mass conservation requires that

$$\dot{\rho} + \rho \operatorname{div}_{\mathbf{x}}(\dot{\mathbf{u}}) = 0, \quad (2.3.1)$$

where ρ^4 denotes the mass per unit volume in the deformed configuration of the continuum body, $\dot{\rho}$ is the derivative of ρ with respect to time and $\operatorname{div}_{\mathbf{x}}(\cdot)$ is the spatial divergence operator.

2.3.2 Momentum Equilibrium

Consider a body $\mathcal{B}$ in the deformed configuration with domain $\varphi(\Omega)$ and boundary $\varphi(\partial\Omega)$ subjected to the action of surface forces, $\mathbf{t}(\mathbf{n}, \mathbf{x})$, expressed per unit of volume, and body forces, $\mathbf{b}(\mathbf{x})$, expressed per unit of volume. The principles of linear and angular momentums balance are satisfied if:

$$\int_{\varphi(\partial\Omega)} \mathbf{t}(\mathbf{n}, \mathbf{x}) \, da + \int_{\varphi(\Omega)} \rho(\mathbf{x}) \mathbf{b}(\mathbf{x}) \, dv = \int_{\varphi(\Omega)} \rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}) \, dv, \quad (2.3.2)$$

$$\int_{\varphi(\partial\Omega)} \mathbf{x} \times \mathbf{t}(\mathbf{n}, \mathbf{x}) \, da + \int_{\varphi(\Omega)} \mathbf{x} \times \rho(\mathbf{x}) \mathbf{b}(\mathbf{x}) \, dv = \int_{\varphi(\Omega)} \mathbf{x} \times \rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}) \, dv, \quad (2.3.3)$$

respectively. Note that the right-hand sides of equations (2.3.2) and (2.3.3) contain the inertial effects, with $\ddot{\mathbf{u}}$ denoting the acceleration field of $\mathcal{B}$. As a result of Cauchy's theorem,

⁴ The dependence on the spatial point $\mathbf{x}$ was omitted for notational convenience.

the balance of linear momentum for $\mathcal{B}$ may be written in terms of the Cauchy stress tensor as the following partial differential equation:

$$\begin{cases} \operatorname{div}_{\mathbf{x}}(\boldsymbol{\sigma}) + \mathbf{b} = \rho \ddot{\mathbf{u}} & \text{in } \varphi(\Omega), \\ \mathbf{t} = \boldsymbol{\sigma} \mathbf{n} & \text{in } \varphi(\partial\Omega). \end{cases} \quad (2.3.4)$$

These equations describe the *strong, local or point-wise form of equilibrium* and establish the physical relation between the forces and stresses and the observed displacements. Furthermore, the upper expression of (2.3.4) is known as *Cauchy's equation of motion*. The above momentum balance equations have been formulated in the spatial configuration. Equivalently, they may also be expressed in the material configuration of $\mathcal{B}$ in terms of the first Piola-Kirchhoff stress tensor:

$$\begin{cases} \operatorname{div}_{\mathbf{p}}(\mathbf{P}) + \mathbf{b}_0 = \rho_0 \ddot{\mathbf{u}} & \text{in } \Omega, \\ \mathbf{t}_0 = \mathbf{P} \mathbf{n}_0 & \text{in } \partial\Omega, \end{cases} \quad (2.3.5)$$

where $\mathbf{b}_0$ is the body force vector per unit of reference volume:

$$\mathbf{b}_0 = J \mathbf{b}, \quad (2.3.6)$$

and ρ_0 is the mass per unit of reference volume:

$$\rho_0 = J \rho. \quad (2.3.7)$$

2.3.3 First Law of Thermodynamics

The *first law of thermodynamics* postulates the principle of the conservation of energy and may be mathematically expressed by the following expression:

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{D} + \rho r - \operatorname{div}_{\mathbf{x}}(\mathbf{q}), \quad (2.3.8)$$

in which the scalar fields e and r represent the specific energy and density of heat production, respectively, the vector field $\mathbf{q}$ is the heat flux and the double contraction $\boldsymbol{\sigma} : \mathbf{D}$ is the stress power per unit volume in the deformed configuration. In other words, according to this energy conservation principle, the rate of internal energy (left-hand side of the equation) must be equal to the sum of the stress power and the heat production minus the spatial divergence of the heat flux (all per unit deformed volume). Energy may change form, but its overall amount must be conserved. That being said, if we admit the particular case of no heat production and heat flux spatially constant, equation (2.3.8) then reduces to

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{D}. \quad (2.3.9)$$

Note that even when thermal effects are dismissed and the problem at hand is purely mechanical, the fundamental laws of thermodynamics still play an important role in continuum mechanics. These laws are being presented in their full form, with no omission of the

thermally-related terms, despite the fact these will be dropped when we address the purely mechanical problem in Section 2.4.3.

2.3.4 Second Law of Thermodynamics

The first law of thermodynamics speaks of energy conservation during a thermodynamic process, but it establishes nothing concerning its direction. A new law must, therefore, be formulated. To mathematically address this issue, a new state variable must be introduced: entropy, denoted s , central to the *second law of thermodynamics*, which, in turn, states the directionality of a given thermodynamic process (in other words, the irreversibility of entropy production). There are several ways this principle can be expressed. Nevertheless, in simple terms, it states that "the entropy of an isolated system can never decrease in any process; it can only increase or stay the same". With that being said, the second law of thermodynamics may be given by the following inequality:

$$\rho \dot{s} + \operatorname{div}_{\mathbf{x}} \left(\frac{\mathbf{q}}{\theta} \right) - \frac{\rho r}{\theta} \geq 0, \quad (2.3.10)$$

where θ denotes the temperature field over $\mathcal{B}$.

2.3.5 Clausius-Duhem Inequality

The *Clausius-Duhem inequality* results from the combination of the first and second laws of thermodynamics, through which one arrives at the following inequality:

$$\boldsymbol{\sigma} : \mathbf{D} - \rho \left(\dot{\psi} + s \dot{\theta} \right) - \frac{1}{\theta} \mathbf{q} \cdot \mathbf{g} \geq 0, \quad (2.3.11)$$

where $\dot{\psi}$ is the time derivative of the specific free energy ψ defined by:

$$\psi = e - \theta s, \quad (2.3.12)$$

and $\mathbf{g}$ is the spatial gradient of the temperature field,

$$\mathbf{g} = \nabla_{\mathbf{x}}(\theta). \quad (2.3.13)$$

The left-hand side of expression (2.3.11) represents the dissipation per unit of deformed volume. Equivalently, the Clausius-Duhem inequality can be expressed in terms of dissipation per unit reference volume, by means of the Kirchhoff stress tensor, as:

$$\boldsymbol{\tau} : \mathbf{D} - \rho \left(\dot{\psi} + s \dot{\theta} \right) - \frac{J}{\theta} \mathbf{q} \cdot \mathbf{g} \geq 0, \quad (2.3.14)$$

which, in other words, forms the material version of expression (2.3.11).

2.4 Constitutive Theory

Up until this point, we have managed to establish a framework (with the physical laws that govern the behaviour of continuum systems) composed of five⁵ partial differential equations:

conservation of mass:	$\dot{\rho} + \rho \operatorname{div}_{\mathbf{x}}(\dot{\mathbf{u}}) = 0$	(1 equation),
balance of linear momentum:	$\operatorname{div}_{\mathbf{x}}(\boldsymbol{\sigma}) + \mathbf{b} = \rho \ddot{\mathbf{u}}$	(3 equations),
first law of thermodynamics:	$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{D} + \rho r - \operatorname{div}_{\mathbf{x}}(\mathbf{q})$	(1 equation).

These are called the *field* or *governing equations* of continuum mechanics. So far, the presented theory may seem remarkably economical; however, the vigilant eye might notice that these five governing equations include sixteen⁶ unknowns:

$\boldsymbol{\sigma}$ (6 unknowns),	$\mathbf{x}$ or $\mathbf{p}$ (3 unknowns),	$\mathbf{q}$ (3 unknowns),
θ (1 unknown),	e (1 unknown),	s (1 unknown), ρ (1 unknown),

where the symmetry of the stress tensor has been imposed by the balance of angular momentum (recall that this balance principle yields $\boldsymbol{\sigma}^T = \boldsymbol{\sigma}$). In other words, the theory is not yet complete since it holds more unknowns than equations to solve them, and it is, thus, necessary to obtain an additional eleven linearly independent equations. These missing equations are called *constitutive relations* and must consider the material of which the body is made. Indeed, the theory described so far is entirely general in the sense that it applies to all matter. However, the specific material that makes up the body plays a vital role in its response. Hence, we must define the laws that capture this dependency and depict different behaviours between different materials. The following pages will briefly review the principles that form the foundation for the constitutive model theory.

2.4.1 Constitutive Axioms

Constitutive relations are assumed to be governed by a set of fundamental principles. That being said, the axioms described in this Section must be satisfied for any constitutive model. Before we go any further, two essential definitions must first be introduced: a *thermokinetic process* of $\mathcal{B}$ is a pair of fields:

⁵ Note that the balance of angular momentum and the Clausius-Duhem inequality, despite providing constraints on material behaviour, are not governing equations.

⁶ We have taken advantage of the symmetrical nature of the Cauchy stress tensor. Notice that if we had instead considered the first Piola-Kirchhoff stress tensor, three additional unknowns would have to be determined. Furthermore, the heat source r and the body forces $\mathbf{b}$ are assumed to be known external interactions of the body with its vicinity.

$$\varphi(\mathbf{p}, t) \quad \text{and} \quad \theta(\mathbf{p}, t),$$

and a *calorodynamic process* of $\mathcal{B}$ is a set of fields:

$$\boldsymbol{\sigma}(\mathbf{p}, t), \quad e(\mathbf{p}, t), \quad s(\mathbf{p}, t), \quad r(\mathbf{p}, t), \quad \mathbf{b}(\mathbf{p}, t) \quad \text{and} \quad \mathbf{q}(\mathbf{p}, t),$$

satisfying the balance of linear momentum and the first and second laws of fundamental thermodynamics. A constitutive relation transforms the history of an arbitrary thermokinetic process into a calorodynamic process (Truesdell, 1984). These processes are intrinsically related to the following three fundamental axioms that every constitutive model must satisfy:

1. *Principle of thermodynamically compatible determinism*: States that, for any given body $\mathcal{B}$ at time t , "the history of the thermokinetic process to which a neighbourhood of a point $\mathbf{p}$ of $\mathcal{B}$ has been subjected determines a calorodynamic process for $\mathcal{B}$ at $\mathbf{p}$ " (Truesdell, 1984). In this respect, the case of *simple materials* is of particular interest. For this class of materials, the local history (history at point $\mathbf{p}$ solely) of $\mathbf{F}$, θ and $\mathbf{g}$ dictates the history of the thermokinetic process for constitutive purposes. That being said, according to the principle of thermodynamically compatible determinism, the local histories of $\mathbf{F}$, θ and $\mathbf{g}$ are sufficient for the definition of a calorodynamic process for $\mathcal{B}$ at $\mathbf{p}$. In other words, the calorodynamic process at point $\mathbf{p}$ is only a function of the history of the thermokinetic process at that exact point and not of the history at its neighbourhood. Therefore, this principle predicts the existence of constitutive functionals $\mathfrak{F}$, $\mathfrak{G}$, $\mathfrak{H}$ and $\mathfrak{I}$ dependent on these histories, such that:

$$\boldsymbol{\sigma}(\mathbf{p}, t) = \mathfrak{F}(\mathbf{F}^t(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^t(\mathbf{p})), \quad (2.4.1)$$

$$\psi(\mathbf{p}, t) = \mathfrak{G}(\mathbf{F}^t(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^t(\mathbf{p})), \quad (2.4.2)$$

$$s(\mathbf{p}, t) = \mathfrak{H}(\mathbf{F}^t(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^t(\mathbf{p})), \quad (2.4.3)$$

$$\mathbf{q}(\mathbf{p}, t) = \mathfrak{I}(\mathbf{F}^t(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^t(\mathbf{p})), \quad (2.4.4)$$

where $(\cdot)^t$ denotes the history of quantity $(\cdot)$ up to time t . Notice that just four of the six fields that compose a calorodynamic are defined. This is due to our assumption that the body forces $\mathbf{b}$ and the heat source r are known external interactions of the body with its environment.

2. *Principle of material objectivity (or frame invariance)*: Postulates that the material response must be independent of the observer. Two motions, φ^* and φ , are related by a change in the observer if its relation can be written as:

$$\varphi^*(\mathbf{p}, t) = \mathbf{y}(t) + \mathbf{Q}(t)(\varphi(\mathbf{p}, t) - \mathbf{x}_0), \quad (2.4.5)$$

where $\mathbf{y}(t)$ is an arbitrary point in space, $\mathbf{Q}(t)$ is a rotation around $\mathbf{x}_0$ and $(\varphi(\mathbf{p}, t) - \mathbf{x}_0)$ is the position vector of $\varphi(\mathbf{p}, t)$ relative to a generic origin $\mathbf{x}_0$. Notice the similarities

between the expression above and equation (2.1.5). Equation (2.4.5) corresponds to a rigid relative movement between the observers which, according to this principle, must not weight on the constitutive laws. In other words, the condition of objectivity imposes certain constraints on the functional form of constitutive relations defined from (2.4.1) to (2.4.4), which ensures that the resulting variables are *objective* (or *frame-indifferent*). These constraint may be expressed by:

$$\boldsymbol{\sigma}^*(\mathbf{p}, t) = \mathfrak{F}(\mathbf{F}^{t*}(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^{t*}(\mathbf{p})), \quad (2.4.6)$$

$$\psi(\mathbf{p}, t) = \mathfrak{G}(\mathbf{F}^{t*}(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^{t*}(\mathbf{p})), \quad (2.4.7)$$

$$s(\mathbf{p}, t) = \mathfrak{H}(\mathbf{F}^{t*}(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^{t*}(\mathbf{p})), \quad (2.4.8)$$

$$\mathbf{q}^*(\mathbf{p}, t) = \mathfrak{J}(\mathbf{F}^{t*}(\mathbf{p}), \theta^t(\mathbf{p}), \mathbf{g}^{t*}(\mathbf{p})). \quad (2.4.9)$$

The deformation gradient corresponding to φ^* , i.e., as viewed by the second observer, relates to $\mathbf{F}$ through:

$$\mathbf{F}^* = \mathbf{Q} \mathbf{F}. \quad (2.4.10)$$

Accordingly, the remaining fields corresponding to the motion φ^* are given by:

$$\boldsymbol{\sigma}^* = \mathbf{Q} \boldsymbol{\sigma} \mathbf{Q}^T, \quad (2.4.11)$$

$$\mathbf{q}^* = \mathbf{Q} \mathbf{q}, \quad (2.4.12)$$

$$\mathbf{g}^* = \mathbf{Q} \mathbf{g}, \quad (2.4.13)$$

whereas the scalar fields, such as temperature θ or entropy s , remain unaffected by a change in observer.

3. *Principle of material symmetry*: A constitutive relation must respect any symmetries described by the material. Generally speaking, the *symmetry group* of a material is the set of density-preserving changes of reference configuration under which the material response functionals remain unchanged. Specifically, the symmetry group of a solid material is a subset of the proper orthogonal group $\mathcal{O}^+$, hence, a set of rotations $\mathbf{Q}$ of the initial configuration that do not affect the functionals of the constitutive model. Note that $\mathcal{O}^+$ is the set of all proper orthogonal rotations $\mathbf{Q}$. Considering $\mathbf{Q} \in \mathcal{I}$ as a generic time-independent rotation, then the subgroup $\mathcal{I}$ of $\mathcal{O}^+$ is the symmetry group of the material defined by the constitutive functional $\mathfrak{F}$, $\mathfrak{G}$, $\mathfrak{H}$ and $\mathfrak{J}$ if the following relations are satisfied:

$$\mathfrak{F}(\mathbf{F}^t, \theta^t, \mathbf{g}^t) = \mathfrak{F}([\mathbf{F} \mathbf{R}]^t, \theta^t, \mathbf{g}^t), \quad (2.4.14)$$

$$\mathfrak{G}(\mathbf{F}^t, \theta^t, \mathbf{g}^t) = \mathfrak{G}([\mathbf{F} \mathbf{R}]^t, \theta^t, \mathbf{g}^t), \quad (2.4.15)$$

$$\mathfrak{H}(\mathbf{F}^t, \theta^t, \mathbf{g}^t) = \mathfrak{H}([\mathbf{F} \mathbf{R}]^t, \theta^t, \mathbf{g}^t), \quad (2.4.16)$$

$$\mathfrak{J}(\mathbf{F}^t, \theta^t, \mathbf{g}^t) = \mathfrak{J}([\mathbf{F} \mathbf{R}]^t, \theta^t, \mathbf{g}^t). \quad (2.4.17)$$

The principle of material symmetry imposes that the symmetries of the constitutive model are consistent with the symmetries of the material whose behaviour it is trying to predict. Frequently, the material at hand is *isotropic*. In that case, its symmetry group must coincide with the entire proper orthogonal group (i.e. $\mathcal{S} \equiv \mathcal{O}^+$), since the response of isotropic materials is the same for any given direction.

2.4.2 Thermodynamics with Internal Variables

In phenomenological theories of the continua's behaviour, there are numerous ways to determine the dissipative effects that follow deformation. The equations presented from (2.4.1) to (2.4.4), written in terms of functionals of the history of $\mathbf{F}$, θ and $\mathbf{g}$, comprise the general constitutive relations that any constitutive model must verify, yet, in the general form in which they have been established, they yield limited practical utility. Here, the history-recording nature of the formulated theory plays a significant limiting role. In fact, from a practical standpoint, the theory of *Thermodynamics with Internal State Variables* comprises a far more elegant approach than the general history functional-based description presented thus far. The premises of this alternative theory is that, at any instant t of a thermodynamical process, the basic local mechanical and thermal variables that define a thermodynamic state ($\boldsymbol{\sigma}$, φ , s and $\mathbf{q}$) at an arbitrary point $\mathbf{p}$ can be determined through constitutive equations coupled with the knowledge of a finite number of *state variables*:

$$\{\mathbf{F}, \theta, \mathbf{g}, \boldsymbol{\alpha}\},$$

in which $\boldsymbol{\alpha}$ is a set of *internal* or *hidden* state variables ($\boldsymbol{\alpha} \equiv \{\alpha_k\}$) and $\mathbf{F}$, θ and $\mathbf{g}$ are the instantaneous values of the deformation gradient, temperature and temperature spatial gradient, respectively. The thermodynamic state depends solely on the instantaneous value of these so-called state variables and, as a result, their past histories do not need to be taken into account. Furthermore, note that the set of internal variables $\boldsymbol{\alpha}$ may include entities of scalar, vectorial and tensorial nature linked with dissipative mechanisms.

Following this hypothesis, together with the fact, as a consequence of the second law of thermodynamics, the specific free energy ψ is independent of $\mathbf{g}$ (Coleman and Gurtin, 1967), we arrive at $\psi = \psi(\mathbf{F}, \theta, \boldsymbol{\alpha})$; accordingly, the time derivative of ψ is:

$$\dot{\psi} = \frac{\partial \psi}{\partial t} = \frac{\partial \psi}{\partial \mathbf{F}} : \dot{\mathbf{F}} + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \sum_k \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k. \quad (2.4.18)$$

Despite its generic notation, α must not be mistaken by a scalar field. As previously stated, each variable α_k may be a scalar, vectorial or tensorial entity, thus, the product operation between $\partial \psi / \partial \alpha_k$ and $\dot{\alpha}_k$ must be chosen accordingly. By writing the stress power as

$$\boldsymbol{\sigma} : \mathbf{D} = \boldsymbol{\sigma} \mathbf{F}^{-T} : \dot{\mathbf{F}}, \quad (2.4.19)$$

and introducing equation (2.4.18) into the Clausius-Duhem inequality (expression 2.3.11)

we obtain:

$$\left(\boldsymbol{\sigma} \mathbf{F}^{-T} - \rho \frac{\partial \psi}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}} - \rho \left(s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} - \rho \sum_k \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k - \frac{1}{\theta} \mathbf{q} \cdot \mathbf{g} \geq 0. \quad (2.4.20)$$

Equivalently, the material version of (2.4.20) reads:

$$\left(\mathbf{P} - \rho_0 \frac{\partial \psi}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}} - \rho_0 \left(s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} - \rho_0 \sum_k \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k - \frac{J}{\theta} \mathbf{q} \cdot \mathbf{g} \geq 0. \quad (2.4.21)$$

According to the principle of thermodynamical determinism, the Clausius-Duhem inequality must hold for any thermokinetic process. Then, the constitutive relations must be such that the inequality (2.4.20) (or its material version 2.4.21) remains valid for any given pair of functions $\dot{\mathbf{F}}, \dot{\theta}$. In particular, assume a arbitrary process for which the temperature is spatially uniform ($\mathbf{g} = \mathbf{0}$), the dissipative mechanisms linked with the internal variables are neglectable ($\dot{\boldsymbol{\alpha}} = \mathbf{0}$) and the deformation gradient is constant ($\dot{\mathbf{F}} = \mathbf{0}$). In this conditions, equation (2.4.21) reduces to:

$$-\rho_0 \left(s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} \geq 0. \quad (2.4.22)$$

Since no conditions are imposed regarding $\dot{\theta}$, its value may be either positive, negative or null. In either case, the only way of assuring that inequality (2.4.22) is always satisfied is if

$$s = - \frac{\partial \psi}{\partial \theta}. \quad (2.4.23)$$

Equation (2.4.23) can be referred to as *entropy constitutive relation*. Alternatively, if we consider that, instead of the deformation gradient, the temperature derivative in order to time is now null, then it can be written that:

$$\mathbf{P} = \rho_0 \frac{\partial \psi}{\partial \mathbf{F}}, \quad (2.4.24)$$

which, in turn, is known as *stress constitutive equation* or, more specifically, the first Piola-Kirchhoff stress constitutive equation. Naturally, alternative representations of the previous equation can be established in terms of the Cauchy stress tensor:

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \mathbf{F}} \mathbf{F}^T, \quad (2.4.25)$$

or in terms of the Kirchhoff stress tensor:

$$\boldsymbol{\tau} = \rho_0 \frac{\partial \psi}{\partial \mathbf{F}} \mathbf{F}^T. \quad (2.4.26)$$

An important point of the internal state variable theory is that it not only rests on the internal state variables but also upon their evolution. That being said, in order to fully characterize the constitutive model, complementary constitutive equations for the *flux variables* $\mathbf{q}/\theta$ and $\dot{\boldsymbol{\alpha}}$ must be defined. Generally, these flux variables are functions of the state variables:

$$\dot{\boldsymbol{\alpha}} = f(\mathbf{F}, \theta, \mathbf{g}, \boldsymbol{\alpha}), \quad (2.4.27)$$

$$\frac{\mathbf{q}}{\theta} = h(\mathbf{F}, \theta, \mathbf{g}, \boldsymbol{\alpha}), \quad (2.4.28)$$

As a final remark, it must be referred that the success of a thermodynamics with internal variables-based constitutive model is entirely reliant on the choice of an adequate set of internal variables. Since no model is comprehensive enough to describe the behaviour of a material under any possible process, it occurs that the internal variables must be chosen according to the specific material in question but also, and equally important, according to the processes under which the model is expected to predict the behaviour of the material. Generally speaking, with further increase in the phenomena (process) complexity, more refined constitutive models and, consequently, an increasing number of internal state variables will be needed. In summary, within the thermodynamics with internal variables theory, two separate approaches can be followed: a *micromechanical* or a *phenomenological* approach. The former involves the determination of mechanisms at the atomic, molecular or crystalline levels, whereas, in the latter, the internal variables are based on the dissipative behaviour observed at the continuum (macroscopic) level. Still, despite the macroscopic nature of the many solids mechanics theories derived from a purely phenomenological approach, in particular cases, it may become essential to consider information about the underlying microscopic dissipative mechanisms.

2.4.3 Purely Mechanical Constitutive Initial Value Problem

In purely mechanical problems, like the ones we intend to study, any thermal effects may be dismissed. As a result, by removing the thermally-related terms from the theory presented in Section 2.4.2, we obtain the following set of *mechanical constitutive equations*:

$$\psi = \psi(\mathbf{F}, \boldsymbol{\alpha}), \quad (2.4.29)$$

$$\mathbf{P} = \rho_0 \frac{\partial \psi}{\partial \mathbf{F}}, \quad (2.4.30)$$

$$\dot{\boldsymbol{\alpha}} = f(\mathbf{F}, \boldsymbol{\alpha}). \quad (2.4.31)$$

If, coupled with the thermally-related terms' discarding, an internal variable approach is used, the generic constitutive problem reduces to a *mechanical constitutive initial value problem*, which may be summarized by the following description: "Given the initial values of the internal variables $\boldsymbol{\alpha}(t)$ and the history of the deformation gradient,

$$\mathbf{F}(t), \quad t \in [t_0, T],$$

find the functions $\mathbf{P}(t)$ and $\boldsymbol{\alpha}(t)$, for the first Piola-Kirchhoff stress and the set of internal

variables, such that the constitutive equations

$$\begin{cases} \mathbf{P}(t) = \rho_0 \left. \frac{\partial \psi}{\partial \mathbf{F}} \right|_t \\ \dot{\boldsymbol{\alpha}}(t) = f(\mathbf{F}(t), \boldsymbol{\alpha}(t)) \end{cases}, \quad (2.4.32)$$

are satisfied for every $t \in [t_0, T]$.” (de Souza Neto et al., 2008)

2.5 Weak Equilibrium Equations

Earlier, in Section 2.3, we established the spatial and material versions of the strong form of equilibrium, given, respectively, by equations (2.3.4) and (2.3.5), which imply a point-wise (or local) equilibrium. Albeit the exact solution of these equations could be obtained for problems with geometries and boundary conditions of little complexity, more often than not, the exact solution of the strong form of equilibrium is quite difficult to obtain. As a result, numerical methods and the estimate of an approximate solution are usually required. To do so, the *weak form of equilibrium* (or *global form of equilibrium*) must first be defined, which can be derived from employing a variational principle to the equilibrium equations. The weak equilibrium formulation is fundamental to the description of the initial boundary value problem (addressed in Section 2.6) and establishes the foundation of the displacement-based finite element procedures for the analysis of solid materials. In the pages that follow, the *Principle of Virtual Work* is the adopted variational principle, and three versions of the weak equilibrium statement are presented: *spatial*, *material* and *quasi-static*.

2.5.1 Spatial Version

The spatial version of the weak equilibrium statement reads:

$$\int_{\varphi(\Omega)} [\boldsymbol{\sigma} : \nabla_{\mathbf{x}}(\boldsymbol{\eta}) - (\mathbf{b} - \rho \ddot{\mathbf{u}}) \cdot \boldsymbol{\eta}] dv - \int_{\varphi(\partial\Omega)} \mathbf{t} \cdot \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}, \quad (2.5.1)$$

where $\boldsymbol{\eta}$ is the virtual displacement vector which belongs to the space of admissible virtual displacements, $\mathcal{V}$.

2.5.2 Material Version

Consider the equation (2.2.10) and the following identity (valid for a generic vector field $\mathbf{a}$):

$$\nabla_{\mathbf{x}}(\mathbf{a}) = \nabla_{\mathbf{p}}(\mathbf{a}) \mathbf{F}^{-1}, \quad (2.5.2)$$

as well as the standard relation for any given scalar field a :

$$\int_{\varphi(\Omega)} a(\mathbf{x}) dv = \int_{\Omega} J(\mathbf{p}) a(\varphi(\mathbf{p})) dv, \quad (2.5.3)$$

By introducing these in equation (2.5.1), we may then establish the material description of the weak form of equilibrium:

$$\int_{\Omega} [\mathbf{P} : \nabla_{\mathbf{p}}(\boldsymbol{\eta}) - (\mathbf{b}_0 - \rho_0 \ddot{\mathbf{u}}) \cdot \boldsymbol{\eta}] dv - \int_{\partial\Omega} \mathbf{t}_0 \cdot \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}. \quad (2.5.4)$$

2.5.3 Quasi-static Version

In this work, we will not address any dynamics of the continuum, which is to say that we may neglect all inertial effects. This assumption leads to the *quasi-static* description of the weak equilibrium statement, whose spatial version can be deduced from (2.5.1):

$$\int_{\varphi(\Omega)} [\boldsymbol{\sigma} : \nabla_{\mathbf{x}}(\boldsymbol{\eta}) - \mathbf{b} \cdot \boldsymbol{\eta}] dv - \int_{\varphi(\partial\Omega)} \mathbf{t} \cdot \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}. \quad (2.5.5)$$

Analogously, from (2.5.4), its material equivalent reads:

$$\int_{\Omega} [\mathbf{P} : \nabla_{\mathbf{p}}(\boldsymbol{\eta}) - \mathbf{b}_0 \cdot \boldsymbol{\eta}] dv - \int_{\partial\Omega} \mathbf{t}_0 \cdot \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}. \quad (2.5.6)$$

In both cases, note that the time-derivative terms were no longer admitted.

2.6 Quasi-Static Initial Boundary Value Problem

Up to this point, we have laid out an extensive set of concepts regarding the continuum mechanics theory and dealt with the generic constitutive initial value problems (Section 2.4) as well as the weak equilibrium statement (Section 2.5). Thus, we can now discuss the weak form of the *fundamental initial boundary value problems*, whose numerical solution will be the subject of study in Section 2.7. Given the nature of the problems we intend to scrutinize in this work, we shall restrict our attention to quasi-static conditions and the purely mechanical behaviour of materials. Foremost, we must refer to the importance of prescribed data, which, fundamentally, turn our problem into one that can be solved. In this regard, it seems convenient to recall the premises of the general theory introduced in Section 2.4.2. Indeed, we must admit that the set of internal variables is known at the initial time t_0 (i.e. $\boldsymbol{\alpha}(\mathbf{p}, t_0) = \boldsymbol{\alpha}_0(\mathbf{p})$) and that the deformation gradient $\mathbf{F}$ is prescribed. As a result, we can then obtain the function $\mathbf{P}(t)$ for the first Piola-Kirchhoff stress tensor as the solution of the mechanical constitutive equations established from (2.4.29) to (2.4.31) and, with equation (2.2.10), the Cauchy stress tensor function $\boldsymbol{\sigma}(t)$ can be subsequently determined.

For this purpose, consider the generic body $\mathcal{B}$ subjected to a prescribed history of body forces (see Figure 2.7):

$$\mathbf{b}(\mathbf{x}, t), \quad t \in [t_0, T]. \quad (2.6.1)$$

Additionally, the following boundary conditions are imposed:

⁷ The dependence of $\mathbf{b}$ on spatial position $\mathbf{x}$ and time t was omitted for visual clarity.

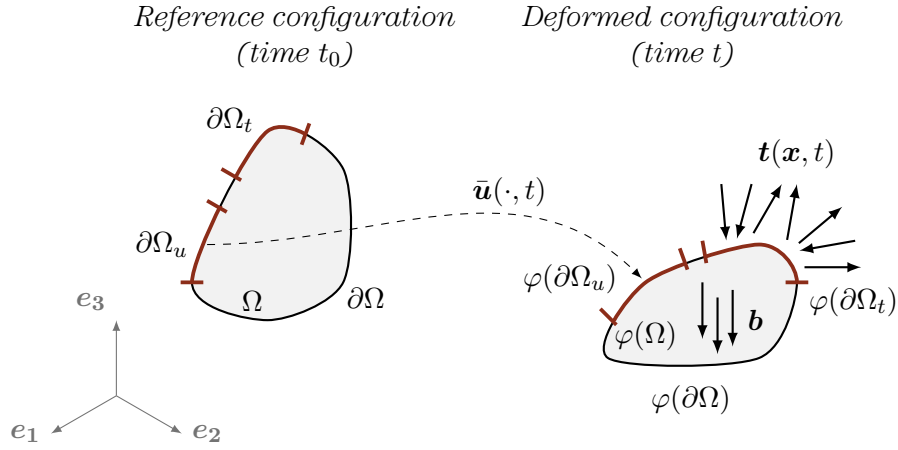


Figure 2.7: Schematic representation of the initial boundary value problem⁷.

1. *Natural boundary conditions*: history of the surface tractions imposed over the the portion of the boundary of $\mathcal{B}$ that occupies $\partial\Omega_t$ ⁸ in its reference configuration and up to time T :

$$\mathbf{t}(\mathbf{x}, t), \quad t \in [t_0, T], \quad \mathbf{x} \in \varphi(\partial\Omega_t). \quad (2.6.2)$$

2. *Essential boundary conditions*: motion imposed over the the portion of the boundary of $\mathcal{B}$ occupying $\partial\Omega_u$ ⁹ in the reference configuration:

$$\bar{\varphi}(\mathbf{p}, t) = \mathbf{p} + \bar{\mathbf{u}}(\mathbf{p}, t), \quad t \in [t_0, T], \quad \mathbf{p} \in \varphi(\partial\Omega_u), \quad (2.6.3)$$

where $\bar{\mathbf{u}}$ is the prescribed boundary displacement field. For simplicity, we may suppose that $\partial\Omega_u \cap \partial\Omega_t = \emptyset$. The set of displacementes that satisfy the essential boundary condition (kinematic constraint) allows us to define the set of *kinematically admissible displacementes* of $\mathcal{B}$:

$$\mathcal{K} = \{\mathbf{u} : \Omega \times \mathcal{R} \rightarrow \mathcal{U} \mid \mathbf{u}(\mathbf{p}, t) = \bar{\mathbf{u}}(\mathbf{p}, t), \quad t \in [t_0, T], \quad \mathbf{p} \in \varphi(\partial\Omega_u)\}. \quad (2.6.4)$$

At last, we can define the fundamental quasi-static initial boundary value problem. Its spatial version is stated by [de Souza Neto et al. \(2008\)](#): "Find a kinematically admissible displacement function, $\mathbf{u} \in \mathcal{K}$, such that, for all $t \in [t_0, T]$, the virtual work equation is satisfied:

$$\int_{\varphi(\Omega, t)} [\boldsymbol{\sigma} : \nabla_{\mathbf{x}}(\boldsymbol{\eta}) - \mathbf{b}(t) \cdot \boldsymbol{\eta}] \, dv - \int_{\varphi(\partial\Omega_t, t)} \mathbf{t}(t) \cdot \boldsymbol{\eta} \, da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}_t, \quad (2.6.5)$$

where the space of virtual admissible displacements at time t is given by:

$$\mathcal{V}_t = \{\boldsymbol{\eta} : \varphi(\Omega, t) \rightarrow \mathcal{U} \mid \boldsymbol{\eta} = \mathbf{0} \text{ on } \varphi(\partial\Omega_u, t)\}. \quad (2.6.6)$$

⁸ In this case, the subscript t refers to *traction*.

⁹ In this case, the subscript u refers to *displacement*.

Alternatively, the material version of quasi-static initial boundary value problem is also defined by [de Souza Neto et al. \(2008\)](#): "Find a kinematically admissible displacement function, $\mathbf{u} \in \mathcal{K}$, such that, for all $t \in [t_0, T]$,

$$\int_{\Omega} [\mathbf{P}(t) : \nabla_{\mathbf{p}}(\boldsymbol{\eta}) - \mathbf{b}_0(t) \cdot \boldsymbol{\eta}] dv - \int_{\partial\Omega_t} \mathbf{t}_0(t) \cdot \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}, \quad (2.6.7)$$

where

$$\mathcal{V} = \{\boldsymbol{\eta} : \Omega \rightarrow \mathcal{U} \mid \boldsymbol{\eta} = \mathbf{0} \text{ on } \partial\Omega_u\}."$$
(2.6.8)

2.7 Finite Element Method

Having established the integral (weak) form of the quasi-static initial boundary value problem, we must, once again, bear in mind that analytical solutions of equations (2.6.5) and (2.6.7) are unrealistic if solid bodies with complex geometries or intricate constitutive laws are to be studied. As a result, we must often resort to numerical (typically computational) methods to determine an admissible (approximate) solution to the problem. In this regard, the finite element method (FEM) is often seen as the benchmark method within solid mechanics. Throughout this Section, two major numerical approximations are described: *time* and *spatial* discretisations. Furthermore, since the original initial boundary value problem reduces to a set of *incremental (generally non-linear) algebraic equations*, the *Newton-Rapshon* algorithm is also presented. Lastly, it must be emphasised that this review is only brief and that no thorough description of the FEM should be expected. For a detailed account on this subject, see, for instance, [Zienkiewicz et al. \(2013\)](#).

2.7.1 Temporal Discretisation

Before going further with the steps related to the application of the FEM, it is worth noting that different descriptions can be made, and, once again, the one we adopt is entirely dependent on the assumptions we make and the type of solid mechanics problems we intend to solve numerically. That being said, it is convenient that we arrange these differences into distinct categories. First, we must take into account the magnitude of deformation. This aspect has already been discussed. In short, we can have finite or infinitesimal deformations, with the major practical difference being that, in the small displacement scenario, we can adopt the simplified infinitesimal strain tensor, $\varepsilon(\mathbf{u})$. Secondly, and more importantly, we need to consider the nature of the underlying material, which yields major consequences to the FEM description, particularly regarding the *strain path's* significance. Here, we can have *elastic* or *hyperelastic* materials, whose constitutive equations are *path-independent*, and *elastoplastic* or *elasto-viscoplastic* materials, for which the constitutive equations of the underlying material model are *path-dependent*.

Frequently, in engineering applications, deformations are assumed infinitesimal and, at the same time, focus often lies over elastic materials behaviour. In this case, the behaviour

and, in particular, the stress tensor is a function of the infinitesimal strain tensor only (without any dependence on internal variables):

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\mathbf{u})). \quad (2.7.1)$$

In more elaborate applications, however, such assumptions may be inaccurate. In fact, the materials' response may depend on the deformation history (and not only on its instantaneous value), i.e., the constitutive equations of the underlying model may be path-dependent. In such circumstances, relying uniquely on the adequate strain measure (be it the deformation gradient or the infinitesimal strain tensor, depending on the displacement scale) ceases to be sufficient and the adoption of an internal variable-based approach becomes inevitable. It happens that the solution of the mechanical constitutive initial value problem (Section 2.4.3) might be difficult to obtain for complex strain paths $\mathbf{F}(t)$ ¹⁰. As a result, an appropriate numerical algorithm for integration of the rate constitutive equations becomes essential. Generally, this numerical integration scheme implies an *incremental* strategy, under which, by adopting a *time* (or *pseudo-time*) *discretisation*, the original time-continuum constitutive equations are transformed into n *time-discrete* increments and the consideration of a specific deformation path along each of the n subintervals.

Within the context of the purely mechanical theory, the principle of thermodynamically determinism (Section 2.4.1) outlines that, for a generic time increment $[t_n, t_{n+1}]$, given the set of internal variables at time t_n , $\boldsymbol{\alpha}_n$, the prescribed deformation gradient at time t_{n+1} , $\mathbf{F}_{n+1}$, must determine the Cauchy stress tensor at the same instant, $\boldsymbol{\sigma}_{n+1}$, uniquely. With this in mind, we may define an *incremental constitutive function*, $\hat{\boldsymbol{\sigma}}$, for the stress tensor, such that:

$$\boldsymbol{\sigma}_{n+1} = \hat{\boldsymbol{\sigma}}(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}), \quad (2.7.2)$$

where $\boldsymbol{\sigma}_{n+1}$ is expected to converge to the exact solution as the strain increments are decreased. The benefit of the application of this temporal discretisation is that, within each increment, the numerical constitutive law is path-independent. In other words, in each subinterval, $\boldsymbol{\sigma}_{n+1}$ is a function of $\mathbf{F}_{n+1}$ alone and the set of internal variables $\boldsymbol{\alpha}$ is constant, in such a way that a similar incremental constitutive function for the internal variables can be defined:

$$\boldsymbol{\alpha}_{n+1} = \hat{\boldsymbol{\alpha}}(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}), \quad (2.7.3)$$

By introducing these time-discrete constitutive laws into the weak form of the initial boundary value problem established in Section 2.6, we can obtain the *incremental boundary value problem*, which, in its spatial version, is stated by de Souza Neto et al. (2008): "Given the field $\boldsymbol{\alpha}_n$ at time t_n and given the body forces ($\mathbf{b}_{n+1}$) and surface traction ($\mathbf{b}_{n+1}$) at t_{n+1} , find a kinematically admissible configuration $\varphi_{n+1}(\Omega) \in \mathcal{K}_{n+1}$ such that the virtual

¹⁰ Recall that we are concerned with the formulation of the FEM under the assumption of large (finite) strains.

work equation

$$\int_{\varphi_{n+1}(\Omega)} [\hat{\boldsymbol{\sigma}}(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}) : \nabla_{\mathbf{x}}^s(\boldsymbol{\eta}) - \mathbf{b}_{n+1} \cdot \boldsymbol{\eta}] dv - \int_{\varphi_{n+1}(\partial\Omega_t)} \mathbf{t}_{n+1} \cdot \boldsymbol{\eta} da = 0, \quad (2.7.4)$$

is satisfied for any $\boldsymbol{\eta} \in \mathcal{V}_{n+1}$, where $\varphi_{n+1}(\Omega)$ is the deformation map at t_{n+1}

$$\mathbf{x}_{n+1} = \varphi_{n+1}(\mathbf{p}) = \mathbf{p} + \mathbf{u}_{n+1}(\mathbf{p}), \quad (2.7.5)$$

and

$$\mathbf{F}_{n+1} = \nabla_p(\varphi_{n+1}) = \mathbf{I} + \nabla_p(\mathbf{u}_{n+1})." \quad (2.7.6)$$

2.7.2 Spatial Discretisation

The spatial discretisation, also called *finite element discretisation*, is the highlight of the FEM and, in short, comprises the division of the domain Ω of a generic body $\mathcal{B}$ into a finite number of non-overlapping subdomains, also called *finite elements*, with each occupying a region $\Omega^{(e)}$, in such a way that Ω is approximated by the union of all finite element domains in what constitutes the discretised solid domain $^h\Omega$ (see Figure 2.8):

$$\Omega \approx ^h\Omega = \bigcup_{e=1}^{n_{elem}} \Omega^{(e)}. \quad (2.7.7)$$

Here, n_{elem} is the number of different finite elements that, together, make up the finite element mesh that corresponds to the discretised domain $^h\Omega$.

Admit a generic finite element (e) defined by a set of n_{nodes} nodes, occupying a region Ω_e of the discretised domain $^h\Omega$. Furthermore, consider $N_i^{(e)}(\mathbf{x})$ as the *shape function* (or *interpolation function*) associated with the respective node i of element (e) . Despite the shape functions of a finite element being dictated by its geometry, they must always satisfy the Kronecker delta (δ_{ij}) property:

$$N_i^{(e)}(\mathbf{x}^j) = \delta_{ij} = \begin{cases} 1, & \text{if } j = i \\ 0, & \text{if } j \neq i \end{cases}, \quad (2.7.8)$$

which states that each shape function $N_i^{(e)}(\mathbf{x})$ must have the unit value of 1 at its respective node i and zero at all other nodes of the element. The shape functions of a generic element (e) may also be arranged in the form of a *interpolation matrix* $\mathbf{N}^{(e)}$, given by:

$$\mathbf{N}^{(e)} = [\text{diag}[N_1^e(\mathbf{x})] \text{diag}[N_2^e(\mathbf{x})] \cdots \text{diag}[N_{n_{nodes}}^e(\mathbf{x})]], \quad (2.7.9)$$

where each diagonal matrix is square and of dimension set by the number of spatial dimen-

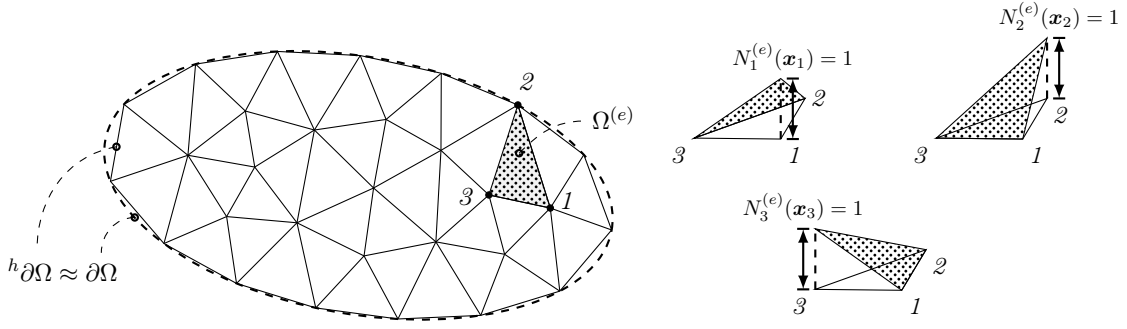


Figure 2.8: Representation of the spatial discretisation of a plane domain by a mesh of triangular finite elements and a schematic representation of the evolution of the shape functions associated with a generic finite element (e).

sions (n_{dim}):

$$\text{diag} [N_i^{(e)}(\mathbf{x})] = \begin{bmatrix} N_i^{(e)}(\mathbf{x}) & 0 & \cdots & 0 \\ 0 & N_i^{(e)}(\mathbf{x}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & N_i^{(e)}(\mathbf{x}) \end{bmatrix}_{n_{dim} \times n_{dim}} \quad (2.7.10)$$

Analogously, it is also possible to define the *global interpolation matrix* $\mathbf{N}^{(g)}$, written in terms of all n_{poin} ¹¹ nodes within the finite element mesh:

$$\mathbf{N}^{(g)} = [\text{diag} [N_1^g(\mathbf{x})] \text{diag} [N_2^g(\mathbf{x})] \cdots \text{diag} [N_{n_{nodes}}^g(\mathbf{x})]], \quad (2.7.11)$$

where the diagonal matrix $\text{diag} [N_i^g(\mathbf{x})]$ can be defined identically to its element version (equation 2.7.10):

$$\text{diag} [N_i^g(\mathbf{x})] = \begin{bmatrix} N_i^{(g)}(\mathbf{x}) & 0 & \cdots & 0 \\ 0 & N_i^{(g)}(\mathbf{x}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & N_i^{(g)}(\mathbf{x}) \end{bmatrix}_{n_{dim} \times n_{dim}} \quad (2.7.12)$$

Naturally, the global shape functions must also satisfy the Kronecker delta property (2.7.8).

Having dealt with the element-based and global interpolation functions and matrices, we may now move on to the analysis of the displacement $\mathbf{u}$, which can be approximated by a discretised version of the displacement field, ${}^h\mathbf{u}$:

$$\mathbf{u}(\mathbf{x}) \approx {}^h\mathbf{u}(\mathbf{x}) = \mathbf{N}^g(\mathbf{x}) \mathbf{u}, \quad \forall {}^h\mathbf{u} \in {}^h\mathcal{K}, \quad (2.7.13)$$

where $\mathbf{u}$ denotes the *global vector of nodal displacements*, given by

$$\mathbf{u} = \{u_1^1, \dots, u_{n_{dim}}^1, \dots, u_1^{n_{poin}}, \dots, u_{n_{dim}}^{n_{poin}}\}^T. \quad (2.7.14)$$

¹¹ Since adjacent elements share nodes, then the total number of nodes in the finite element mesh is $n_{poin} < n_{elem} \times n_{nodes}$.

in which each generic component u_i^j associated with nodal points on $\partial\Omega_u$ must satisfy the prescribed kinematic constraints. Note that, from the finite element discretisation h of the domain Ω , the discrete subset ${}^h\mathcal{K}$ can be generated (and subsequently used to replace the functional set $\mathcal{K}$):

$${}^h\mathcal{K} = \left\{ {}^h\mathbf{u}(\mathbf{x}) = \sum_{j=1}^{n_{\text{poin}}} \mathbf{u}^j N_j^g(\mathbf{x}) \mid \mathbf{u}^j = \bar{\mathbf{u}}(\mathbf{x}^j) \text{ if } \mathbf{x}^j \in \partial\Omega_u \right\};, \quad (2.7.15)$$

where $\mathbf{u}^j$ and $\bar{\mathbf{u}}(\mathbf{x}^j)$ are the displacement vector and the prescribed displacement at node j , respectively. Equivalently, any virtual displacement ${}^h\boldsymbol{\eta} \in {}^h\mathcal{V}$ is defined as:

$$\boldsymbol{\eta}(\mathbf{x}) \approx {}^h\boldsymbol{\eta}(\mathbf{x}) = \mathbf{N}^g(\mathbf{x}) \boldsymbol{\eta}, \quad \forall {}^h\boldsymbol{\eta} \in {}^h\mathcal{V}, \quad (2.7.16)$$

where the global vector of virtual displacements $\boldsymbol{\eta}$ reads:

$$\boldsymbol{\eta} = \{\eta_1^1, \dots, \eta_{n_{\text{dim}}}^1, \dots, \eta_1^{n_{\text{poin}}}, \dots, \eta_{n_{\text{dim}}}^{n_{\text{poin}}}\}^T. \quad (2.7.17)$$

and ^{h} denotes the finite-dimensional subset that reduces $\mathcal{V}$ to:

$${}^h\mathcal{V} = \left\{ {}^h\boldsymbol{\eta}(\mathbf{x}) = \sum_{j=1}^{n_{\text{poin}}} \boldsymbol{\eta}^j N_j^g(\mathbf{x}) \mid \boldsymbol{\eta}^j = 0 \text{ if } \mathbf{x}^j \in \partial\Omega_u \right\}, \quad (2.7.18)$$

meaning that the components of $\boldsymbol{\eta}$ associated with nodal points belonging to $\partial\Omega_u$ must vanish.

At this point, it is convenient to introduce the *global discrete symmetric gradient operator*, denoted $\mathbf{B}^g$. Additionally, because of the general large-scale displacement driven nature of the continuum theory described throughout this Chapter, we must as well consider the *global discrete spatial gradient operator*, which, in turn, is referred to as $\mathbf{G}^g$. Both of these matrices provide great importance while establishing the discrete initial boundary value problem (or, more precisely, its incremental counterpart). For instance, consider two-dimensional problems, such as plane stress and plane strain. In these circumstances, these matrices are given by:

$$\mathbf{B}^g = \begin{bmatrix} N_{1,1}^g & 0 & N_{2,1}^g & 0 & \cdots & N_{n_{\text{poin}},1}^g & 0 \\ 0 & N_{1,2}^g & 0 & N_{2,2}^g & \cdots & 0 & N_{n_{\text{poin}},2}^g \\ N_{1,2}^g & N_{1,1}^g & N_{2,2}^g & N_{2,1}^g & \cdots & N_{n_{\text{poin}},2}^g & N_{n_{\text{poin}},1}^g \end{bmatrix}, \quad (2.7.19)$$

$$\mathbf{G}^g = \begin{bmatrix} N_{1,1}^g & 0 & N_{2,1}^g & 0 & \cdots & N_{n_{\text{poin}},1}^g & 0 \\ 0 & N_{1,1}^g & 0 & N_{2,1}^g & \cdots & 0 & N_{n_{\text{poin}},1}^g \\ N_{1,2}^g & 0 & N_{2,2}^g & 0 & \cdots & N_{n_{\text{poin}},2}^g & 0 \\ 0 & N_{1,2}^g & 0 & N_{2,2}^g & \cdots & 0 & N_{n_{\text{poin}},2}^g \end{bmatrix}, \quad (2.7.20)$$

in which any generic component $N_{i,j}^g$ translates to:

$$N_{i,j}^g = \frac{\partial N_i^g}{\partial x_j}. \quad (2.7.21)$$

Lastly, the element counterpart of these *global deformation matrices* can also be defined:

$$\mathbf{B}^{(e)} = \begin{bmatrix} N_{1,1}^{(e)} & 0 & N_{2,1}^{(e)} & 0 & \cdots & N_{n_{poin},1}^{(e)} & 0 \\ 0 & N_{1,2}^{(e)} & 0 & N_{2,2}^{(e)} & \cdots & 0 & N_{n_{poin},2}^{(e)} \\ N_{1,2}^{(e)} & N_{1,1}^{(e)} & N_{2,2}^{(e)} & N_{2,1}^{(e)} & \cdots & N_{n_{poin},2}^{(e)} & N_{n_{poin},1}^{(e)} \end{bmatrix}, \quad (2.7.22)$$

$$\mathbf{G}^{(e)} = \begin{bmatrix} N_{1,1}^{(e)} & 0 & N_{2,1}^{(e)} & 0 & \cdots & N_{n_{poin},1}^{(e)} & 0 \\ 0 & N_{1,1}^{(e)} & 0 & N_{2,1}^{(e)} & \cdots & 0 & N_{n_{poin},1}^{(e)} \\ N_{1,2}^{(e)} & 0 & N_{2,2}^{(e)} & 0 & \cdots & N_{n_{poin},2}^{(e)} & 0 \\ 0 & N_{1,2}^{(e)} & 0 & N_{2,2}^{(e)} & \cdots & 0 & N_{n_{poin},2}^{(e)} \end{bmatrix}. \quad (2.7.23)$$

At this stage, we are now capable of establishing the discretised virtual work expression, through the adequate replacement, in equation (2.7.4), of the domain of the body (Ω) and the associated functional sets ($\mathcal{H}$ and $\mathcal{V}$) for their respective discretised counterparts:

$$\int_{\varphi_{n+1}({}^h\Omega)} \left[\hat{\boldsymbol{\sigma}}^T(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}) \mathbf{B}^g \boldsymbol{\eta} - \mathbf{b}_{n+1} \cdot \mathbf{N}^g \boldsymbol{\eta} \right] dv - \int_{\varphi_{n+1}(\partial {}^h\Omega_t)} \mathbf{t}_{n+1} \cdot \mathbf{N}^g \boldsymbol{\eta} da = 0, \quad \forall \boldsymbol{\eta} \in {}^h\mathcal{V}, \quad (2.7.24)$$

which can be rearranged as:

$$\left\{ \int_{\varphi_{n+1}({}^h\Omega)} [(\mathbf{B}^g)^T \hat{\boldsymbol{\sigma}}(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}) - (\mathbf{N}^g)^T \mathbf{b}_{n+1}] dv - \int_{\varphi_{n+1}(\partial {}^h\Omega_t)} (\mathbf{N}^g)^T \mathbf{t}_{n+1} da \right\}^T \cdot \boldsymbol{\eta} = 0, \quad \forall \boldsymbol{\eta} \in {}^h\mathcal{V}. \quad (2.7.25)$$

Since the above must be satisfied for all $\boldsymbol{\eta} \in {}^h\mathcal{V}$, then the term between the curly brackets ($\{\cdot\}$), on the left-hand side of the equation, must vanish. As the product of the standard finite element discretisation of the incremental boundary value problem, (2.7.25) embodies the *incremental boundary value finite element problem*. Then, the following step is to find the kinematically admissible global nodal displacement vector $\mathbf{u}_{n+1}$ at time t_{n+1} that satisfies the incremental equilibrium equation:

$$\mathbf{r}(\mathbf{u}_{n+1}) \equiv \mathbf{f}_{int}^g(\mathbf{u}_{n+1}) - \mathbf{f}_{ext,n+1}^g = 0, \quad (2.7.26)$$

where $\mathbf{f}_{int}^g$ and $\mathbf{f}_{ext,n+1}^g$ are the *global vectors of internal and external forces*, respectively, and can be obtained from the assembly of their element counterparts:

$$\mathbf{f}_{int}^g = \bigvee_{e=1}^{n_{elem}} \mathbf{f}_{int}^{(e)} \quad (2.7.27)$$

$$\mathbf{f}_{ext}^g = \bigvee_{e=1}^{n_{elem}} \mathbf{f}_{ext}^{(e)} \quad (2.7.28)$$

which, in short, means that each component of a global force vector is equal to the sum of the corresponding components of the element force vector of all elements that share that global node. Here, $\mathbf{f}_{int}^{(e)}$ and $\mathbf{f}_{ext}^{(e)}$ denote the *element internal* and *external nodal force vectors*, respectively, which are given by:

$$\mathbf{f}_{int}^{(e)} = \int_{\varphi_{n+1}(h\Omega^{(e)})} (\mathbf{B}^{(e)})^T \hat{\boldsymbol{\sigma}}(\boldsymbol{\alpha}_n, \mathbf{F}_{n+1}) dv, \quad (2.7.29)$$

$$\mathbf{f}_{ext}^{(e)} = \int_{\varphi_{n+1}(h\Omega^{(e)})} (\mathbf{N}^{(e)})^T \mathbf{b}_{n+1} dv + \int_{\varphi_{n+1}(\partial h\Omega^{(e)})} (\mathbf{N}^{(e)})^T \mathbf{t}_{n+1} da. \quad (2.7.30)$$

Alternatively, a material configuration may also be considered, for which the material counterparts of equations (2.7.29) and (2.7.30) are:

$$\mathbf{f}_{int}^{(e)} = \int_{h\Omega^{(e)}} (\mathbf{G}^{(e)})^T \hat{\mathbf{P}}(\hat{\boldsymbol{\alpha}}, \mathbf{F}_{n+1}) dv, \quad (2.7.31)$$

$$\mathbf{f}_{ext}^{(e)} = \int_{h\Omega^{(e)}} (\mathbf{N}^{(e)})^T \mathbf{b}_{0,n+1} dv + \int_{\partial h\Omega^{(e)}} (\mathbf{N}^{(e)})^T \mathbf{t}_{0,n+1} da. \quad (2.7.32)$$

Additionally, it is worth mentioning that equation (2.7.26) is generally non-linear, which explains the significance of the Newton-Raphson method (see Section 2.7.3).

Generally, the exact integrals of equations (2.7.29) and (2.7.30) are numerically evaluated through a quadrature rule known as the *Gaussian quadrature rule*, which, coupled with the use of natural coordinates $\boldsymbol{\xi}$ (as well as the compact mathematical nature of the shape functions), yields a great level of automation within the FEM framework. The use of natural coordinates provides the integration over a standard domain Γ , such that $\mathbf{x} : \Gamma \rightarrow \Omega^{(e)}$ maps the standard domain Γ onto the element domain $\Omega^{(e)}$ (see Figure 2.9). With that being said, the Gaussian quadrature with n_{gaussp} *Gauss points* approximates the integral of a generic function $g(\mathbf{x})$ over the element domain $\Omega^{(e)}$ through the following weighted sum:

$$\int_{\Omega^{(e)}} g(\mathbf{x}) d\mathbf{x} = \int_{\Gamma} g(\mathbf{x}(\boldsymbol{\xi})) j(\boldsymbol{\xi}) d\boldsymbol{\xi} \approx \sum_{i=1}^{n_{gaussp}} w(\boldsymbol{\xi}_i) g(\mathbf{x}(\boldsymbol{\xi}_i)) j(\boldsymbol{\xi}_i), \quad (2.7.33)$$

where $j(\boldsymbol{\xi})$ is the determinant of the Jacobian of the transformation $\mathbf{x}$:

$$j(\boldsymbol{\xi}) = \det \left(\frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}} \right), \quad (2.7.34)$$

$\boldsymbol{\xi}_i$ stands for the natural coordinates of the Gauss point i and $w(\boldsymbol{\xi}_i)$ is the corresponding

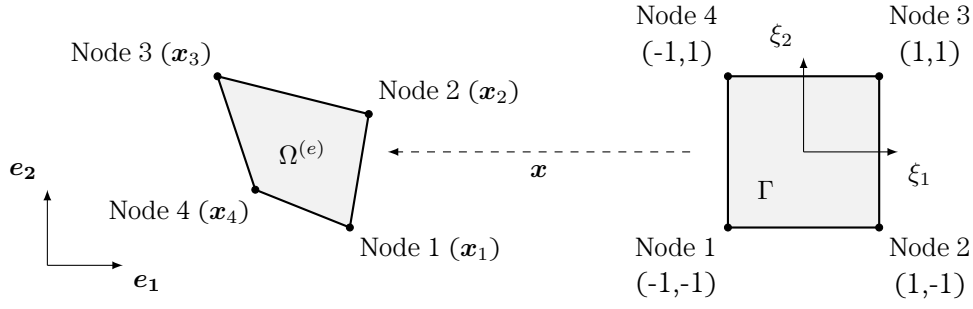


Figure 2.9: Schematic representation of the mapping of the standard domain Γ onto the element domain $\Omega^{(e)}$ through the transformation function $\mathbf{x}$ for a generic bi-linear quadrilateral element.

weights. Equivalently, the Gaussian quadrature rule also allows the evaluation of the integral of a function $g(\mathbf{x}^b)$ over the element boundary, $\partial\Omega^{(e)}$, in which case the previous transformation $\mathbf{x}$ may now be regarded as $\mathbf{x}^b : \partial\Gamma \rightarrow \partial\Omega^{(e)}$, which denotes the boundary transformation (note the indicative superscript b). The determinant of the Jacobian now reads:

$$j^b(\boldsymbol{\xi}^b) = \det\left(\frac{\partial \mathbf{x}^b}{\partial \boldsymbol{\xi}}\right), \quad (2.7.35)$$

and, accordingly, considering n_{gaussb} points, the boundary version of expression (2.7.33) is:

$$\int_{\partial\Omega^{(e)}} g(\mathbf{x}^b) d\mathbf{x}^b = \int_{\partial\Gamma} g(\mathbf{x}^b(\boldsymbol{\xi}^b)) j^b(\boldsymbol{\xi}^b) d\boldsymbol{\xi}^b \approx \sum_{i=1}^{n_{gaussb}} w_i^b g_i j_i^b. \quad (2.7.36)$$

All in all, by applying the Gaussian quadratures with n_{gaussp} and n_{gaussb} Gauss points for integrals over the element domain ($\Omega^{(e)}$) and a arbitrary portion of its corresponding boundary ($\partial\Omega_t^{(e)}$), respectively, the numerical computation of the element forces (2.7.29) and (2.7.30) gives:

$$\mathbf{f}_{int}^{(e)} \approx \sum_{i=1}^{n_{gaussp}} w_i j_i (\mathbf{B}_i^{(e)})^T \boldsymbol{\sigma}_{n+1,i}, \quad (2.7.37)$$

$$\mathbf{f}_{ext}^{(e)} \approx \sum_{i=1}^{n_{gaussp}} w_i j_i (\mathbf{N}_i^{(e)})^T \mathbf{b}_{n+1,i} + \sum_{i=1}^{n_{gaussb}} w_i^b j_i^b (\mathbf{N}_i^{(e),b})^T \mathbf{t}_{n+1,i}^b. \quad (2.7.38)$$

In Section 2.7.1, we spoke on the body forces and surface tractions at time t_{n+1} as a key part of the temporal discretisation and its resulting incremental boundary value problem, but we have yet to make any comments on how these quantities are implemented at each timestamp t_n . As imposed variables, different strategies may be adopted. However, we frequently implement a *proportional loading* scheme, under which $\mathbf{b}_{n+1}$ and $\mathbf{t}_{n+1}$ are given by:

$$\mathbf{b}_{n+1} = \lambda_{n+1} \tilde{\mathbf{b}} \quad (2.7.39)$$

$$\mathbf{t}_{n+1} = \lambda_{n+1} \tilde{\mathbf{t}} \quad (2.7.40)$$

where λ_{n+1} is the prescribed load factor, fixed for a specific time t_{n+1} , and $\tilde{\mathbf{b}}$ and $\tilde{\mathbf{t}}$ are the prescribed fields (constant in time).

2.7.3 Newton-Rapshon Method

As previously stated, the discretised version of the incremental boundary value problem (equation 2.7.26) is generally non-linear. Therefore, we must resort to the Newton-Rapshon method, which, due to its quadratic rates of asymptotic convergence, provides a robust and efficient iterative solution for non-linear incremental finite element problems.

Each iteration of this method involves the linearisation of the non-linear incremental finite element equation (or, alternatively, the discrete version of the linearised boundary value problem). With that being said, the linearised virtual work equation for large strain problems reads:

$$\left\{ \int_{\varphi_{n+1}(^h\Omega)} (\mathbf{G}^g)^T \mathbf{a} \mathbf{G}^g dv \right\} \delta \mathbf{u} = - \int_{\varphi_{n+1}(^h\Omega)} [(\mathbf{B}^g)^T \boldsymbol{\sigma}_{n+1} - (\mathbf{N}^g)^T \mathbf{b}_{n+1}] dv + \int_{\varphi_{n+1}(\partial^h\Omega_t)} (\mathbf{N}^g)^T \mathbf{t}_{n+1} da, \quad (2.7.41)$$

where $\mathbf{a}$ denotes the matrix of components of the *spatial tangent modulus*. Alternatively, if a material approach is followed instead, the counterpart of the previous equation comes as:

$$\left\{ \int_{^h\Omega} (\mathbf{G}^g)^T \mathbf{A} \mathbf{G}^g dv \right\} \delta \mathbf{u} = - \int_{^h\Omega} [(\mathbf{G}^g)^T \mathbf{P}_{n+1} - (\mathbf{N}^g)^T \mathbf{b}_{0,n+1}] dv + \int_{\partial^h\Omega_t} (\mathbf{N}^g)^T \mathbf{t}_{0,n+1} da, \quad (2.7.42)$$

where $\mathbf{A}$ is the *consistent material tangent modulus* and the material counterpart of $\mathbf{a}$.

Considering a generic iteration (k) of the Newton-Rapshon method, upon linearisation we may write:

$$\begin{aligned} \mathbf{r}(\mathbf{u}_{n+1}^{(k)}) &\approx \left(\mathbf{u}_{n+1}^{(k-1)} \right) + \frac{\partial \mathbf{r}}{\partial \mathbf{u}_{n+1}} \bigg|_{\mathbf{u}_{n+1}^{(k-1)}} \left(\mathbf{u}_{n+1}^{(k)} - \mathbf{u}_{n+1}^{(k-1)} \right) \\ &= \mathbf{r}^{(k-1)} + \mathbf{K}_T \left(\mathbf{u}_{n+1}^{(k)} - \mathbf{u}_{n+1}^{(k-1)} \right) \\ &= \mathbf{r}^{(k-1)} + \mathbf{K}_T \delta \mathbf{u}^{(k)}, \end{aligned} \quad (2.7.43)$$

which, according to equation (2.7.26), yields:

$$\mathbf{K}_T \delta \mathbf{u}^{(k)} = -\mathbf{r}^{(k-1)}, \quad (2.7.44)$$

where the global displacement vector at the previous iteration $\mathbf{u}_{n+1}^{(k-1)}$ is known, $\mathbf{K}_T$ is the *global tangent stiffness matrix* and $\mathbf{r}^{(k-1)}$ is the *residual force* given, in terms of $\mathbf{u}_{n+1}^{(k-1)}$, by:

$$\mathbf{r}^{(k-1)} \equiv \mathbf{f}_{int}^g(\mathbf{u}_{n+1}^{(k-1)}) - \mathbf{f}_{ext,n+1}^g . \quad (2.7.45)$$

Solving (2.7.44) and obtaining $\delta\mathbf{u}^{(k)}$, the global nodal displacement vector is then properly updated for the corresponding iteration through:

$$\mathbf{u}_{n+1}^{(k)} = \mathbf{u}_{n+1}^{(k-1)} + \delta\mathbf{u}^{(k)} . \quad (2.7.46)$$

This iterative procedure is repeated until iteration (m), for which the following *convergence criterion* is verified:

$$\left\| \frac{\mathbf{r}^{(m)}}{\mathbf{f}_{ext,n+1}^g} \right\| \leq \epsilon_{tol} , \quad (2.7.47)$$

where ϵ_{tol} is a pre-imposed *equilibrium convergence tolerance*. This tolerance must be sufficiently small so that the corresponding displacement vector $\mathbf{u}_{n+1}^{(m)}$ provides is sufficiently close to the solution of:

$$\mathbf{u}_{n+1} = \mathbf{u}_{n+1}^{(m)} . \quad (2.7.48)$$

Note that, as any other iterative scheme, the Newton-Rapshon iterative process requires a starting point for the itera steps of each increment. A common approach is to adopt the converged displacement vector og the previous increment as the the initial guess of the current increment, that gives:

$$\mathbf{u}_{n+1}^{(0)} = \mathbf{u}_n . \quad (2.7.49)$$

2.8 Second-Order Continuum Mechanics

Up until this point, we have comprehensively exposed the main features of the classical continuum mechanics theory; however, in the context of this dissertation, the contents exposed thus far are incomplete. In this regard, one key distinction must be established. Indeed, the theory presented in the previous Sections encompasses the classical first-order continuum theories (otherwise known as Cauchy continuum), for which the constitutive response at a given point depends on the strain (based on the deformation gradient) and the internal variables at that specific point (disregarding any thermal effects). For this reason, the approach associated with such theories is inherently local. Fundamentally, the standard first-order continuum formulation assumes that the underlying micro-structural phenomena dictating the material response take place at length scales substantially smaller than that of the macroscopic structure, and, thus, that the strain field at the microscopic region of a given material point is uniform. However, when the deformation field wavelength

at the macroscopic level approaches the material characteristic length, associated with the micro-structural length scale, such assumption can not be made and first-order continuum theories become inadequate for an accurate representation of the material response. On the other hand, *second-order continuum theories*, which account for the second gradient of the displacement field and consequently introduce the material characteristic length, are intrinsically *non-local*, while still preserving the local nature of the constitutive laws. Note that, with this framework, the behaviour at a given point is inevitably dependent on the neighbouring points enclosed in the region delimited by the defined length.

In this work, complex micro-structural behaviour is to be examined through a second-order homogenisation framework, therefore, the understanding of the second-order continuum mechanics is of significant importance. In particular, the concepts of second gradient of the displacement field and higher-order stress tensor are fundamental for the introduction of the second-order homogenisation (Section 3.4). That being said, it should be noted that the overall second-order description here presented is brief. The finite element solution for the second-order equilibrium problem, for instance, is completely overlooked. For a more detailed account of this subject, the interested reader is referred to [Rodrigues Lopes \(2019\)](#) and [Rodrigues Lopes and Andrade Pires \(2021\)](#).

2.8.1 Second Gradient of the Displacement Field

In line with the originally presented classical first-order continuum mechanics theory, consider now a second-order continuum body, in its reference configuration, occupying the region Ω , and subjected to external body forces, $\mathbf{b}_0$, external boundary tractions, $\mathbf{t}_0$, double tractions $\mathbf{r}_0$ on part of its boundary, $\partial\Omega^N$, and line forces $\mathbf{s}_0$ on Γ^N . In addition to the already presented deformation gradient $\mathbf{F}$, the constitutive behaviour of this second-order continuum is driven by the *second gradient of the displacement field*, $\mathbf{G}$, which is given by:

$$\nabla_{\mathbf{p}} \mathbf{F} = \nabla_{\mathbf{p}} (\nabla_{\mathbf{p}} \mathbf{u}) \Rightarrow G_{ijk} = \frac{\partial^2 u_i}{\partial p_j \partial p_k}. \quad (2.8.1)$$

Note that when a second gradient $\mathbf{G}$ is included in the description of the solid deformation kinematics, the infinitesimal volume element associated with a given material point exhibits second-order deformation modes, which are schematically presented in Figure 2.10.

2.8.2 Weak Equilibrium Equation

Following the *Virtual Work Principle*, the weak equilibrium equation reads as follows:

$$\begin{aligned} \int_{\Omega} \left(\mathbf{P} : \delta \mathbf{F} + \mathbf{Q} : \delta \mathbf{G} \right) dV &= \int_{\Omega} \mathbf{b}_0 \cdot \delta \mathbf{u} dV + \int_{\partial\Omega^N} \mathbf{t}_0 \cdot \delta \mathbf{u} dA \\ &+ \int_{\partial\Omega^N} \mathbf{r}_0 \cdot D_0 \delta \mathbf{u} dA + \int_{\Gamma^N} \mathbf{s}_0 \cdot \delta \mathbf{u} dA, \end{aligned} \quad (2.8.2)$$

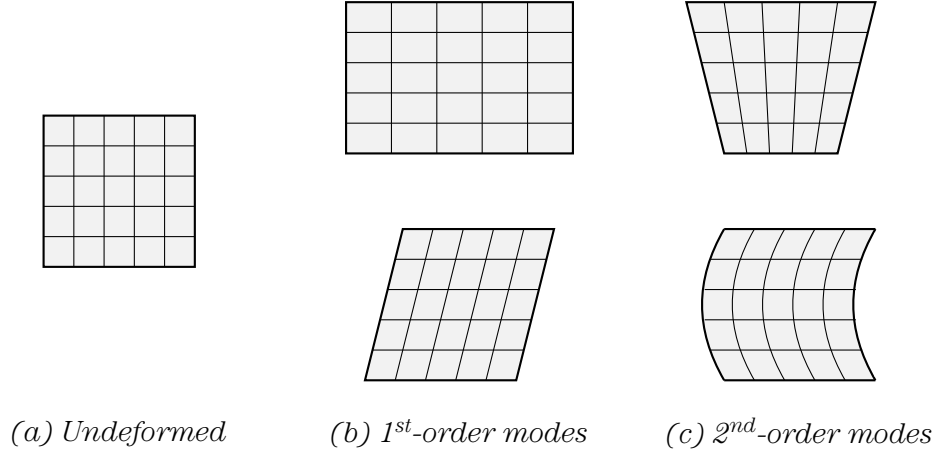


Figure 2.10: Representation of typical first- and second-order deformation modes.

where $D_0 \delta \mathbf{u} = \nabla_{\mathbf{p}} \delta \mathbf{u} \cdot \mathbf{n}_0$ denoted the normal displacement gradient, which is dual to the double tractions $\mathbf{r}_0$. In addition, the higher-order stress tensor $\mathbf{Q}$, which is dual to the second gradient $\mathbf{G}$ (analogously to the first Piola-Kirchhoff stress tensor being dual the deformation gradient) is also included.

2.8.3 Strong Equilibrium

After some algebraic manipulations (detailed in [Rodrigues Lopes \(2019\)](#)), and by standard variational arguments, the strong form of the equilibrium problem is determined from its weak version and is expressed by the following set of equations:

$$\mathbf{b}_0 = \operatorname{div}(\operatorname{div} \mathbf{Q}) - \operatorname{div} \mathbf{P}, \quad \text{in } \Omega \quad (2.8.3)$$

$$\mathbf{t}_0 = \mathbf{P} \cdot \mathbf{n}_0 - \operatorname{div} \mathbf{Q} \cdot \mathbf{n}_0 + \operatorname{div}^t \mathbf{n}_0 (\mathbf{Q} \cdot \mathbf{n}_0) \cdot \mathbf{n}_0 - \operatorname{div}^t (\mathbf{Q} \cdot \mathbf{n}_0), \quad \text{on } \partial\Omega \quad (2.8.4)$$

$$\mathbf{r}_0 = (\mathbf{Q} \cdot \mathbf{n}_0) \cdot \mathbf{n}_0, \quad \text{on } \partial\Omega \quad (2.8.5)$$

$$\mathbf{s}_0 = \|(\mathbf{Q} \cdot \mathbf{n}_0) \cdot \mathbf{m}\|, \quad \text{on } \Gamma \quad (2.8.6)$$

where div^t denotes the tangential divergence operator and $\mathbf{m}$ is the unit vector tangent to the surface $\partial\Omega$ and normal to the line $\Gamma^{\mathbf{n}_0}$.

3

Multi-Scale Models Based on Computational Homogenisation

Over the last decades, with the increasing adoption of composite materials and polycrystalline materials involving complex microstructural phenomena, as well as with conventional phenomenological (macroscopic) constitutive theories seemingly reaching their descriptive capability, there has been a clear shift in focus towards the development of more accurate constitutive models. Although conventional approaches are still present, when we attempt to establish constitutive models capable of describing the behaviour of materials undergoing complex deformation histories, traditional theories do not suffice, and alternative frameworks must be found. This is the case for the nonlinear mechanical response of heterogeneous materials, which may result from several phenomena, namely plasticity, phase-transformation or crack nucleation and propagation. Attempting to model the behaviour of solids undergoing such nonlinearities purely through macroscopic approaches leads to significant discrepancies between the predicted and empirically observed material responses. Generally, when dealing with inelastic or history-dependent phenomena, a certain degree of energy dissipation can be expected, which arises from irreversible interactions between different microstructural constituents. Indeed, internal (strain) energy constitutes an essential element of the underlying thermodynamics (de Souza Neto and Feijóo, 2006; Hill, 1963). Hence, to develop more precise and accurate constitutive models, the material's microstructure cannot be dissociated from the overall governing physics, which is to say that the microstructural details must be considered.

In order to introduce the effects of the underlying heterogeneous microstructure on the large-scale response of the material, *Multi-Scale Models* (MSM) are often employed, with which the limitations of classical phenomenological theories are overcome through the interchange of information between different length scales. In this work, we will focus on *Multi-Scale Models based on Computational Homogenisation*, where the equivalent or effective macroscopic quantities at a particular macro-scale point are defined as volume av-

erages of their microscopic counterparts over a *Representative Volume Element* (RVE). In the following Sections, the general concept of multi-scale models based on coupled and decoupled approaches, as well as the definition of a Representative Volume Element are introduced. Then, the main ingredients of first-order homogenisation are presented, followed by its extension into a second-order homogenisation scheme. Finally, the numerical tools employed in this dissertation are briefly exposed, and an outline of the performed numerical analyses is also presented.

3.1 Coupled and Decoupled Multi-Scale Schemes

Before going further into the formulation of large strain multi-scale constitutive models based on computational homogenisation, it is worth drawing a distinction between two different approaches of multi-scale modelling and their respective workflows: coupled and decoupled multi-scale schemes. In either case, the micro-scale boundary value problem's solution must be known to solve the macro-scale equilibrium problem. Nevertheless, there are some key differences in how this relationship between scales is established in each of the two aforementioned schemes, and the adoption of a particular one derives from the type of analysis that is pursued.

In a decoupled multi-scale approach, as its name suggests, the lower and upper length scales' equilibrium problems are solved separately, in such a way that one of the scales, usually the smaller one, is computed beforehand. By conducting several micro-scale studies, the parameters that conduct the large-scale material behaviour can be determined and a calibrated macroscopic constitutive law is then established in an empirical fashion. To some extent, this approach may be interpreted as the computational equivalent of classical experimental procedures, where the role of the traditional test coupon is now carried out by the RVE of each microscopic analysis. In this context, [Watanabe and Terada \(2010\)](#) provide a detailed description of the decoupled multi-scale scheme procedure.

Alternatively, coupled multi-scale studies may also be performed, in which the solution of both scales is computed in a concurrent manner. To do so, a single RVE is attached to each integration point of the macroscopic mesh. Each RVE is then subjected to its respective local macroscopic deformation gradient and its equilibrium state is subsequently found, after which each point's macroscopic stress tensor may be determined through computational homogenisation of the corresponding microscopic counterparts over the RVE domain (see Figure 3.1). A thorough description of this procedure can be found in the work of [Smit et al. \(1998\)](#). This scheme implies several micro-scale calculations (in equal number to the number of integration points at the macro-scale) which may lead to analyses of overall significant computational cost. For this reason, decoupled numerical methods and their statistically calibrated constitutive laws occasionally emerge as the preferable route for the analysis of the nonlinear behaviour of heterogeneous materials.

In the context of this work, numerical studies under both coupled and decoupled approaches were performed. In a first stage, a coupled multi-scale scheme, specifically, a *Cou-*

pled Multi-Scale Finite Element Analysis (FE²), where a finite element discretisation is employed at both length scales, was followed to obtain the macroscopic results presented in 5, as well as the corresponding deformation history. Subsequently, standalone micro-scale analyses of individual RVEs were performed, under the respective local deformation gradient collected from the prior coupled analyses, in what constitutes a decoupled multi-scale approach.

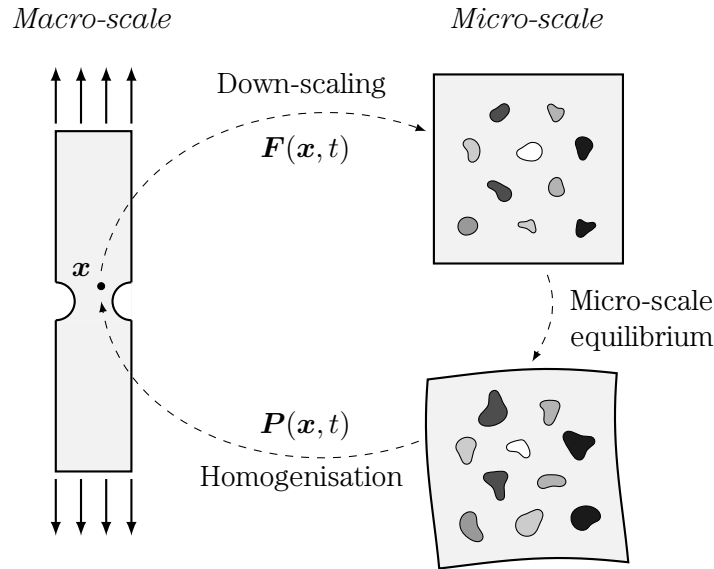


Figure 3.1: Schematic representation of a coupled multi-scale model.

3.2 Representative Volume Element

As previously mentioned, the idea behind multi-scale modelling implies an exchange of information between two or more length scales, in this case, the macro and micro-scale, which is established through an RVE and homogenisation of the adequate properties. Therefore, in order to properly comprehend how this bridge between scales is set and how the underlying material microstructure is accounted for in the macroscopic constitutive response, the concept of Representative Volume Element must be further dissected. The idea of an RVE was firstly introduced by Hill (1963), but since then many definitions have been proposed. A compilation of some may be found in the work of Gitman et al. (2007). In particular, Nemat-Nasser and Hori (1993) describe an RVE for a material point of a continuum body as "a material volume which is statistically representative of the infinitesimal material neighbourhood of that material point". Here, the key word is *representative*. Indeed, the RVE must incorporate all statistically microstructural features, so that its behaviour, in an average sense, constitutes a truthful representation of that of the large-scale material. Evidently, the concept of RVE is intimately related to its size, which, in fact, is an issue that requires particular care. While it is true that the RVE must be sufficiently large in order to accurately portray the material's microstructure, its size must also allow an affordable analysis in terms

of computational burden. In this sense, the RVE's definition proposed by Drugan and Willis (1996) is also worth mentioning as it directly targets this size aspect. It states that the RVE is the smallest material volume element that represents the mean constitutive response with sufficient accuracy. Moreover, the concept of an RVE relies on the *Scale Separation Principle*, which states that the size of the RVE (denoted s_{RVE}) must be much larger than its micro-constituents (of characteristic length l), so that it is representative of the material's microstructure and, at the same time, much smaller than the macroscopic continuum body, i.e. (Hashin, 1983),

$$l \ll s_{RVE} \ll L. \quad (3.2.1)$$

Additionally, the RVE may also include cracks, voids, inclusions, grain boundaries or any other defects. As a result, the undeformed domain of a generic RVE, Ω_μ , may be split into two distinct regions, such that:

$$\Omega_\mu = \Omega_\mu^s \cup \Omega_\mu^v, \quad (3.2.2)$$

where Ω_μ^s and Ω_μ^v denote the solid and the void regions, respectively. Here, the subscript μ is used to identify a micro-scale quantity, thus allowing the clear distinction of any macroscopic entity from its microscopic counterpart without the need of adding unnecessary variables. Following this notation, together with the one from Chapter 2, the boundary of the RVE is $\partial\Omega_\mu$.

3.3 First-Order Homogenisation Formulation

In this Section, the formulation of the multi-scale problem based on first-order computational homogenisation is presented. The *Method of Multi-Scale Virtual Power* (Blanco et al., 2016a) is followed, and the derived formulation is thus variationally consistent across scales. Recall that a schematic representation of the following formulation is shown in Figure 3.1¹.

3.3.1 Homogenised Deformation Gradient

As we have already established, the transition of the appropriate strain and stress measures from the micro to the macro-scale is made possible through the adoption of homogenisation procedures. In this framework, the macroscopic quantities at a particular point $\mathbf{x}$ can be computed as the volume averages of the local microscopic counterparts, that is, the equivalent properties found in the corresponding RVE. That being said, the *homogenised* or

¹ While Figure 3.1 was initially introduced to illustrate the idea of a generic coupled multi-scale model, it actually targets the first-order homogenisation scheme; as we will see in further Sections, the second-order homogenisation scheme involves the interchange of additional strain and stress measures between the macro and micro-scale.

macroscopic deformation gradient, $\mathbf{F}$, at a given material point $\mathbf{p}$ of the continuum body relates to its microscopic counterpart, $\mathbf{F}_\mu$, by:

$$\mathbf{F}(\mathbf{x}, t) = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \mathbf{F}_\mu(\mathbf{p}_\mu, t) \, dv, \quad (3.3.1)$$

where Ω_μ denotes the domain of the RVE in its reference configuration, the scalar $v_{0,\mu}$ is the volume of the undeformed RVE, and $\mathbf{p}_\mu$ is a generic infinitesimal spatial point at the RVE domain. Recalling the description of the deformation gradient established in equation (2.1.14), the previous expression (3.3.1) may be rewritten as follows:

$$\mathbf{F}(\mathbf{x}, t) = \mathbf{I} + \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \nabla_{\mathbf{p}}[\mathbf{u}_\mu(\mathbf{p}_\mu, t)] \, dv. \quad (3.3.2)$$

Invoking Gauss theorem, the integration over Ω_μ can be replaced by an integration over the RVE's boundary, such that

$$\mathbf{F}(\mathbf{x}, t) = \mathbf{I} + \frac{1}{v_{0,\mu}} \int_{\partial\Omega_\mu} \mathbf{u}_\mu(\mathbf{p}_\mu, t) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_\mu) \, da, \quad (3.3.3)$$

where $\mathbf{n}_{0,\mu}$ is the outward unit vector normal to the boundary of the microscopic domain in the reference configuration, thus allowing us to express the macroscopic deformation gradient as a function of the microscopic displacement field $\mathbf{u}_\mu$ and the RVE's boundary.

3.3.2 Multi-Scale Kinematics

Since the macroscopic deformation gradient is enforced to the RVE, i.e., $\mathbf{F}(\mathbf{x}, t)$ is prescribed, equations (3.3.2) and (3.3.3) place restrictions on the possible resulting microscopic displacement fields. As a result, we can express the condition of *kinematic admissibility* as

$$\mathbf{u}_\mu \in \mathcal{K}_\mu^*, \quad (3.3.4)$$

where $\mathcal{K}_\mu^*$ denotes the *minimally constrained set of kinematically admissible microscopic displacements*, which, given equation (3.3.3), comprise

$$\mathcal{K}_\mu^* \equiv \left\{ \mathbf{u}_\mu, \text{ sufficiently regular} \mid \int_{\partial\Omega_\mu} \mathbf{u}_\mu(\mathbf{p}_\mu, t) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_\mu) \, da = v_{0,\mu} [\mathbf{F}(\mathbf{x}, t) - \mathbf{I}] \right\} \quad (3.3.5)$$

Without loss of generality, the microscopic displacement field may be decomposed into its linear part, or *linear displacement*, which depends directly on the prescribed macroscopic deformation gradient, and the *displacement fluctuation*, $\tilde{\mathbf{u}}_\mu$, as follows:

$$\mathbf{u}_\mu(\mathbf{p}_\mu, t) = [\mathbf{F}(\mathbf{x}, t) - \mathbf{I}] \cdot \mathbf{p}_\mu + \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu, t). \quad (3.3.6)$$

Since the prescribed macroscopic deformation gradient is assumed constant throughout the RVE (recall that we are admitting the first-order homogenisation and, thus, first-order continuum mechanics), the linear displacement is known, in a such a way that the fluctuation field $\tilde{\mathbf{u}}_\mu$ is the unknown variable of the microscopic equilibrium problem.

Substituting (3.3.6) into the expression (2.1.14), the microscopic deformation gradient $\mathbf{F}_\mu$ may be expressed in terms of the displacement fluctuation field $\tilde{\mathbf{u}}_\mu$ as:

$$\mathbf{F}_\mu(\mathbf{x}, t) = \mathbf{F}(\mathbf{x}, t) + \nabla_{\mathbf{p}} [\tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu, t)] . \quad (3.3.7)$$

Introducing (3.3.1) into the decomposition above, we obtain:

$$\mathbf{F}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x}, t) + \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \nabla_{\mathbf{p}} [\tilde{\mathbf{u}}_\mu(\mathbf{x}, t)] dv , \quad (3.3.8)$$

The *minimal kinematically admissible constraint* is then given by

$$\int_{\Omega_\mu} \nabla_{\mathbf{p}} \tilde{\mathbf{u}}_\mu [(\mathbf{x}, t)] dv = \mathbf{0} , \quad (3.3.9)$$

which, following the Gauss theorem once again, leads to

$$\int_{\partial\Omega_\mu} \tilde{\mathbf{u}}_\mu(\mathbf{x}, t) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_\mu) da = \mathbf{0} . \quad (3.3.10)$$

The *minimally constrained space of displacement fluctuations* is therefore defined by:

$$\tilde{\mathcal{K}}_\mu^* \equiv \left\{ \tilde{\mathbf{u}}_\mu, \text{ sufficiently regular } \mid \int_{\partial\Omega_\mu} \tilde{\mathbf{u}}_\mu(\mathbf{x}, t) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_\mu) da = \mathbf{0} \right\} . \quad (3.3.11)$$

As we will see in further detail in Section 3.3.4, the application of the minimal kinematically admissible constraint yields the *uniform traction* boundary condition. Nonetheless, additional constraints may be placed, and, as a consequence, we may also define the resulting *actual set of kinematically admissible fluctuation fields*, $\tilde{\mathcal{K}}_\mu$, that satisfies the following extension of the condition stated in (3.3.4):

$$\tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{K}}_\mu \subset \tilde{\mathcal{K}}_\mu^* . \quad (3.3.12)$$

3.3.3 Hill-Mandel Principle of Macro-Homogeneity

Up until this point, the link between scales has been established solely by the homogenisation of micro-scale properties; however, this bridge is not yet complete. In that sense, the *Hill-Mandel Principle* connects both scales by establishing an energetic equivalence between the two coupled scales. To be precise, it states that the macroscopic stress power must be equal to the volume average of the microscopic stress power over the RVE. Within the Method of Multi-Scale Virtual Power based on a standard first-order homogenisation formulation, the Hill-Mandel Principle is synonymous with *Principle of Multi-Scale Virtual Power*, which postulates the equivalence of the virtual power across scales:

$$\mathbf{P}(\mathbf{x}, t) : \dot{\mathbf{F}}(\mathbf{x}, t) = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \mathbf{P}_\mu(\mathbf{p}_\mu, t) : \dot{\mathbf{F}}_\mu(\mathbf{p}_\mu, t) dv , \quad (3.3.13)$$

where $\dot{\mathbf{F}}$ is the macroscopic deformation gradient rate (or virtual macroscopic deformation gradient) and $\dot{\mathbf{F}}_\mu$ is its microscopic counterpart. Recalling equation (3.3.7), the time derivative microscopic deformation gradient analogously relates to its macroscopic equivalent by:

$$\dot{\mathbf{F}}_\mu(\mathbf{x}, t) = \dot{\mathbf{F}}(\mathbf{x}, t) + \nabla_{\mathbf{p}} [\dot{\mathbf{u}}_\mu(\mathbf{p}_\mu, t)] . \quad (3.3.14)$$

Combining the previous two expressions, it follows that

$$\mathbf{P}(\mathbf{x}, t) : \dot{\mathbf{F}}(\mathbf{x}, t) = \mathbf{P}(\mathbf{x}, t) : \dot{\mathbf{F}}(\mathbf{x}, t) + \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \mathbf{P}_\mu(\mathbf{p}_\mu, t) : \nabla_{\mathbf{p}} [\dot{\mathbf{u}}_\mu(\mathbf{p}_\mu, t)] \, dv , \quad (3.3.15)$$

and, as a result:

$$\int_{\Omega_\mu} \mathbf{P}_\mu(\mathbf{p}_\mu, t) : \nabla_{\mathbf{p}} [\dot{\mathbf{u}}_\mu(\mathbf{p}_\mu, t)] \, dv = 0, \quad \forall \dot{\mathbf{u}}_\mu \in \mathcal{V}_\mu , \quad (3.3.16)$$

where $\mathcal{V}_\mu$ stands for the *space of virtual kinematically admissible displacements* of the RVE, which coincides with actual space of kinematically admissible fluctuations, i.e., $\mathcal{V}_\mu \equiv \tilde{\mathcal{K}}_\mu$.

Through integration by parts of the left-hand side of equation (3.3.16) and considering the absence of body forces on the voids present in the RVE, i.e.,

$$\mathbf{b}_{0,\mu}(\mathbf{p}_\mu, t) = 0, \quad \forall \mathbf{p}_\mu \in \Omega_\mu^v , \quad (3.3.17)$$

it follows from the strong form of equilibrium at the micro-scale² (which can be derived from 2.3.5):

$$\begin{aligned} \int_{\Omega_\mu} \mathbf{P}_\mu(\mathbf{p}_\mu, t) : \nabla_{\mathbf{p}} [\dot{\mathbf{u}}_\mu(\mathbf{p}_\mu, t)] \, dv &= \int_{\partial\Omega_\mu} \mathbf{t}_{0,\mu}(\mathbf{p}_\mu, t) \cdot \dot{\mathbf{u}}_\mu \, da \\ &+ \int_{\Omega_\mu^s} \mathbf{b}_{0,\mu}(\mathbf{p}_\mu, t) \cdot \dot{\mathbf{u}}_\mu \, dv \end{aligned} \quad (3.3.18)$$

Considering (3.3.16) and that both terms on the right-hand side of the expression above are independent of each other, the Hill-Mandel principle is verified if and only if

$$\int_{\partial\Omega_\mu} \mathbf{t}_{0,\mu}(\mathbf{p}_\mu, t) \cdot \dot{\mathbf{u}}_\mu \, da = 0, \quad \forall \dot{\mathbf{u}}_\mu \in \mathcal{V}_\mu, \quad \text{and} \quad (3.3.19)$$

$$\int_{\Omega_\mu^s} \mathbf{b}_{0,\mu}(\mathbf{p}_\mu, t) \cdot \dot{\mathbf{u}}_\mu \, dv = 0, \quad \forall \dot{\mathbf{u}}_\mu \in \mathcal{V}_\mu . \quad (3.3.20)$$

Through (3.3.19) and (3.3.20), resulting from the Hill-Mandel principle, one may then interpret the body and surface forces, $\mathbf{b}_{0,\mu}$ and $\mathbf{t}_{0,\mu}$, respectively, as reactions of the kinematical constraints enforced on the RVE.

² Recall that any concept of the CMT theory addressed in Chapter 2 remains valid at the micro-scale.

3.3.4 Micro-Scale Boundary Conditions

As the final ingredient of the microscopic equilibrium problem, we must now discuss the possible kinematical constraints that might be imposed on the RVE. In Section 3.3.2 we introduced the space $\tilde{\mathcal{K}}_\mu$, the actual set of kinematically admissible displacement fluctuations, which depends on the adopted boundary condition and constitutes a subset of the minimal constrained space of displacement fluctuations $\tilde{\mathcal{K}}_\mu^*$. In other words, by choosing a particular boundary condition, one is fundamentally filtering a specific actual set $\tilde{\mathcal{K}}_\mu$, which, in turn, must restrict the solution of the microscopic problem in such a way the multi-scale model accurately reproduces the material's true behaviour. In this Section, the following four different boundary conditions will be discussed:

1. *Taylor condition*: ${}^{\text{Tay}}\tilde{\mathcal{K}}_\mu$;
2. *Linear boundary condition*: ${}^{\text{Lin}}\tilde{\mathcal{K}}_\mu$;
3. *Periodic boundary condition*: ${}^{\text{Per}}\tilde{\mathcal{K}}_\mu$;
4. *Uniform traction boundary condition*: ${}^{\text{Uni}}\tilde{\mathcal{K}}_\mu$.

The boundary conditions listed above are ranked from most to least restrictive, that is, ranked in order of decreasing *stiffness*. This means that the Taylor condition embodies the largest amount of kinematical constraints, thus increasing the RVE's stiffness, while the uniform traction boundary condition, on the other hand, leads to the least kinematically constrained RVE. This is the reason why, previously, in Section 3.3.2, we matched the minimally constrained space of displacement fluctuations to the space resulting from the adoption of the uniform traction boundary condition in the microscopic equilibrium problem. With that being said, we may write:

$${}^{\text{Tay}}\tilde{\mathcal{K}}_\mu \subset {}^{\text{Lin}}\tilde{\mathcal{K}}_\mu \subset {}^{\text{Per}}\tilde{\mathcal{K}}_\mu \subset {}^{\text{Uni}}\tilde{\mathcal{K}}_\mu \equiv \tilde{\mathcal{K}}_\mu^* . \quad (3.3.21)$$

Taylor Condition

Out of the four conditions listed above, the Taylor condition is the simplest and most kinematically restrictive one and it imposes that the displacement fluctuation is null over the entire domain of the RVE:

$$\tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu, t) = \mathbf{0}, \quad \forall \mathbf{p}_\mu \in \Omega_\mu . \quad (3.3.22)$$

Recalling the decomposition stated in (3.3.6), the microscopic displacement field, $\mathbf{u}_\mu$, becomes:

$$\mathbf{u}_\mu(\mathbf{p}_\mu, t) = [\mathbf{F}(\mathbf{x}, t) - \mathbf{I}] \cdot \mathbf{p}_\mu, \quad \forall \mathbf{p}_\mu \in \Omega_\mu^s , \quad (3.3.23)$$

which means that, under the adoption of Taylor condition, $\mathbf{u}_\mu$ will vary linearly with its reference position $\mathbf{p}_\mu$ over all its solid domain (see Figure 3.2), and, following (3.3.7), the microscopic deformation gradient matches with the macroscopic deformation gradient:

$$\mathbf{F}_\mu(\mathbf{p}_\mu, t) = \mathbf{F}(\mathbf{x}, t), \quad \forall \mathbf{p}_\mu \in \Omega_\mu^s. \quad (3.3.24)$$

It must be emphasized that this condition satisfies the consequences of the Hill-Mandel principle stated in (3.3.19) and (3.3.20), as well as equation (3.3.10).

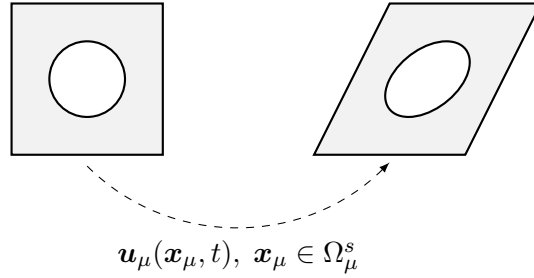


Figure 3.2: Schematic representation of the deformation of an RVE under the Taylor condition.

All in all, this condition results in a homogeneous strain, regardless of the microstructure. Indeed, a downside of the Taylor model is its disregard for the interactions between the microstructural elements of the RVE. For this reason, the resulting RVE may fail to characterise the material heterogeneities and lead to an overly stiff macroscopic behaviour of the material.

Ultimately, the set of kinematically admissible displacement fluctuations is given by:

$$\text{Tay } \tilde{\mathcal{K}}_\mu \equiv \left\{ \tilde{\mathbf{u}}_\mu, \text{ sufficiently regular} \mid \tilde{\mathbf{u}}_\mu = \mathbf{0}, \quad \forall \mathbf{p}_\mu \in \Omega_\mu^s \right\}. \quad (3.3.25)$$

Linear Boundary Condition

The linear boundary condition relaxes the condition imposed by the Taylor model and contrasts with it by enforcing a null displacement fluctuation over the RVE boundary, instead of its whole solid domain:

$$\tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu, t) = \mathbf{0}, \quad \forall \mathbf{p}_\mu \in \partial\Omega_\mu, \quad (3.3.26)$$

which leads to a microscopic displacement field $\mathbf{u}_\mu$ that varies linearly with the material coordinate $\mathbf{p}_\mu$ belonging to the RVE boundary $\partial\Omega_\mu$, i.e.,

$$\mathbf{u}_\mu(\mathbf{p}_\mu, t) = [\mathbf{F}(\mathbf{x}, t) - \mathbf{I}] \cdot \mathbf{p}_\mu, \quad \forall \mathbf{p}_\mu \in \partial\Omega_\mu, \quad (3.3.27)$$

A schematic representation of this hypothesis is shown in Figure 3.3.

As a result, the set of kinematically admissible microscopic displacement fluctuations reduces to:

$$^{\text{Lin}}\tilde{\mathcal{K}}_\mu \equiv \left\{ \tilde{\mathbf{u}}_\mu, \text{ sufficiently regular} \mid \tilde{\mathbf{u}}_\mu = \mathbf{0}, \forall \mathbf{p}_\mu \in \partial\Omega_\mu \right\}. \quad (3.3.28)$$

Similarly to the previous model, this condition also verifies equations (3.3.10) and (3.3.19); however, equation (3.3.20) is only satisfied in the absence of body forces and accelerations, which, in a quasi-static formulation, is a sensible assumption.

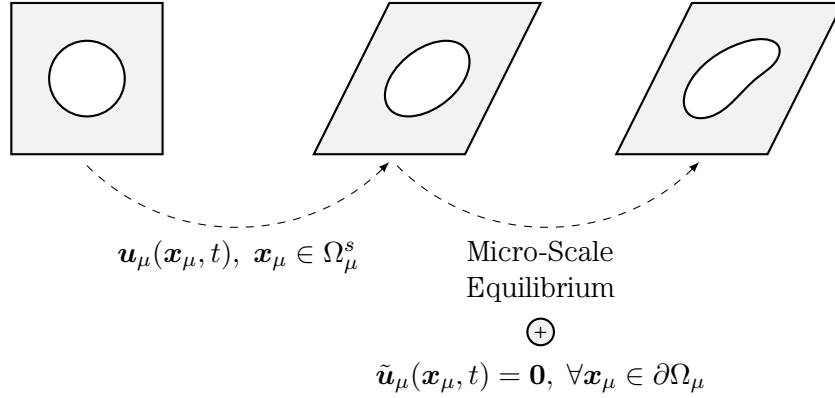


Figure 3.3: Schematic representation of the deformation of an RVE under the linear boundary condition.

Periodic Boundary Condition

The periodic boundary condition is generally used to model the response of materials with periodic microstructures. For such materials, the microstructure may be portrayed as a pattern of RVEs. Assuming that this periodicity remains true while the deformation occurs, then the resulting displacements on opposite boundary sides must be compatible.

In this context, the microscopic boundary is split into n_{pairs} pairs of RVE boundary sides, i.e.,

$$\partial\Omega_\mu = \bigcup_{i=1}^{n_{pairs}} \partial\Omega_{\mu,i}, \quad (3.3.29)$$

where the subscript i identifies the pair. Each pair i of directly opposing boundary sides is composed by a positive and a negative part, $\partial\Omega_{\mu,i}^+$ and $\partial\Omega_{\mu,i}^-$, respectively, with outward unit normal vectors given by $\mathbf{n}_{0,\mu,i}^+$ and $\mathbf{n}_{0,\mu,i}^-$ (see Figure 3.4), such that

$$\partial\Omega_{\mu,i} = \partial\Omega_{\mu,i}^+ \cup \partial\Omega_{\mu,i}^-. \quad (3.3.30)$$

Accordingly, equation (3.3.29) may be rewritten as:

$$\partial\Omega_\mu = \bigcup_{i=1}^{n_{pairs}} (\partial\Omega_{\mu,i}^+, \partial\Omega_{\mu,i}^-). \quad (3.3.31)$$

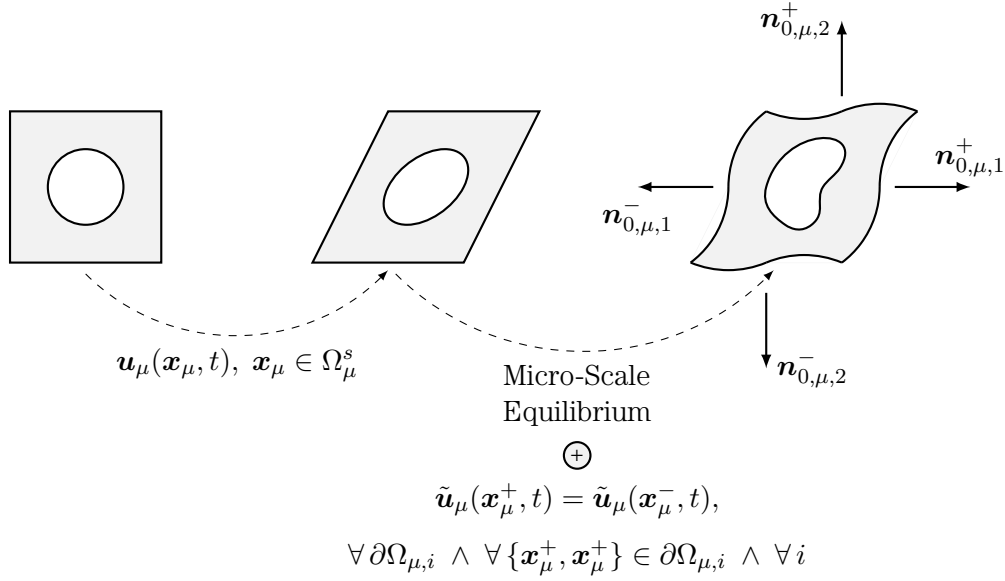


Figure 3.4: Schematic representation of the deformation of an RVE under the periodic boundary condition.

For each point $\mathbf{p}_\mu^+ \in \partial\Omega_{\mu,i}^+$, there also exists a corresponding point $\mathbf{p}_\mu^- \in \partial\Omega_{\mu,i}^-$, for which, in general, that is, for any arbitrary pair i , it must be verified that

$$\mathbf{n}_{0,\mu,i}^+ = -\mathbf{n}_{0,\mu,i}^-. \quad (3.3.32)$$

As stated above, the displacement fluctuations on opposite boundary sides cannot be prescribed independently. In detail, it should be remarked that the periodic microstructure is obtained from the periodic repetition of the RVE. With that in mind, the displacement fluctuation field has to be periodic on the boundary of the RVE.

Following the criteria established above, the periodic boundary condition can be outlined as:

$$\tilde{u}_\mu(\mathbf{p}_\mu^+, t) = \tilde{u}_\mu(\mathbf{p}_\mu^-, t), \quad (3.3.33)$$

which immediately verifies equation (3.3.10).

The resulting space of kinematically admissible displacement fluctuations is:

$$\text{Per } \tilde{\mathcal{K}}_\mu \equiv \left\{ \tilde{u}_\mu, \text{ sufficiently regular} \mid \tilde{u}_\mu(\mathbf{p}_\mu^+, t) = \tilde{u}_\mu(\mathbf{p}_\mu^-, t), \right. \\ \left. \forall \partial\Omega_{\mu,i} \wedge \forall \{\mathbf{p}_\mu^+, \mathbf{p}_\mu^+\} \in \partial\Omega_{\mu,i} \right\}. \quad (3.3.34)$$

Once again, (3.3.20) requires the absence of both body forces and accelerations. However, in contrast with the Taylor model and linear boundary condition, equation (3.3.19) is only verified if the external surface traction field on the boundary of the RVE is *anti-periodic*, that is,

$$\mathbf{t}_{0,\mu}(\mathbf{x}_{\mu,i}^-, t) = -\mathbf{t}_{0,\mu}(\mathbf{x}_{\mu,i}^+, t). \quad (3.3.35)$$

As previously established, the average properties obtained through the homogenisation scheme are sensitive to the adopted RVE size. In short, the smaller the RVE, the less representative it is of its respective infinitesimal material neighbourhood, and the more the homogenised properties deviate from their true values. A notable aspect of the periodic boundary condition, relatively to other models, is the fact its resulting homogenised properties converge faster to their real values, with an increasing RVE size (Kanit et al., 2003; Terada et al., 2000), which allows for the adoption of smaller RVEs (thus reducing the consequent necessary computational effort) when the periodic boundary condition is employed. In detail, the macroscopic responses obtained with the uniform traction boundary model and the linear boundary condition form a convergence envelope, where the uniform traction boundary condition establishes the lower limit and the linear boundary condition the upper one, and the periodic boundary condition's homogenised response lies between both (see Figure 3.5).

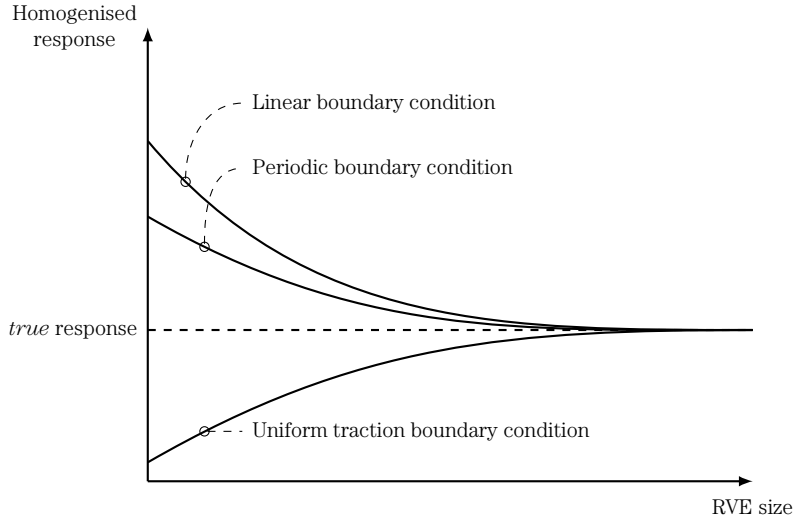


Figure 3.5: Convergence of the homogenised response with increasing RVE size for different boundary conditions, observed in first-order homogenisation schemes.

Uniform Traction Boundary Condition

The uniform traction boundary condition results in the least constrained solution of the microscopic equilibrium problem and its resulting space is, in fact, equivalent to the minimally constrained space of displacement fluctuations. Considering this, we may simply write:

$$^{\text{Uni}}\tilde{\mathcal{K}}_{\mu} \equiv \tilde{\mathcal{K}}_{\mu} \equiv \left\{ \tilde{\mathbf{u}}_{\mu}, \text{ sufficiently regular} \mid \int_{\partial\Omega_{\mu}} \tilde{\mathbf{u}}_{\mu}(\mathbf{x}, t) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_{\mu}) d\mathbf{a} = \mathbf{0} \right\}. \quad (3.3.36)$$

3.3.5 Homogenised Stress Tensor

After the microscopic equilibrium state is found, and the resulting microscopic displacement fluctuations field determined, the corresponding microscopic stress tensor may also

be found. To be precise, since a material approach is being followed, the microscopic first Piola-Kirchhoff stress tensor is computed. Subsequently, the *homogenised* or *macroscopic first Piola-Kirchhoff stress tensor* may be obtained through an analogous homogenisation scheme to that of Section 3.3.1:

$$\mathbf{P}(\mathbf{x}, t) = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \mathbf{P}_\mu(\mathbf{p}_\mu, t) dv. \quad (3.3.37)$$

Developing the right-hand side of the expression above through integration by parts, and introducing the strong form of equilibrium, the expression (3.3.36) may be rewritten in terms of the relevant microscopic quantities:

$$\mathbf{P}(\mathbf{x}, t) = \frac{1}{v_{0,\mu}} \left(\int_{\partial\Omega_\mu} \mathbf{t}_{0,\mu} \otimes \mathbf{p}_\mu da - \int_{\Omega_\mu} \mathbf{b}_{0,\mu} \otimes \mathbf{p}_\mu dv \right). \quad (3.3.38)$$

Finally, macroscopic Cauchy stress tensor might be obtained by the relation expressed in equation (2.2.10). This expression may be rearranged and $\boldsymbol{\sigma}$ is thus expressed in terms of the homogenised first Piola-Kirchhoff stress tensor and the homogenised deformation gradient as:

$$\boldsymbol{\sigma} = \frac{1}{\det(\mathbf{F})} \mathbf{P} \mathbf{F}^T. \quad (3.3.39)$$

3.4 Second-Order Homogenisation Formulation

Having fully discussed the conventional first-order computational homogenisation formulation, we are now at a position to advance into the second-order homogenisation scheme. The concept of second-order computational homogenisation was initially introduced by Kouznetsova et al. (2002), Kouznetsova (2002) and Kouznetsova et al. (2004), and since then several distinct formulations have been proposed in the literature (Blanco et al., 2016a; Luscher, 2010; Rodrigues Lopes and Andrade Pires, 2021). Multi-Scale models based on second-order computational homogenisation are simply an extension of the ones based upon the first-order scheme, and the overall idea is relatively similar, with the only major difference resting on the kinematical information passed from the macro-scale to the microscopic equilibrium problem (and, as a consequence, from the micro to the macro-scale as well). Evidently, this particularity leads to substantial differences between both formulations and, naturally, between its results. In short, the macro-scale description is based on the second-order continuum theory (Section 2.8) where, in addition to the deformation gradient $\mathbf{F}$, the second gradient of the displacements, denoted $\mathbf{G}$, is also accounted for and inserted into the micro-scale (see Figure 3.6), which, in turn, is still modelled by a first-order continuum model. Note that while the micro-scale modelling may still rest on the first-order continuum mechanics, the macro-scale has to be considered a second-order continuum (this framework defines the *standard* second-order homogenisation scheme, which contrasts with the *fully* second-order multi-scale model, in which the second-order approach is adopted at both scales; note that the latter is outside the scope of this work and

will not be discussed - the interested reader is referred to the works of [Rodrigues Lopes \(2019\)](#) and [Rodrigues Lopes and Andrade Pires \(2021\)](#)). With this approach a second-order constitutive law is directly obtained from the homogenisation process, without the need to formulate any of its underlying equations and, thus, a standard first-order constitutive model can be used at the RVE level. While in first-order homogenisation is indifferent the absolute length of the RVE, in a second-order scheme the RVE length implies the natural introduction of a material characteristic length, and introducing the influence of the absolute size of the microstructure in the homogenised non-local response. Additionally, the scale separation principle, which postulates that the RVE size must be much smaller than the macroscopic structural length (recall Section 3.2), is relaxed under the adoption of the second-order framework, since a linear variation of the macro-deformation is assumed within the RVE. For this reason, the second-order homogenisation is particularly suitable for the analysis of very small structures [Rodrigues Lopes \(2019\)](#).

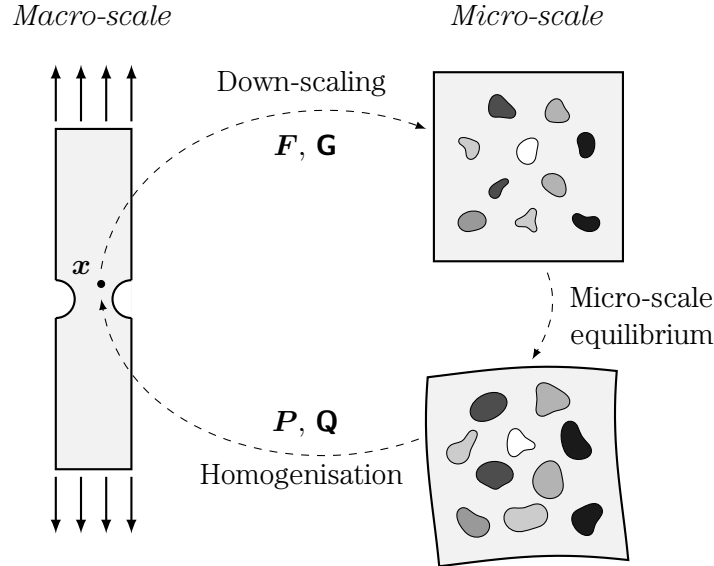


Figure 3.6: Schematic representation of a coupled multi-scale model based on second-order homogenisation.

In the present work, the formulation proposed by [Rodrigues Lopes and Andrade Pires \(2021\)](#) is employed. It is presented in this Section in order to clarify the assumptions behind the models used throughout the dissertation, the advantages of second-order homogenisation, and the differences obtained when compared to first-order homogenisation. That being said, the following topics do not constitute a complete and self-supporting review of the second-order homogenisation scheme formulation. If the reader desires a more comprehensive account on the formulation of multi-scale models based on second-order homogenisation, the works of [Rodrigues Lopes \(2019\)](#); [Rodrigues Lopes and Andrade Pires \(2021\)](#) are heavily recommended.

3.4.1 Kinematic Homogenisation

Following the description discussed throughout Section 3.3, the kinematic homogenisation is worth revisiting as we now must also consider the macroscopic second deformation gradient. As observed for the first-order homogenisation, the homogenised deformation gradient, $\mathbf{F}$, is still obtained by volume averaging of its microscopic counterpart field (equations 3.3.1 and 3.3.2). For the *homogenised* or *macroscopic second gradient*, however, the procedure is not as straightforward. In fact, given that the micro-scale kinematics are based on the first-order continuum theory, the microscopic second gradient $\mathbf{G}_\mu$ is not considered, and, as a result, the macroscopic second gradient cannot simply be averaged from its microscopic counterpart. Therefore, following the proposal of Rodrigues Lopes (2019); Rodrigues Lopes and Andrade Pires (2021), the macroscopic second gradient reads:

$$\mathbf{G} = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \nabla_{\mathbf{p}} [\mathbf{u}_\mu(\mathbf{p}_\mu)] \otimes \mathbf{p}_\mu \cdot \mathbf{J}^{-1} dv. \quad (3.4.1)$$

where $\mathbf{J}$ is the *second-order moment of volume tensor*:

$$\mathbf{J} = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \mathbf{p}_\mu \otimes \mathbf{p}_\mu dv. \quad (3.4.2)$$

3.4.2 Multi-Scale Kinematics

Taking into account the macroscopic second-order deformation gradient, the microscopic displacement field can now be decomposed into both linear displacement and displacement fluctuation parts, but also a *quadratic displacement*, and thus written in terms of the relevant macro-scale quantities as:

$$\mathbf{u}_\mu(\mathbf{p}_\mu) = \mathbf{u}_M + (\mathbf{F} - \mathbf{I}) \cdot \mathbf{p}_\mu + \frac{1}{2} \mathbf{G} : (\mathbf{p}_\mu \otimes \mathbf{p}_\mu - \mathbf{J}) + \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu), \quad \forall \mathbf{p}_\mu \in \Omega_\mu, \quad (3.4.3)$$

While the term $(-1/2 \mathbf{G} : \mathbf{J})$ might be required for an accurate characterisation of the external power per volume unit, it may also induce a rigid body movement in the RVE (Blanco et al., 2016a). Since inertia and external body forces are not admitted in this presentation, it is appropriate to neglect this term and expression (3.4.3) of the microscopic displacement field becomes:

$$\mathbf{u}_\mu(\mathbf{p}_\mu) = \mathbf{u}_M + (\mathbf{F} - \mathbf{I}) \cdot \mathbf{p}_\mu + \frac{1}{2} \mathbf{G} : (\mathbf{p}_\mu \otimes \mathbf{p}_\mu) + \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu), \quad \forall \mathbf{p}_\mu \in \Omega_\mu, \quad (3.4.4)$$

The microscopic deformation gradient is derived from (3.4.4):

$$\mathbf{F}_\mu(\mathbf{p}_\mu) = \nabla_{\mathbf{p}} [\mathbf{u}_\mu(\mathbf{p}_\mu)] + \mathbf{I} = \mathbf{F} + \mathbf{G} \cdot \mathbf{p}_\mu + \nabla_{\mathbf{p}} \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu), \quad \forall \mathbf{p}_\mu \in \Omega_\mu. \quad (3.4.5)$$

Without loss of generality, the origin of the micro-coordinate system is conveniently considered located at the RVE's centroid, such that

$$\int_{\Omega_\mu} \mathbf{p}_\mu dv = \mathbf{0}. \quad (3.4.6)$$

Introducing the definition of the microscopic displacement gradient, equation (3.4.5), into the expression (3.3.1) of the homogenised deformation gradient, and taking into account the result from the assumption that the centroid of the RVE is located at the origin of the microscopic coordinate system, we may write:

$$\mathbf{F} = \mathbf{F} + \frac{1}{v_{0,\mu}} \left[\mathbf{G} \cdot \int_{\Omega_{\mu}^s} \mathbf{p}_{\mu} dv + \int_{\Omega_{\mu}} \nabla_{\mathbf{p}} [\tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu})] \right] \Leftrightarrow \int_{\Omega_{\mu}} \nabla_{\mathbf{p}} \tilde{\mathbf{u}}_{\mu} = \mathbf{0}, \quad (3.4.7)$$

which can also be expressed as the following boundary condition:

$$\int_{\Omega_{\mu}} \nabla_{\mathbf{p}} [\tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu})] = \int_{\partial\Omega_{\mu}} \tilde{\mathbf{u}}_{\mu} \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_{\mu}) da = \mathbf{0}, \quad (3.4.8)$$

and is identical to the uniform traction boundary condition (or minimal kinematically admissible constraint) and leads to the minimally constrained space of displacement fluctuations defined in the first-order homogenisation scheme (3.4.8 is equal to the minimal constraint 3.3.10).

Analogously, introducing (3.4.5) into (3.4.1) and considering the definitions of equations (3.4.3) and (3.4.6) yields the volumetric constraint:

$$\int_{\Omega_{\mu}} \nabla_{\mathbf{p}} [\tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu})] \otimes \mathbf{p}_{\mu} \cdot \mathbf{J}^{-1} dv = \mathbf{0}. \quad (3.4.9)$$

Developing the expression above with integration by parts, it is split into a volumetric and a boundary integral terms:

$$\int_{\partial\Omega_{\mu}} [\tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu}) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_{\mu}) \otimes \mathbf{p}_{\mu}] \cdot \mathbf{J}^{-1} da - \int_{\Omega_{\mu}} \tilde{\mathbf{u}}(\mathbf{p}_{\mu}) dv \otimes \mathbf{J}^{-1} = \mathbf{0}. \quad (3.4.10)$$

Therefore, in this case, the constraints that define the kinematically admissible space are given by equation (3.4.8) and equation (3.4.10). That being said, the minimally constrained space of displacement fluctuations (previously expressed by (3.3.11) in the first-order homogenisation procedure) is now defined as:

$$\begin{aligned} \mathcal{K}_{\mu}^* \equiv \left\{ \tilde{\mathbf{u}}_{\mu}, \text{ sufficiently regular } \mid \int_{\partial\Omega_{\mu}} \tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu}) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_{\mu}) da = \mathbf{0} \wedge \right. \\ \left. \int_{\partial\Omega_{\mu}} [\tilde{\mathbf{u}}_{\mu}(\mathbf{p}_{\mu}) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_{\mu}) \otimes \mathbf{p}_{\mu}] \cdot \mathbf{J}^{-1} da - \int_{\Omega_{\mu}} \tilde{\mathbf{u}}(\mathbf{p}_{\mu}) dv \otimes \mathbf{J}^{-1} = \mathbf{0} \right\}. \end{aligned} \quad (3.4.11)$$

3.4.3 Micro-Scale Boundary Conditions

Again, according to the boundary conditions adopted in the micro-scale equilibrium problem, different sets (or, more accurately, subsets) of displacement fluctuations may be defined.

Periodic Boundary Condition

The main idea behind the periodic boundary condition remains the same to the detailed for the first-order homogenisation scheme (see Figure 3.4); however, within the second-order homogenisation scheme, additional considerations must be admitted so that the kinematic admissibility is still guaranteed.

The periodic boundary condition is defined by:

$$\tilde{\mathbf{u}}(\mathbf{p}_\mu^+) = \tilde{\mathbf{u}}(\mathbf{p}_\mu^-), \quad \forall \mathbf{p}_\mu^+ \in \partial\Omega_\mu^+, \quad \forall \mathbf{p}_\mu^- \in \partial\Omega_\mu^-, \quad (3.4.12)$$

and

$$\mathbf{n}_{0,\mu}(\mathbf{p}_\mu^+) = -\mathbf{n}_{0,\mu}(\mathbf{p}_\mu^-), \quad \forall \mathbf{p}_\mu^+ \in \partial\Omega_\mu^+, \quad \forall \mathbf{p}_\mu^- \in \partial\Omega_\mu^-. \quad (3.4.13)$$

From these equations, the minimal kinematical admissibility criterion stated in equation (3.4.8) is automatically satisfied.

In order to also satisfy the minimal constraint (3.4.10), it is convenient to prescribe each of its terms independently, i.e.:

$$\int_{\partial\Omega_\mu} [\tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu) \otimes \mathbf{n}_{0,\mu}(\mathbf{p}_\mu) \otimes \mathbf{p}_\mu] da = \mathbf{0}, \quad (3.4.14)$$

$$\int_{\Omega_\mu} \tilde{\mathbf{u}}(\mathbf{p}_\mu) dv = \mathbf{0}. \quad (3.4.15)$$

Considering solely RVEs with either rectangular or cubic shapes, defined by a constant normal vector on each surface, expression (3.4.14) can be developed and adequately simplified to:

$$\int_{\partial\Omega_\mu^{+,s}} \tilde{\mathbf{u}}(\mathbf{p}_\mu) da = 0, \quad \text{for each positive surface } s. \quad (3.4.16)$$

Therefore, within the second-order homogenisation framework, the actual space of kinematically admissible displacement fluctuations for the periodic boundary condition is:

$$\begin{aligned} \text{Per } \tilde{\mathcal{K}}_\mu \equiv \left\{ \tilde{\mathbf{u}}_\mu, \text{ sufficiently regular} \mid \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu^+) = \tilde{\mathbf{u}}_\mu(\mathbf{p}_\mu^-), \int_{\Omega_\mu} \tilde{\mathbf{u}}(\mathbf{p}_\mu) dv = \mathbf{0}, \right. \\ \left. \int_{\partial\Omega_\mu^{+,s}} \tilde{\mathbf{u}}(\mathbf{p}_\mu) da = 0, \quad \text{for each positive surface } s. \right\}. \end{aligned} \quad (3.4.17)$$

Direct Boundary Condition

For the sake of completeness, it is worth addressing the direct boundary condition, whose first-order homogenisation equivalent is the linear boundary condition. This condition is simply defined by:

$$\tilde{\mathbf{u}}(\mathbf{p}_\mu) = \mathbf{0}, \quad \forall \mathbf{p}_\mu \in \partial\Omega_\mu, \quad (3.4.18)$$

and immediately verifies both constraints (3.4.8) and (3.4.14). Therefore, only the volumetric constraint (3.4.15) needs to be additionally imposed in order to satisfy all minimal constraints. With that being said, the resulting set of kinematically admissible displacement fluctuations is:

$$\text{Dir } \tilde{\mathcal{H}}_\mu \equiv \left\{ \tilde{\mathbf{u}}_\mu, \text{ sufficiently regular} \mid \tilde{\mathbf{u}}(\mathbf{p}_\mu) = \mathbf{0}, \forall \mathbf{p}_\mu \in \partial\Omega_\mu, \int_{\Omega_\mu} \tilde{\mathbf{u}}(\mathbf{p}_\mu) \, dv = \mathbf{0} \right\}. \quad (3.4.19)$$

3.4.4 Higher-Order Stress Tensor Homogenisation

The *homogenised higher-order stress tensor* $\mathbf{Q}$ is given by:

$$\mathbf{Q} = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} (\mathbf{P}_\mu \otimes \mathbf{p}_\mu)^S \, dv, \quad (3.4.20)$$

whereas the homogenised first Piola-Kirchhoff stress tensor is still computed as the volume average of its counterpart microscopic stress field (expression 3.3.37).

3.5 Numerical Implementation

With the topics presented in this Chapter, together with those from Chapter 2 (particularly, its Section 2.7) we are now well-equipped to address the numerical implementation and solution of the multi-scale equilibrium problem. A numerical solution of the weak equilibrium problems at both scales can be obtained using the finite element method. While the macro-scale problem is mostly treated as a standard finite element problem, additional numerical treatment is required to solve the microscopic equilibrium problem. As a matter of fact, the only difference between a typical finite element formulation and the macro-scale finite element analysis lies on the capturing of the constitutive behaviour at the macro-integration points, which, in the case of the macro-scale problem, is obtained by means of homogenisation procedures from the underlying RVEs attached to each of the integration points. Nevertheless, with most of the underlying principles of the numerical micro-scale equilibrium problem being somewhat similar to those found in the standard finite element formulation, which were detailed in Section 2.7, and since the scope of the present work is not a numerical implementation of the multi-scale theory based on computational homogenisation, we will not expose this particular subject any further.

3.5.1 Links Program

In this work, all analyses will be carried out using **Links** (Large Strain Implicit Non-Linear Finite Element Analysis of Solids Linking Scales), a multi-scale finite element analysis program developed by the research group CM2S (Computational Multi-Scale Modelling of Solids and Structures). The general inputs and outputs of **Links** related to the analyses conducted in the context of this work are schematically represented in Figure 3.7.

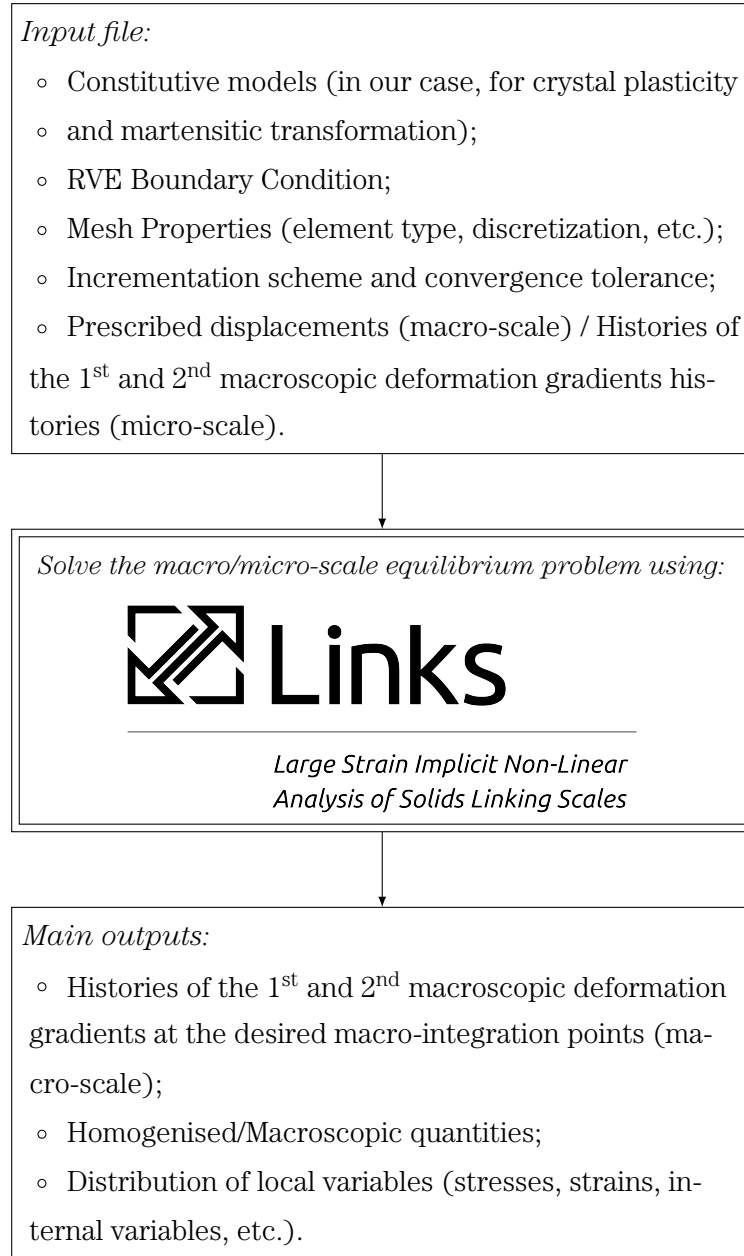
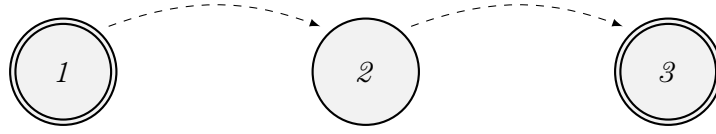


Figure 3.7: Summary of the stages that dictate the workflow of the numerical analyses conducted within the context of this work.

One aspect that must be paid particular attention to is the notion of "micro-scale analyses" and how they contrast with their macroscopic counterpart, that is, "multi-scale analyses". As we have established in Section 3.1, in a coupled multi-scale scheme, both scales are computed simultaneously, and the macroscopic response is obtained via the solution and subsequent homogenisation of the micro-scale equilibrium found in the RVEs attached to the integration points of the specimen's finite element mesh. However, here, and particularly in the diagram above, we refer to macro and micro-scale as two individual stages, with different inputs and outputs. This is because here, and throughout the remainder of this work, we associate "micro-scale analysis" to the analysis of a specific, isolated RVE (or

macro-integration point), which corresponds to the second half of the numerical analyses carried out and discussed in Chapter 6. This is the reason why, as we will see in the Chapters ahead, different RVE boundary conditions might be selected for each of the numerical analyses' stages. Figure 3.8 aims to expand this idea and clarify how both stages of the numerical analyses relate to each other in a sequential manner.



1. Solve the first-order coupled multi-scale analysis for each specimen;
2. Extract the histories of the 1st and 2nd macroscopic deformation gradients at the macro-integration point i ;
3. Solve the micro-scale analysis of the RVE attached to the macro-integration point i with periodic first- and second-order homogenisation.

Figure 3.8: Summary of the inputs and outputs involved in the analyses conducted with **Links** within the context of this work.

3.6 A Detailed Outline of the Numerical Analyses

In the previous Section, a brief description of the numerical analyses carried out in the context of this work (and discussed in Chapters 5 and 6) was presented. In light of the presentation of these results in later Chapters, it is appropriate to illustrate in a clear and concise fashion the key steps and decisions that make up the bulk of the numerical analyses workflow. That being said, Figure 3.9 lays down a schematic representation detailing each of these steps.

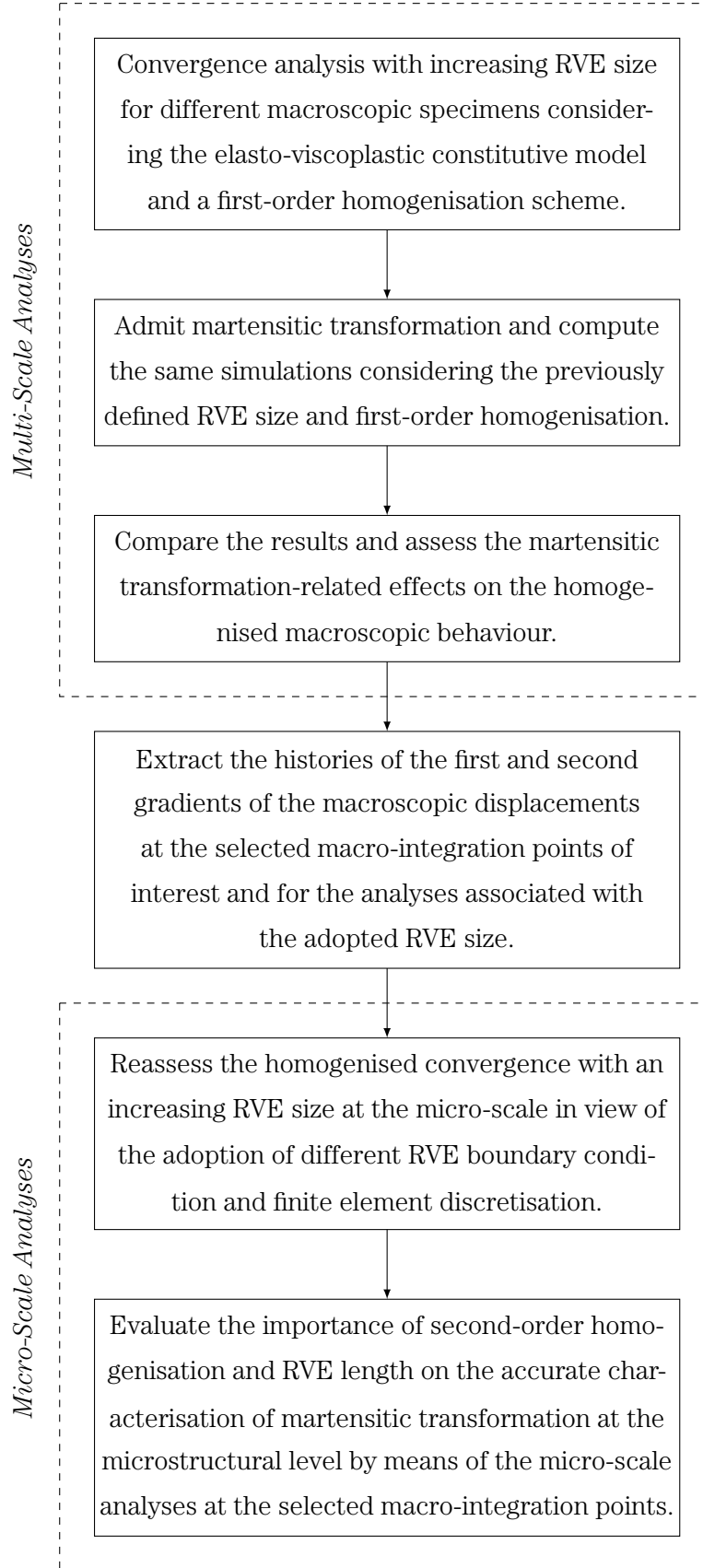


Figure 3.9: Schematic representation detailing each of the steps and decisions that outline the bulk of the numerical analyses workflow for a given specimen.

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4

Crystal Plasticity and Martensitic Transformation Constitutive Models

In this Chapter, the constitutive models associated with crystal plasticity and martensitic transformation phenomena are presented. Firstly, a review of some introductory concepts regarding crystalline materials is briefly exposed. Then, a slip-plasticity continuum law is presented, and subsequently extended to encompass the mechanically-induced martensitic transformations in a fully coupled scheme. Lastly, a short account of the computational implementation of the presented constitutive model is also discussed, with emphasis on particular issues entailed with the rate-independent limit and their impact on the crystal plasticity continuum model.

4.1 Brief Introduction to Crystalline Materials

Given the nature of the constitutive models addressed in this Chapter, a brief review of some concepts related to crystalline materials is of the utmost importance. As we mentioned in Chapter 2, solid materials comprise very intricate systems composed by molecules of atoms and subatomic particles, which are generally arranged in a very particular manner. On this basis, crystalline materials can be characterised by a discrete translation symmetry at the atomic level (Engler and Randle, 2009). In other words, the atomic structure of a crystalline material may be reduced to an elementary block of arranged atoms, usually referred to as a *unit cell*, whose repetition in a specific pattern along the three-dimensional space produces a *crystal lattice*. Figure 4.1 presents the notion of a generic three-dimensional lattice, along with its corresponding unit cell highlighted in grey.

The architecture of a unit cell, and of a crystal lattice for that matter, can be mathematically defined by a set of three noncoplanar linearly independent vectors, $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ and the angles α , β and γ between them. All these parameters are also depicted in Figure 4.1. Thereby, the position of each lattice point, denoted $\mathbf{r}$ can be obtained as,

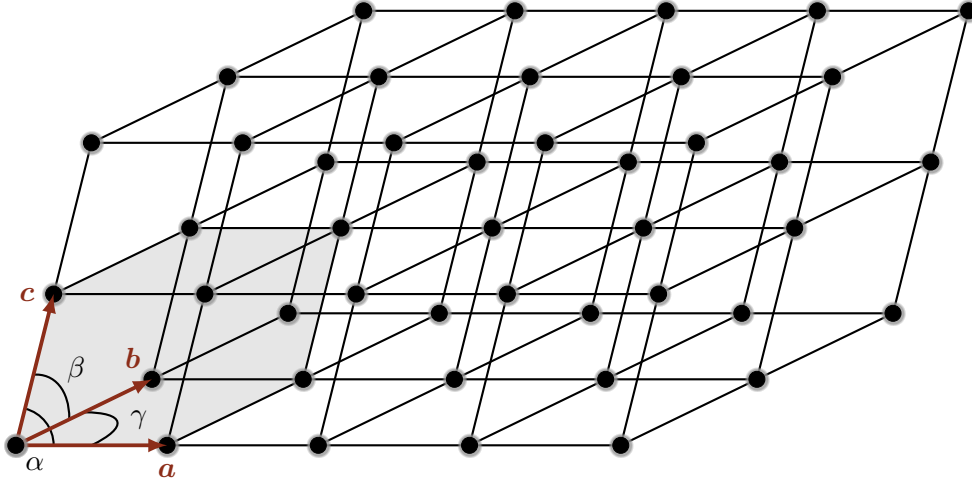


Figure 4.1: Schematic representation of a lattice and its respective unit cell for a generic crystalline system.

$$\mathbf{r} = \mathbf{o} + k_a \mathbf{a} + k_b \mathbf{b} + k_c \mathbf{c}, \quad k_i \in \mathbb{Z}, \quad i = a, b, c, \quad (4.1.1)$$

where $\mathbf{o}$ is the spatial position of an arbitrary origin of the crystalline system.

Expanding the aspect of the repetition of a unit cell and consequent periodicity within a crystal lattice, it is essential that we speak of the property of crystal *symmetry*. Stemming from its own definition, previously stated, translational symmetry may be observed in crystalline systems. In the crystalline system sketched in Figure 4.1, this detail is rather apparent. However, other symmetry modes may be outlined, in such a way that, in the most general case, crystals exhibit compound symmetries (Engler and Randle, 2009). Other symmetry modes include rotational/mirror symmetries. In the crystalline system depicted in Figure 4.1, for example, a rotation of 180° of the crystal about the axis defined by the lattice vector $\mathbf{b}$ produces exactly the same crystal, which corresponds to a two-fold symmetry around that axis^{1,2}. All in all, there are seven unique configurations of the unit cell parameters, which results in seven different types of *crystal systems*, which are detailed in Table 4.1.

Each crystal system, recognised by its respective unit cell parameters, depicts a specific global geometrical configuration. That being said, in order to fully characterize the structure of the crystalline system of the material at hand, the geometric arrangement of the lattice points, that is, the *lattice centerings*, must be touched upon. Briefly, the four different lattice centerings are:

¹ Although the crystalline system depicted in Figure 4.1 serves as a generic representation of a three-dimensional lattice, its configuration actually complies with the unit cell parameters of a *monoclinic* crystal system with *primitive* lattice centering.

² Other rotational symmetries include rotations of 60° (six-fold), 90° (four-fold) and 120° (three-fold) around a specific axis with the crystal remaining unchanged.

1. *Primitive (P)*: Lattice points on the corners of the unit cell;
2. *Body-centered (B)*: Lattice points on the corners of the unit cell and its center;
3. *Face-centered (F)*: Lattice points on the corners and centers of the faces of the unit cell;
4. *Base-centered (C)*: Lattice points on the corners and on the center of the basis of the cell.

Combining these two properties, i.e., the crystal system together with the lattice centering, we establish the concept of a *Bravais Lattice*. Since certain combinations lead to precisely the same lattice, there are solely fourteen unique Bravais lattices, which are also listed in Table 4.1. Nevertheless, only two of these are relevant in the context of these work: the *face-centered cubic* and the *body-centered cubic* Bravais lattices (denoted, respectively, FCC and BCC) and their respective unit cells are represented in Figure 4.2.

Table 4.1: Characterization of the 7 possible crystal systems and corresponding 14 Bravais lattices.

<i>Crystal System</i>	<i>Unit Cell Parameters</i>	<i>Lattice Centering</i>
Triclinic	$a \neq b \neq c$	Primitive
	$\alpha \neq \beta \neq \gamma$	
Monoclinic	$a \neq b \neq c$	Primitive
	$\alpha = \beta = 90^\circ \neq \gamma$	Base-centered
Orthorombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive
		Body-centered
		Face-centered
		Base-centered
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive
		Body-centered
Rhombohedral	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	Primitive
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	Primitive
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive
		Body-centered
		Face-centered

The understading of the material behaviour at the atomic scale is crucial for an accurate modelling of complex phenomena; however, at such length scales, matter is evidently discontinuous and, therefore, the continuum hypothesis, central to the validity of CMT, does

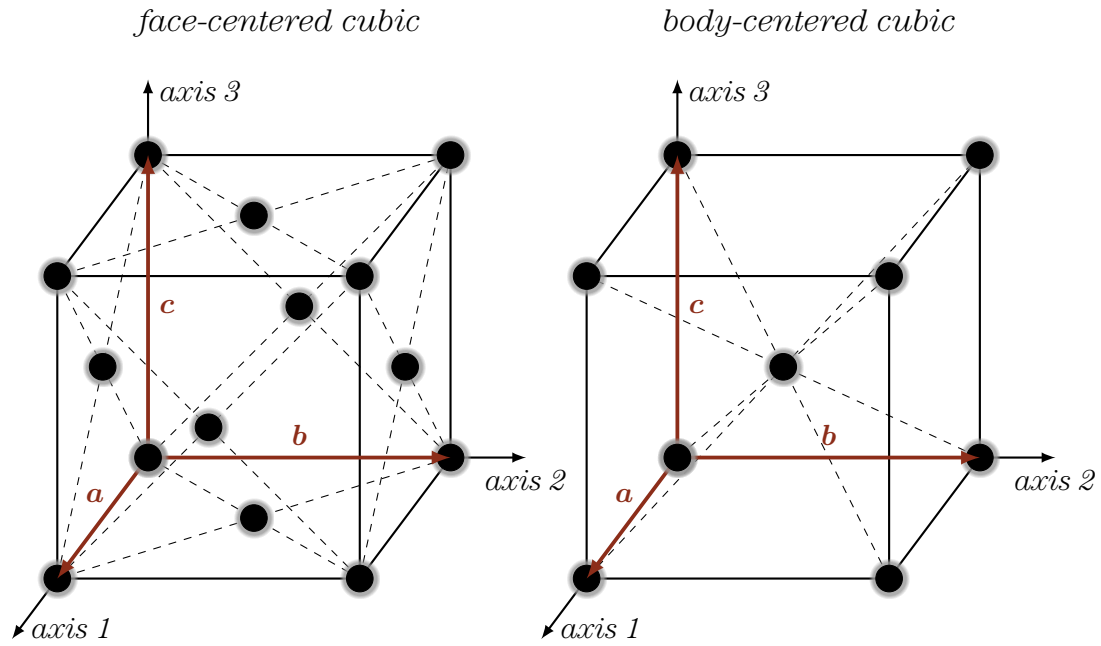


Figure 4.2: Schematic representation of the unit cells associated with face-centered cubic and body-centered cubic Bravais lattices.

not apply. Furthermore, as we originally established in Chapter 2, these theories do not provide a sensible approach to the modelling of the real material behaviour, as the required computational power would be excessively high. That being said, the constitutive model presented in the following Sections considers the micromechanical behaviour of the material at the lattice level, where matter may still be regarded as continuous.

4.2 Slip Plasticity

The elastoplastic behaviour of solid materials may be modelled under several frameworks and techniques, and the adoption of a particular one comes as a result of the specific material whose behaviour we wish to predict. Perhaps, the biggest differentiating factor is the assumption or not of an isotropic response. As a matter of fact, the hypothesis of isotropic finite elastoplasticity and its resulting framework have been widely accepted, given that, in many cases, the isotropy hypothesis leads to an acceptably accurate depiction of the inelastic phenomena and the real material behaviour. However, for some materials, and particularly for *single crystal* alloys, the response is highly anisotropic, hence, alternative frameworks must be found (de Souza Neto et al., 2008). In this Section, the mathematical formulation of the single crystal plasticity constitutive model at large strains and for a rate-independent slip-plasticity continuum law is presented. The elastic domain is modelled with an anisotropic hyperelastic law and self- and latent- hardening are also considered in the evolution of the plastic domain.

Although many mechanisms are important to the plastic deformation of single crystals, the most relevant one comes from the sliding of crystal blocks along certain crystallographic

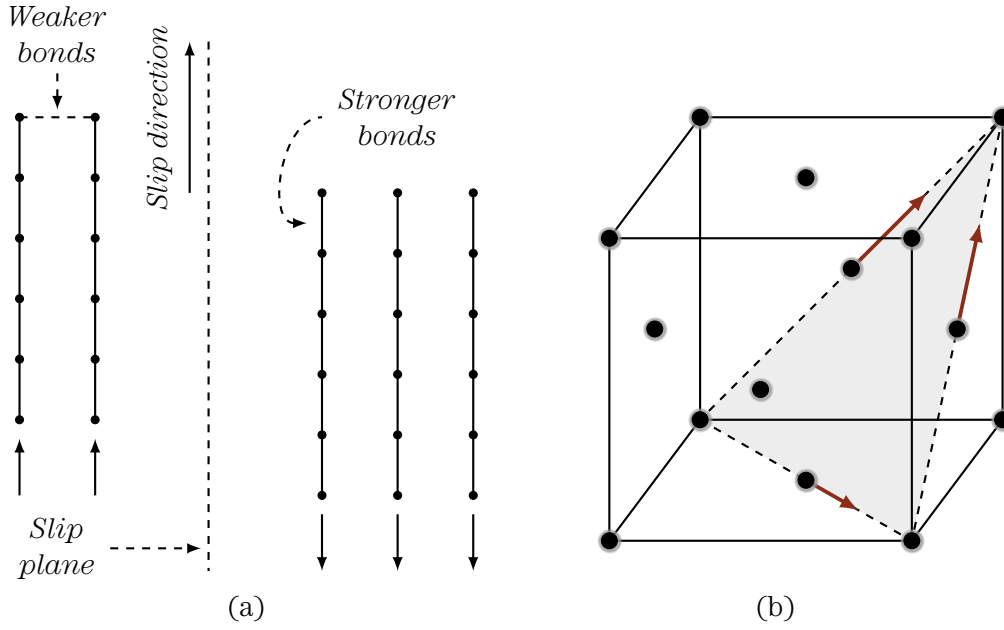


Figure 4.3: Slip planes and directions: (a) general slip plasticity concept; (b) slip systems in FCC crystals (one of the four slip planes with its three in-plane slip directions).

planes. Smaller interatomic distances entail stronger atomic bonds, which, naturally, are more difficult to break. In that sense, this crystallographic plasticity mechanism, otherwise known as *crystallographic slip*, happens between the planes with greater atomic density, also known as *slip planes*, whose atoms exhibit significantly stronger bonds than those between atoms of neighbouring slip planes. Additionally, it also occurs that the sliding (slip) follows the directions that display the highest linear atomic density within a particular slip plane, usually referred to as *slip directions*. Each slip plane has its specific set of plane directions, in such a way that a particular pair composed by a slip plane and one of its associated slip directions defines a *slip system*. In detail, once a shear stress of a given slip plane reaches its respective critical value, the weaker bonds between it and the neighbouring plane are temporarily broken, the blocks of atoms on the opposing sides of the slip interface slide relatively to one another, and new bonds are subsequently established (Dieter, 1988). In Figure 4.3, crystallographic slip is schematically represented.

As a final remark, we must emphasise that other plastic deformation mechanisms do, in fact, exist, and may even be of significant importance under certain conditions. One of such mechanisms is *twinning*. That being said, for FCC crystals, the primary plasticity mechanism is slip, which can be attributed to the high degree of symmetry of their cubic lattices (Dieter, 1988). As a result, the modelling of the FCC continuum crystal plasticity here presented completely disregards twinning and any other plasticity deformation mechanism other than slip plasticity.

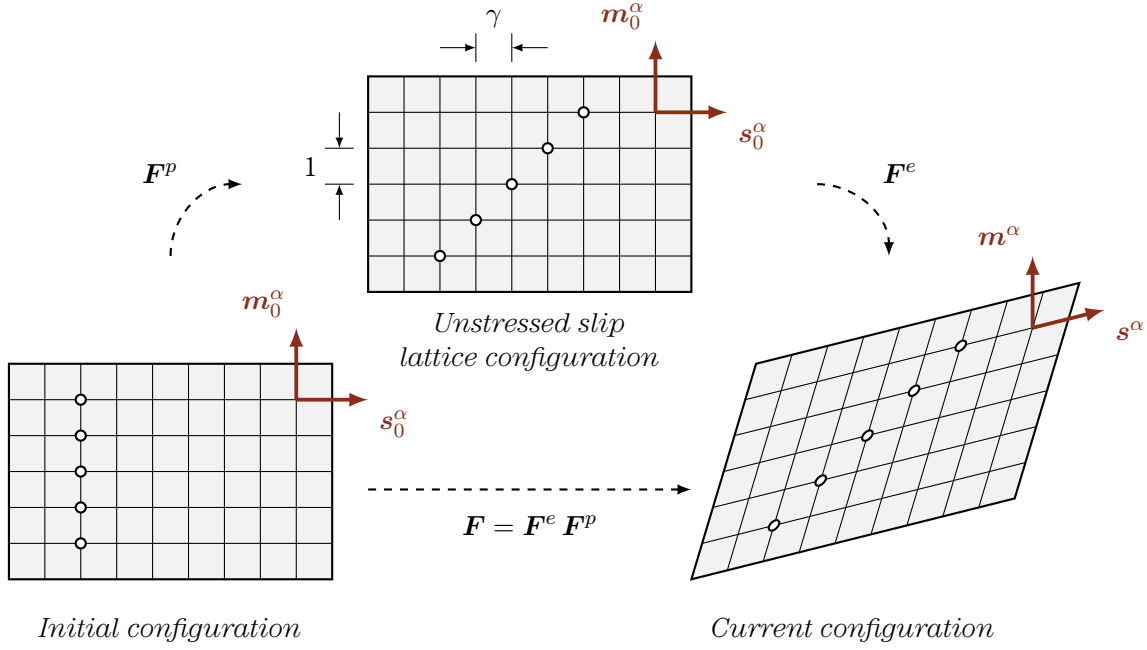


Figure 4.4: Schematic representation of the multiplicative decomposition of the deformation gradient. Note that the grid and circles *do not* represent the crystal lattice, but rather the sliding motion between neighbouring crystal blocks.

4.2.1 Multiplicative Decomposition of the Deformation Gradient

As a starting point to the description of the theory and mathematical formulation of the single crystal plasticity constitutive model, the hypothesis of *multiplicative decomposition of the deformation gradient* $\mathbf{F}$ (also known as the *Lee-Kröner decomposition*) is introduced. The deformation gradient is decomposed into the *elastic* and *plastic deformation gradients*, respectively denoted as $\mathbf{F}^e$ and $\mathbf{F}^p$:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p. \quad (4.2.1)$$

This hypothesis was firstly introduced by Lee and Liu (1967) and Lee (1969), and assumes the existence of a local (pointwise³) unstressed intermediate configuration, defined relatively to the initial configuration by the plastic deformation gradient $\mathbf{F}^p$. Analogously, this configuration can also be obtained through the elastic unloading of the final configuration (de Bortoli, 2017). It is worth emphasising that, in the intermediate unstressed configuration, only the deformation associated with the plastic slip is accounted for, in such a way that the lattice distortion and rotation are only given by the elastic deformation gradient $\mathbf{F}^e$.

Recalling the concept of spatial velocity gradient $\mathbf{L}$ (introduced in Section 2.1.7 by the expressions 2.1.37 and 2.1.38) and incorporating the multiplicative deformation of the de-

³ Note that, generally, the intermediate unstressed configuration can only be physically defined locally, because there is no global displacement field related to $\mathbf{F}^p$ that verifies the compatibility conditions (Vieira, 2018).

formation gradient, we arrive at the following additive decomposition of $\mathbf{L}$,

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e \mathbf{L}^p (\mathbf{F}^e)^{-1}, \quad (4.2.2)$$

where $\mathbf{L}^e$ and $\mathbf{L}^p$ are the *elastic* and *plastic velocity gradients*, respectively defined as,

$$\mathbf{L}^e = \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1}, \quad (4.2.3)$$

$$\mathbf{L}^p = \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1}. \quad (4.2.4)$$

Furthermore, it is worth noting that while the velocity gradient $\mathbf{L}$ is a spatial (i.e., deformed) quantity, the plastic velocity gradient $\mathbf{L}^p$ is defined in the intermediate unstressed configuration.

Returning to the illustrative scheme presented in Figure 4.4, $\mathbf{m}^\alpha$ denotes the unit vector normal to slip plane and $\mathbf{s}^\alpha$ the unit vector parallel to the slip direction, where α defines a particular slip system. In this regard, we must notice that the generic initial slip system α (defined by the pair $\{\mathbf{s}_0^\alpha, \mathbf{m}_0^\alpha\}$) remains unchanged during the linear transformation between the initial and unstressed intermediate configurations.

As a closing remark, it is paramount to clarify that the multiplicative decomposition of the deformation gradient not only provides a convenient mathematical instrument to extend the standard additive split of the strain tensor, but it is also well-founded, in the physical sense, by the slip theory of crystals (Asaro, 1983b; Peirce et al., 1982; Reina and Conti, 2014).

4.2.2 Plastic Flow Rule

Assuming that a given crystal experiences plastic deformation, then its corresponding plastic deformation gradient $\mathbf{F}^p$ is evidently non-null. Under these circumstances, considering a plastic slip of magnitude γ^α associated with the slip system $\{\mathbf{s}_0^\alpha, \mathbf{m}_0^\alpha\}$, we can write,

$$\mathbf{F}^p = \mathbf{I} + \gamma^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha, \quad (4.2.5)$$

whose inverse is given by:

$$(\mathbf{F}^p)^{-1} = \mathbf{I} - \gamma^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha. \quad (4.2.6)$$

Thereby, combining the expressions (4.2.4), (4.2.5) and (4.2.6), the plastic velocity gradient may be defined in the following manner:

$$\mathbf{L}^p = \dot{\gamma}^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha, \quad (4.2.7)$$

where $\dot{\gamma}^\alpha$ denotes the rate of plastic slip in the slip system α . Assuming a general lattice with n_{slip} slip systems, the expression (4.2.7) becomes,

$$\mathbf{L}^p = \sum_{\alpha=1}^{n_{slip}} \dot{\gamma}^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha. \quad (4.2.8)$$

Thus, recalling (4.2.4), we may write the plastic deformation gradient as:

$$\dot{\mathbf{F}}^p = \left[\sum_{\alpha=1}^{n_{slip}} \dot{\gamma}^\alpha \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha \right] \mathbf{F}^p. \quad (4.2.9)$$

4.2.3 FCC Slip: Schmid Law and Schmid Resolved Shear Stress

Until this point, the general mechanism of plastic slip has been adequately established; however, we have yet to address the stresses required to induce crystallographic slip. For the case of FCC crystal structures, plastic activity, that is, slip, may begin on any crystal system once the component of stress parallel to the corresponding slip direction reaches a specific critical value, also known as the *critical resolved shear stress*. This principle is known as *Schmid law*, and, in short, it states that crystallographic sliding occurs on a generic slip system α when,

$$\tau^\alpha = \tau_y^\alpha, \quad (4.2.10)$$

where τ_y^α and τ^α define, respectively, the aforementioned critical resolved shear stress and the *Schmid resolved shear stress* of a generic slip system α , with the latter being defined as follows:

$$\tau^\alpha = \boldsymbol{\sigma} : (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha), \quad (4.2.11)$$

with both Cauchy stress tensor, $\boldsymbol{\sigma}$, and the dyadic product, $\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha$, being established in the deformed configuration. In other words, the Schmid resolved shear stress consists of the shear force transferred to the slip plane α (defined by $\mathbf{m}^\alpha$) along the direction $\mathbf{s}^\alpha$. Frequently, and as we will write from now on, the dyadic product that identifies each slip system may be alternatively expressed as:

$$\mathbf{M}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha, \quad (4.2.12)$$

$$\mathbf{M}_0^\alpha = \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha. \quad (4.2.13)$$

In FCC crystals, there are a total of twelve unique slip systems. The initial unrotated slip systems for a FCC crystalline structure are defined in Table 4.2.

Lastly, it is worth noting that for BCC crystal structures, the Schmid resolved shear stress and related Schmid law are not applicable and a more complex law that uses the so-called *non-Schmid effects* must be employed (Yalcinkaya et al., 2008). In this work, however, we are solely concerned with the modelling of plastic slip in FCC austenite phases (as we will see in further sections, the produced BCC martensite phase, resulting from the plasticity-induced austenite to martensite phase-transformation, is only modelled considering simply

Table 4.2: Octahedral slip systems in FCC single crystals represented under the Miller index notation.

α	$\mathbf{m}_0^\alpha$	$\mathbf{s}_0^\alpha$	α	$\mathbf{m}_0^\alpha$	$\mathbf{s}_0^\alpha$
1	[1,1,1]	$[\bar{1},0,1]$	7	$[\bar{1},1,1]$	$[\bar{1},0,\bar{1}]$
2	[1,1,1]	$[0,1,\bar{1}]$	8	$[\bar{1},1,1]$	$[0,\bar{1},1]$
3	[1,1,1]	$[1,\bar{1},0]$	9	$[\bar{1},1,1]$	$[1,1,0]$
4	$[1,\bar{1},1]$	$[1,0,\bar{1}]$	10	$[1,1,\bar{1}]$	$[1,0,1]$
5	$[1,\bar{1},1]$	$[\bar{1},\bar{1},0]$	11	$[1,1,\bar{1}]$	$[\bar{1},1,0]$
6	$[1,\bar{1},1]$	$[0,1,1]$	12	$[1,1,\bar{1}]$	$[0,\bar{1},\bar{1}]$

its elastic domain). Nonetheless, it should be kept in mind that the modelling of the slip plasticity of BCC lattices is indeed possible and would require taking the aforementioned non-Schmid effects into account (Vieira de Carvalho et al., in submission).

4.2.4 Anisotropic Elasticity

As we initially established in the introductory paragraph of Section 4.2, the isotropic assumption for the formulation of finite elastoplasticity may lead to a significantly inaccurate prediction of the true material response. This applies not only to the description of inelastic phenomena, such as plasticity, but to the elastic domain as well, since the behaviour of a single crystal is highly dependent on its crystallographic structure and orientation. Furthermore, during thermomechanical loading, the elastic distortion in a single crystal may be deemed infinitesimal; however, the produced elastic rotations have significant impact on the texture development of the grain and, therefore, can not be neglected (Vieira de Carvalho et al., in submission). The constitutive model here presented is then formulated under an appropriate anisotropic finite strain elastoplasticity. In detail, we have adopted an anisotropic *Saint Venant-Kirchhoff* hyperelastic law, based on a quadratic strain energy function Ψ , that is given by Kim (2014):

$$\Psi = \frac{1}{2} \mathbf{E}^e : \mathbf{D}^e : \mathbf{E}^e , \quad (4.2.14)$$

where $\mathbf{E}^e$ denotes the Green-Lagrange elastic strain tensor,

$$\mathbf{E}^e = \frac{1}{2} \left[(\mathbf{F}^e)^T \mathbf{F}^e - \mathbf{I} \right] = \frac{1}{2} (\mathbf{C}^e - \mathbf{I}) , \quad (4.2.15)$$

and $\mathbf{C}^e$ is the right Cauchy-Green elastic strain tensor. In the case of cubic single crystals, the anisotropic elasticity $\mathbf{D}^e$, which constitutes a symmetric fourth-order tensor, is defined by three independent materials parameters denoted D_{11} , D_{12} and D_{44} , that remain constant throughout all deformation. The matrix representation of $\mathbf{D}^e$ is:

$$\mathbf{D}^e = \begin{bmatrix} D_{11} & D_{12} & D_{12} & 0 & 0 & 0 \\ & D_{11} & D_{12} & 0 & 0 & 0 \\ & & D_{11} & 0 & 0 & 0 \\ & & & D_{44} & 0 & 0 \\ \text{sym} & & & & D_{44} & 0 \\ & & & & & D_{44} \end{bmatrix}. \quad (4.2.16)$$

The conjugate quantity of the Green-Lagrange elastic strain tensor, $\mathbf{E}^e$, is the second Piola-Kirchhoff stress tensor, which is defined in the intermediate configuration and relates with strain energy function as,

$$\mathbf{S} = \tilde{\rho} \frac{\partial \Psi}{\partial \mathbf{E}^e} = \mathbf{D}^e : \mathbf{E}^e, \quad (4.2.17)$$

where $\tilde{\rho}$ denotes the mass density in the intermediate configuration.

Evidently, the adoption of a particular elastic law has a significant influence on the resolved stresses. On that note, considering that only the elastic deformation gradient contributes to the stress, the Cauchy stress tensor may then be expressed in terms of the second Piola-Kirchhoff stress tensor:

$$\boldsymbol{\sigma} = \frac{1}{J^e} \mathbf{F}^e \mathbf{S} (\mathbf{F}^e)^T, \quad (4.2.18)$$

where J^e denotes the determinant of the elastic deformation gradient, $\mathbf{F}^e$. Furthermore, it is also important that the evolution of the crystallographic slip systems during the elastic deformation is properly defined. In this regard, the current (deformed) counterparts of the initial unit vectors $\mathbf{s}_0^\alpha$ and $\mathbf{m}_0^\alpha$ for a generic slip system α are, respectively, given by:

$$\mathbf{s}^\alpha = \mathbf{F}^e \mathbf{s}_0^\alpha, \quad (4.2.19)$$

$$\mathbf{m}^\alpha = (\mathbf{F}^e)^{-T} \mathbf{m}_0^\alpha. \quad (4.2.20)$$

The previously defined plastic flow rule is established in the intermediate configuration; however, the Schmid resolved stress, expressed in equation (4.2.11), is defined in the current configuration. For this reason, in order to achieve a consistent formulation, the Schmid resolved stress must also be defined in the intermediate configuration:

$$\tau^\alpha = J^e \boldsymbol{\sigma} : (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha), \quad (4.2.21)$$

with which we are now able to rewrite the Schmid equation for FCC crystals:

$$\begin{aligned}
\tau^\alpha &= J^e \boldsymbol{\sigma} : (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \\
&= J^e \frac{1}{J^e} \mathbf{F}^e \mathbf{S} (\mathbf{F}^e)^T : \left(\mathbf{F}^e \mathbf{s}_0^\alpha \otimes (\mathbf{F}^e)^{-T} \mathbf{m}_0^\alpha \right) \\
&= (\mathbf{F}^e)^T \mathbf{F}^e \mathbf{S} (\mathbf{F}^e)^T (\mathbf{F}^e)^{-T} : (\mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha) \\
&= \mathbf{C}^e \mathbf{S} : \mathbf{M}_0^\alpha.
\end{aligned} \tag{4.2.22}$$

4.2.5 Yield Function

As we previously established, the onset of plastic crystallographic slip is defined, for FCC crystals, by the Schmid law (equation 4.2.10), which, in short, states that plastic flow may develop in any slip system whose respective resolved stress reaches a critical value. This behaviour can be mathematically expressed by a *yield function*, Φ_p , whose value output is negative while the material response is within the elastic domain and becomes zero once plastic flow is imminent, that is, once the critical value is reached. Since FCC crystals have $n_{slip} = 12$ slip systems, we must actually establish n_{slip} yield functions, which may be generically written as,

$$\Phi_p^\alpha(\tau^\alpha, \tau_y^\alpha) = \tau^\alpha - \tau_y^\alpha, \quad \alpha = 1, \dots, n_{slip}. \tag{4.2.23}$$

In this context, the following *loading/unloading criteria* must also be satisfied⁴:

$$\Phi_p^\alpha \leq 0, \quad \dot{\gamma}^\alpha \geq 0, \quad \dot{\gamma}^\alpha \Phi_p^\alpha = 0. \tag{4.2.24}$$

Lastly, note that the critical resolved shear stress τ_y^α may depend on the temperature, strain rate and history of the deformation process. Moreover, the latter also implies that τ_y^α may differ between different slip systems. This subject is expanded in the following Section.

4.2.6 Latent and Self Hardening

Before any plastic deformation occurs, it is fair to assume that all slip systems share the same initial yield strength, τ_{y0}^α . This critical value usually increases during plastic deformation, under a phenomenon called *hardening*. Therefore, hardening rules must be established, so that the relation between the critical resolved shear stresses and the history of plastic deformation, crucial to the modelling of inelastic phenomena, can be adequately defined. In this context, and following the problem exposed in the final part of Section 4.2.5, experimental evidence shows that different slip systems evolve at different rates (Kocks, 1970), depending on their coplanarity properties. In this context, the concepts of *self* and *latent hardening* are of significant importance. In detail, the impact of an incremental plastic slip on the yield strength of coplanar systems, that is, systems that share the same normal unit vector $\mathbf{m}$, is known as self hardening, whereas its influence on non-coplanar slip systems is defined as latent hardening, which is usually of greater magnitude than that of its antonym.

⁴ Observe that the summation of the repeated index is not implied in the last equation.

In order to take into account both hardening concepts, the rate of evolution of the critical resolved shear stress for a particular slip system is frequently modelled by the following expression (Asaro and Needleman, 1985):

$$\dot{\tau}_y^\alpha = \sum_{\beta=1}^{n_{slip}} \left(h^{\alpha\beta} \dot{\gamma}^\beta \right), \quad \alpha = 1, \dots, n_{slip}, \quad (4.2.25)$$

where $\dot{\gamma}^\beta$ is the rate of the plastic multiplier (or plastic slip) of the slip system β and $h^{\alpha\beta}$ denotes the hardening coefficients, which change during the plastic deformation. Furthermore, note that only the *active* slip systems impact the evolution rate of the critical resolved shear stress, as, for all the remaining, $\dot{\gamma}^\beta = 0$.

The hardening coefficients account for the slope of the hardening law, $h(\gamma)$, as well as the coplanarity between different slip systems, and are defined as,

$$h^{\alpha\beta} = q h(\gamma) + (1 - q) h(\gamma) \chi^{\alpha\beta}, \quad (4.2.26)$$

in which γ is the *accumulated slip*, q is the *latent hardening parameter*, and $\chi^{\alpha\beta}$ defines the slip system coplanarity ($\chi^{\alpha\beta} = 1$ if α and β are coplanar and $\chi^{\alpha\beta} = 0$ otherwise).

The total accumulated plastic slip γ is an hardening (internal) variable, which is given by,

$$\gamma = \int_0^t \sum_{\alpha=1}^{n_{slip}} \dot{\gamma}^\alpha dt. \quad (4.2.27)$$

Under these conditions, the matrix of hardening coefficients can be rewritten as follows:

$$h^{\alpha\beta} = \mathbf{A}^{\alpha\beta} h(\gamma), \quad (4.2.28)$$

with $\mathbf{A}^{\alpha\beta}$ being the *coplanarity matrix*, which reads,

$$\mathbf{A}^{\alpha\beta} = \begin{cases} 1, & \text{if } \|\mathbf{m}^\alpha \times \mathbf{m}^\beta\| = 0 \\ q, & \text{if } \|\mathbf{m}^\alpha \times \mathbf{m}^\beta\| \neq 0 \end{cases}. \quad (4.2.29)$$

The latent hardening parameter q is usually specified within the interval $q \in [1, 1.4]$, in such a way that, for $q = 1$, the isotropic hardening assumption is reproduced, and, for $q > 1$, both self and latent hardening may occur.

Lastly, the slope hardening parameter $h(\gamma)$ requires the adoption of a particular hardening law. In this work, we opted for the Nadai-Ludwik hardening law (Perdahcioglu and Geijselaers, 2012):

$$\tau_y(\gamma) = \tilde{\tau}_y + K (\gamma_0 + \gamma)^m, \quad (4.2.30)$$

where $\tilde{\tau}_y$, K , γ_0 and m denote, respectively, the critical resolved stress offset (or initial yield stress), the deformation resistance (hardening parameter), the accumulated slip offset and

the hardening exponent. The slope of the hardening law is then computed as the derivative of the expression above and is given by:

$$h(\gamma) = m \cdot K (\gamma_0 + \gamma)^{m-1} . \quad (4.2.31)$$

4.3 Mechanically-Induced Martensitic Transformation

Having fully discussed the FCC single crystal plasticity model, we are well-equipped to approach the subject of martensitic transformation. In the context of this work, we direct our attention to the modelling of ferrous alloys that undergo irreversible phase transformations, when subjected to isothermal mechanical loadings, and in which the martensitic transformation occurs in the metastable retained austenite. This is the case of fully austenitic and multiphase steels that include metastable austenite, such as, for instance, transformation-induced plasticity (TRIP) steels.

In this Chapter, a continuum model for such transformations is formulated, considering both evolution of slip dislocations in the austenite phase (mechanism described by the constitutive model presented in Section 4.2) and the local martensite domain formation. Lastly, it should be noted that the material here presented does not provide an exhaustive description of this subject, therefore, if the interested reader desires a more detailed approach, it is referred to [de Bortoli \(2017\)](#) and [Vieira de Carvalho et al. \(in submission\)](#).

4.3.1 Phenomenological Aspects of the Martensitic Transformation

To properly formulate the martensitic transformation continuum model, it is paramount that we firstly expose the associated relevant phenomena, which mostly takes place at the crystal lattice scale. In fact, the link between parent (austenite) and product (martensite) lattice properties comes as a result of the atomic behaviour observed at the lattice-scale.

In short, a structural transformation may be classified as martensitic if the atomic displacements, i.e., the movement of the atoms from the lattice under transformation, result in an homogeneous deformation. With this in mind, the martensitic transformation may then be classified as *displacive*, as opposed to *reconstructive*, which allows a lattice correspondence to be established, thus mapping the atomic positions from the parent to the product lattice. In fact, while in a reconstructive (diffusional) transformation atoms change relative positions, which poses a non-conservative transformation, in the displacive (or shear) case each atom preserves precisely the same set of neighbours. Moreover, the preferred correspondence in a given transformation is generally that leading to the smallest atomic displacements. For the FCC-to-BCT (face-centered cubic to body centered tetragonal) martensitic transformation in steels, for instance, the correspondence with the smallest atomic displacements is given by *Bain correspondence* ([Bain, 1924](#)), and the associated principal stretches are given by [Turteltaub and Suiker \(2006\)](#):

$$\alpha_{tr} = \sqrt{2} \frac{a^M}{a^A} , \quad \beta_{tr} = \frac{c^M}{a^A} , \quad (4.3.1)$$

where a^A is the austenite (FCC) lattice parameter, and a^M and c^M are the martensite (BCT) lattice parameters. However, recalling what has already been established in prior Sections, in the context of this work, we are only concerned with the BCC martensite crystalline structure. Indeed, the martensite *tetragonality* is directly correlated to the alloy's carbon content, in such a way that higher carbon contents lead to the practically linear increase of the long BCT axis relatively to any of its other axis, and resulting tetragonality (Nishiyama, 1978). This relation is due to the fact martensite comprises a supersaturated solid solution of carbon, such that any excess causes the crystalline structure to strain from BCC to a BCT. Therefore, in low carbon steels, such as material adopted for this work, the BCT martensite can be approximated to a body-centered cubic structure. In these circumstances, $c^M \approx a^M$ and the second principal stretch of equation (4.3.1) becomes:

$$\beta_{tr} = \frac{a^M}{a^A}. \quad (4.3.2)$$

Phenomenological Theory of Martensite Crystallography

The development of a model capable of predicting the crystallographical features of martensitic transformation has been subject of intense research. Currently, the most acknowledged theory is the *Phenomenological Theory of Martensite Crystallography* (PTMC), initially proposed by Wechsler (1953) and Bowles and Mackenzie (1954), and later improved by Ball and James (1987), who, by resorting to an energy minimisation perspective, obtained the same predictions.

Considering a specific combination of parent and product lattices, the PTMC predicts a set of possible systems for the martensitic transformation, $\mathfrak{S}_{tr}$, and each system $i \in \mathfrak{S}_{tr}$ is characterized by a habit plane with a unit normal vector $\mathbf{n}_0^i$ and a shear direction $\mathbf{s}_0^i$.

Stemming from a set of imposed compatibility equations, the PTMC postulates that the transformation deformation gradient for each system i is defined as,

$$\mathbf{F}^{tr,i} = \mathbf{F}^{tr,A} + \mathbf{b}_0^i \otimes \mathbf{n}_0^i = \mathbf{I} + \mathbf{b}_0^i \otimes \mathbf{n}_0^i, \quad (4.3.3)$$

where $\mathbf{F}^{tr,A} = \mathbf{I}$ is the *transformation deformation gradient* in the austenite and $\mathbf{b}_0^i$ is the (average) shape strain vector. The martensitic transformation can be split into shear and expansion; the decomposition of the shape strain vector into an habit plane shear of magnitude ν in the direction $\mathbf{s}_0^i$ and an expansion of magnitude δ in the direction $\mathbf{n}_0^i$ is schematically represented in Figure 4.5. Accordingly, the transformation deformation gradient may also be expressed as,

$$\mathbf{F}^{tr,i} = \mathbf{I} + \nu \mathbf{s}_0^i \otimes \mathbf{n}_0^i + \delta \mathbf{n}_0^i \otimes \mathbf{n}_0^i, \quad (4.3.4)$$

On this topic, it is worth noting the similarity between the transformation deformation gradient $\mathbf{F}^{tr,i}$ with the plastic deformation gradient $\mathbf{F}^p$ of equation (4.2.5) and the associated correspondence of the vectors $\mathbf{b}_0^i$ and $\mathbf{n}_0^i$ with the plastic slip unit vectors $\mathbf{s}^\alpha$ and $\mathbf{m}^\alpha$, respectively. In fact, the major difference is that, in this case, the transformation vectors $\mathbf{b}_0^i$

and $\mathbf{n}_0^i$ are *not orthogonal*, as a result of a nonzero volumetric component of the martensitic transformation phenomenon.

Therefore, at a given material point, the overall deformation that encompasses all potential concurrent transformation systems can be described by computing the weighted average of each transformation deformation gradient, such that,

$$\mathbf{F}^{tr} = \mathbf{I} + \sum_{i \in \mathfrak{S}_{tr}} (\xi^i \mathbf{N}_0^i), \quad (4.3.5)$$

where the transformation tensor $\mathbf{N}_0^i$ is defined by $\mathbf{N}_0^i = \mathbf{b}_0^i \otimes \mathbf{n}_0^i$, and ξ^i denotes the martensitic volume fraction in each system $i \in \mathfrak{S}_{tr}$. This *transformation multiplier* $\xi^i \in [0, 1]$ consists of a *monotonically increasing* function that monitors the status of a given ongoing transformation. Note that the monotonically increasing nature of the transformation multipliers reflect the previously stated transformation irreversibility, which reads,

$$\dot{\xi}^i \geq 0, \quad \forall i \in 1, \dots, |\mathfrak{S}_{tr}| \quad (4.3.6)$$

Following these definitions, the martensite and austenite total volume fractions naturally come as,

$$\xi^m = \sum_{i \in \mathfrak{S}_{tr}} \xi^i, \quad (4.3.7)$$

$$\xi^a = 1 - \xi^m, \quad (4.3.8)$$

such that $\xi^m = 0$ implies that the material is locally fully austenitic; $\xi^m = 1$ means that the transformation has completed and the corresponding local material point is fully martensitic; and, lastly, intermediate values of ξ^m depict a still ongoing martensitic transformation.

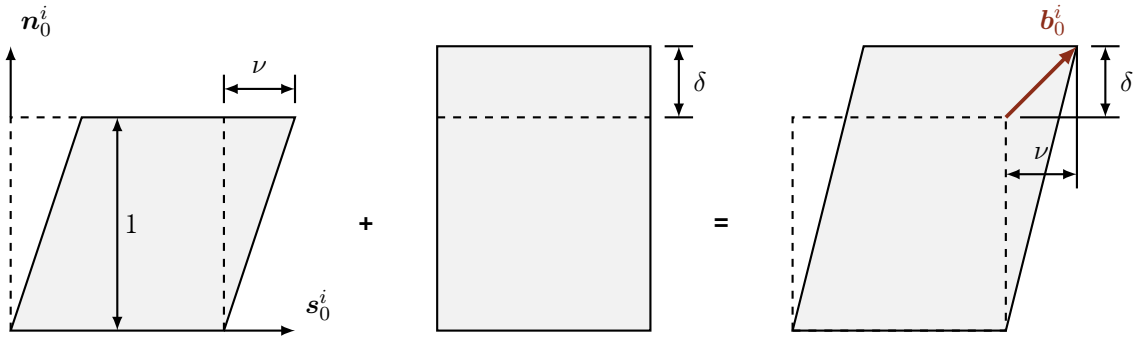


Figure 4.5: Decomposition of the total transformation deformation depicted by the vector $\mathbf{b}_0^i$ for a given system i into a habit plane shear component in the direction $\mathbf{s}_0^i$ and a volumetric component normal to the habit plane, $\mathbf{n}_0^i$.

Patel and Cohen's Transformation Criteria

Patel and Cohen (1953), observed that mechanical loadings influence the transformation starting temperature, and proposed that such behaviour came as a result of the work done between applied stresses and transformation displacements. On those terms, they then derived a simple transformation criterion limited to small strains and uniaxial stress states, and based on the mechanical loading contribution to the total thermodynamical driving force. This phenomenon came to be known as a *stress-assisted transformation*.

According to this assumption, we may define a *critical energy*, whose magnitude must be met in order for the transformation to begin. As we have exposed in Figure 4.6, this energy bound consists of a material property, as it depends on both parent and product phases' relative chemical free energies, which is inherently temperature-dependent. From the aforementioned Figure, we can observe that, at temperature M_s , the transformation starts spontaneously, whereas for a temperature T_0 both phases are in thermodynamical equilibrium. From that point on, that is, for temperatures above T_0 , the austenite phase has a lower chemical free energy and is, consequently, more stable than the martensite phase, meaning that under such conditions, martensitic transformation is usually not possible. In the temperature range between M_s and T_0 , the chemical free energy difference between both phases is insufficient for the spontaneous transformation to occur; however, an external mechanical loading can provide the remaining energy necessary, $\Delta G_{\text{mech}}|_T$, which, as it is shown, increases with the rise in temperature. That being said, we may conclude that, for a given temperature, ΔG_{mech} denoted the external stress power required for

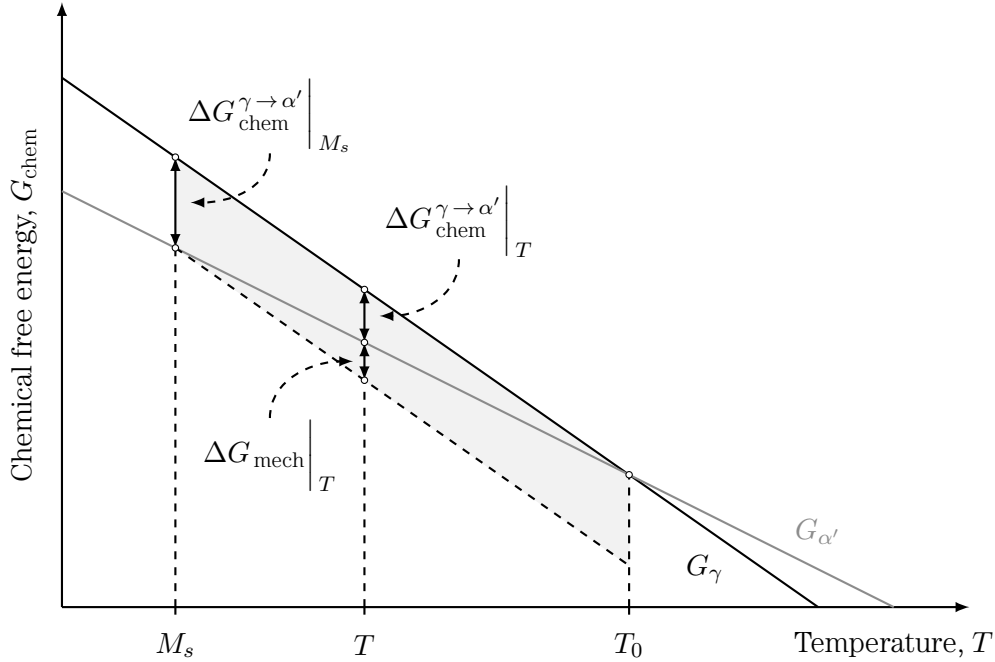


Figure 4.6: Austenite (γ) and martensite (α') chemical free energy evolution in terms of the temperature, T . Between M_s and T_0 , martensitic transformations can be induced by energy from external mechanical loadings.

the transformation initiation.

4.3.2 Extended Lee-Kröner Decomposition

The martensitic transformation constitutive model here presented is evidently coupled with the plastic slip model presented in Section 4.2. On that note, in order to account for both the austenite slip and martensitic transformations, the multiplicative decomposition of the deformation gradient (originally presented in equation 4.2.1) is now extended as follows:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^{tr} \mathbf{F}^p . \quad (4.3.9)$$

Following the scheme exposed in Figure 4.4, this extended decomposition entails the existence of *two* intermediate unstressed configurations, that is, one additional to the already presented for the plastic slip constitutive model, which is referred to as the *unstressed transformation lattice configuration*.

4.3.3 Thermodynamical Formulation

Our first step in this thermodynamical formulation is admitting the *hypothesis of separability*, which states that the elastic and inelastic parts of the specific free energy can be decomposed in an additively manner (Gurtin et al., 2010). With that in mind, and neglecting the defect energy, the specific free energy ψ (presented in Section 2.4.2) may be regarded as a function of solely the elastic deformation gradient, such that,

$$\psi = \psi (\mathbf{F}^e) , \quad (4.3.10)$$

and its time derivative, that is, its rate, is reduced from equation (2.4.18) to:

$$\dot{\psi} = \frac{\partial \psi}{\partial \mathbf{F}^e} : \dot{\mathbf{F}}^e . \quad (4.3.11)$$

Combining the above with the deformation gradient multiplicative decomposition, equation (4.3.9) and the general material version (reference configuration) of the Clausius-Duhem inequality (equation 2.4.21), under the assumption of an isothermal process, the following expression of the dissipation rate $\dot{D}$ can be derived (see Vieira de Carvalho et al. (in submission)):

$$\begin{aligned} \dot{D} = & (\mathbf{F}^e)^T \rho_0 \frac{\partial \psi}{\partial \mathbf{F}^e} (\mathbf{F}^{tr})^{-T} : \dot{\mathbf{F}}^{tr} \\ & + (\mathbf{F}^{tr})^{-T} (\mathbf{F}^e)^T \rho_0 \frac{\partial \psi}{\partial \mathbf{F}^e} (\mathbf{F}^{tr})^{-T} (\mathbf{F}^p)^{-T} : \dot{\mathbf{F}}^p \geq 0 , \end{aligned} \quad (4.3.12)$$

from which the *work conjugate stress of the transformation deformation gradient*, $\mathbf{T}$, can be defined as follows:

$$\mathbf{T} = (\mathbf{F}^e)^T \mathbf{P} (\mathbf{F}^p)^T = (\mathbf{F}^e)^T \boldsymbol{\tau} \mathbf{F}^{-T} (\mathbf{F}^p)^T . \quad (4.3.13)$$

Combining the expressions (2.2.13) and (2.2.18), the Kirchhoff stress tensor, $\boldsymbol{\tau}$, which actually defines the push-forward equivalent of the second Piola-Kirchhoff stress tensor, may be written for the present case as,

$$\boldsymbol{\tau} = \mathbf{F}^e \mathbf{S} (\mathbf{F}^e)^T, \quad (4.3.14)$$

and the transformation conjugate stresses can then be expressed as follows,

$$\mathbf{T} = \mathbf{C}^e \mathbf{S} (\mathbf{F}^{tr})^{-T}. \quad (4.3.15)$$

4.3.4 Transformation Functions

In Section 4.2.5 we discussed the subject regarding the onset of plastic crystallographic slip and presented the yield functions required to correctly model such behaviour. Here, analogously, the same concept is introduced for the martensitic transformation. As we have already discussed, and can be clearly observed in Figure 4.6, for a given temperature within the range between M_s and T_0 , the martensitic transformation requires a critical mechanical energy ΔG_{mech} (per unit reference volume). In this context, a constitutive model that dissipates exactly this amount of energy over the course of the martensitic transformation can be formulated by the introduction of $|\mathfrak{S}_{tr}|$ *transformation functions* that may be generically written as,

$$\Phi_{tr}^i (T^i, \Delta G_{\text{mech}}) = \mathbf{T} : \mathbf{N}_0^i - \Delta G_{\text{mech}} = T^i - \Delta G_{\text{mech}}, \quad (4.3.16)$$

coupled with the usual loading/unloading criteria⁵:

$$\Phi_{tr}^i \leq 0, \quad \dot{\xi}^i \geq 0, \quad \dot{\xi}^i \Phi_{tr}^i = 0, \quad i = 1, \dots, |\mathfrak{S}_{tr}|. \quad (4.3.17)$$

Above, the quantity T^i is the projection of the transformation conjugate stress tensor into the transformation system i , i.e., $T^i = \mathbf{T} : \mathbf{N}_0^i$. With that being said, T^i can then be understood as the martensitic transformation equivalent of the resolved Schmid stresses in slip plasticity.

From equation (4.3.5), the transformation flow rule reads,

$$\dot{\mathbf{F}}^{tr} = \sum_{i=1}^{|\mathfrak{S}_{tr}|} \left(\dot{\xi}^i \mathbf{N}_0^i \right) = \sum_{i=1}^{|\mathfrak{S}_{tr}|} \left(\dot{\xi}^i \frac{\partial \Phi_{tr}^i}{\partial \mathbf{T}} \right), \quad (4.3.18)$$

in which $\mathbf{b}_0^i$ and $\mathbf{n}_0^i$ are considered constant during the transformation.

4.3.5 Dissipation Consistency

From the expressions (4.3.12) and (4.3.16), it follows that,

$$\dot{D} = \mathbf{T} : \dot{\mathbf{F}}^{tr} = \sum_{i=1}^{|\mathfrak{S}_{tr}|} \left(\dot{\xi}^i T^i \right) = \Delta G_{\text{mech}} \sum_{i=1}^{|\mathfrak{S}_{tr}|} \left(\dot{\xi}^i \right). \quad (4.3.19)$$

⁵ Again, summation of the repeated index is not implied in the last equation.

Through the integration of this dissipation rate throughout the martensitic transformation, starting from a fully austenitic state ($\xi^m = 0$) until a fully martensitic material ($\xi^m = 1$),

$$\begin{aligned} D &= \int_{t_0}^{t_f} \dot{D}(t) dt = \Delta G_{\text{mech}} \int_{t_0}^{t_f} \sum_{i=1}^{|\mathfrak{S}_{tr}|} \dot{\xi}^i dt = \Delta G_{\text{mech}} \int_{t_0}^{t_f} \dot{\xi}^m dt \\ &= \Delta G_{\text{mech}} \left(\xi^m \Big|_{t=t_f} - \xi^m \Big|_{t=t_0} \right) = \Delta G_{\text{mech}}, \end{aligned} \quad (4.3.20)$$

we are then able to conclude that the total mechanical energy dissipated during the course of the transformation is equal to the energy density required for the activation of martensitic transformation.

4.3.6 Martensite Anisotropic Elasticity

Generally, a transformed, that is, martensitic system i reveals different elastic properties than those from its parent austenite phase. Following the procedure presented in [Turteltaub and Suiker \(2006\)](#), the elasticity tensors $\mathbf{D}^{e,i}$ of the martensite transformed in each system i can be determined as the weighted average of the elasticity tensors of both variants. However, this operation requires that both tensors are defined in the same vector basis. [Vieira de Carvalho et al. \(in submission\)](#) expounds this subject to great detail and derives the following expression:

$$\mathbf{D}^e(\xi^i) = \frac{1}{1 + \delta \xi^m} \left[\xi^a \mathbf{D}^{e,a} + (1 + \delta) \sum_{i=1}^{|\mathfrak{S}_{tr}|} (\xi^i \mathbf{D}^{e,i}) \right], \quad (4.3.21)$$

which relates the resulting elasticity tensor $\mathbf{D}$ with those of the austenite phase, $\mathbf{D}^{e,a}$, and of the martensite transformation system, $\mathbf{D}^{e,i}$.

In this context, it is worth noting that, while for a BCT (tetragonal) martensite structure the different orientations of the martensite variants would impact the resulting elasticity tensor, in the case of FCC-to-BCC transformations, with isotropy in both phases and resulting martensitic phase and austenite of similar stiffnesses, the effective stiffness tensor must be equal to $\mathbf{D}^{e,a}$.

4.3.7 Coupling of Austenite Slip Plasticity and Martensitic Transformation Evolution

To conclude this presentation of the martensitic transformation constitutive model, it must be emphasized that the austenite slip plasticity is incorporated into the model in a fully coupled scheme. In fact, in the current model, it is admitted that plasticity may occur in the austenite phase before the beginning of any transformation, depending on the particular alloy and conditions such as temperature, which has been evidenced in metastable austenitic stainless steels ([Perdahcioglu et al., 2008a,b](#)) and TRIP steels ([Chatterjee and Bhadeshia,](#)

2007). Furthermore, it should be noted that once transformation ceases, that is, $\xi^m = 1$ ⁶, the resulting martensite phase only behaves within the elastic domain for the remainder of the deformation process (martensite plasticity is ignored in the current formulation). For this reason, given the presence of plastic behaviour uniquely in the austenitic phase, the slip plasticity flow rule (equation 4.2.9) must be reassessed in order to account for the local volume fraction of the remaining austenite, ξ^a , thus becoming,

$$\dot{\mathbf{F}}^p = \left[\xi^a \sum_{\alpha=1}^{n_{slip}} (\dot{\gamma}^\alpha \mathbf{M}_0^\alpha) \right] \mathbf{F}^p. \quad (4.3.22)$$

4.4 Final Remarks on Computational Treatment and Rate-Dependent Formulation

The computational framework of the fully coupled constitutive model presented until this point, and implemented in **Links**, is outside the scope of this work. Nevertheless, one particular aspect regarding plastic slip and the adopted yield function, which involves the consideration of a *rate-dependent* or a *rate-independent* formulation, must still be discussed.

Focusing on the materials of concern in the context of this work, single crystal alloys exhibit a great resistance to rate-dependent phenomena such as, for instance, creep failure under high-service temperatures. As a result, it might seem the better approach to adopt a rate-independent formulation within the implemented model; however, rate-independent formulations embody several algorithmic inconveniences, particularly regarding the determination of the set of active systems during deformation.

For these reasons, a rate-dependent formulation is used in the constitutive model here presented and implemented in **Links**, which actually encompasses a much more versatile approach. In short, a *viscous slip rate law*, known as *Peric's law* (Peric, 1993), is adopted:

$$\dot{\gamma}^\alpha = f_p^\alpha (\tau^\alpha, \tau_y^\alpha) = \begin{cases} \frac{1}{\mu_p} \left(\frac{\tau^\alpha}{\tau_y^\alpha} - 1 \right)^{1/\epsilon_p} & \text{if } \tau^\alpha > \tau_y^\alpha, \\ 0 & \text{otherwise} \end{cases}, \quad (4.4.1)$$

where ϵ_p and $1/\mu$ denote the non-dimensional rate-sensitivity and a viscosity-like material parameter (of dimension time), respectively. Note that for the limits of these parameters, that is, when $\epsilon_p \rightarrow 0$ and $\mu_p \rightarrow 0$, the rate-independent case is recovered, which displays the versatility of the rate-dependent formulation. However, it should be emphasised that for this limit, the aforementioned rate-independent problems are equally recovered. The analyses carried out in this work considered this rate-independent, limit case, coupled with several computational techniques that solve, to a large extent, the associated convergence problems.

⁶ Since monotonically increasing loading scenarios are considered, the transformation proceeds on any given system i until its completion.

Analogously, an explicit law for the rate of martensite transformation can also be defined, $\dot{\xi}^i = f_{tr}^i(T^i, \Delta G_{\text{mech}})$, and one possible transformation rate law can be directly obtained from the above, by replacing τ^α with T^i , τ_y^α with ΔG_{mech} , ϵ_p with ϵ_{tr} and μ_p with μ_{tr} .

Besides this particular issue, no other computational related subject will be discussed. On that note, for a thorough description of the computational treatment of both constitutive models here presented, see [Vieira de Carvalho et al. \(in submission\)](#).

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5

Determination of the RVE Size for Multi-Scale Homogenisation Convergence and Analysis of the Macroscopic Results

In Chapter 3, the concept of a Representative Volume Element was introduced and the idea of the convergence of the homogenised macroscopic results with the increase in the RVE size was also briefly exposed (see Figure 3.5). Fundamentally, the homogenisation technique assumes a certain degree of periodicity regarding the material microstructure over the entirety of the macro-scale domain; however, in reality, and particularly with polycrystalline heterogeneous materials, truly periodic microstructural morphologies are seldom found. As a result, the adopted RVE must provide a rich sampling of all micro-heterogeneities present in the material whose behaviour we aim to predict, otherwise the resulting macroscopic quantities may carry significant discrepancies relatively to their true values. Conversely, from a practical standpoint, the adoption of smaller RVEs is also fruitful as it implies the need for less computational power. Time and resources are limited, therefore, the determination of the RVE size that is statistically representative of the whole material and leads to acceptable macroscopic results is paramount. The subject of homogenisation convergence with the RVE size and applied boundary condition is studied to great detail by Terada et al. (2000), while Kanit et al. (2003) proposed a statistical approach to the determination of the RVE size.

5.1 Introduction

In this Chapter, three distinct macroscopic problems are analysed: (i) the bending of a slender cantilever beam, (ii) a double-notched specimen under plane strain and, lastly, (iii) a butterfly specimen subjected to shear. Within the context of this first stage of numerical analyses, each of these specimens is subjected to a prescribed displacement and its

simulations are performed under a FE^2 multi-scale model based on the standard first-order homogenisation formulation, from which the effective macroscopic results can be observed and the deformation state histories, $\mathbf{F}$ and $\mathbf{G}$, can be captured at the selected interest points. Given that a single multi-scale analysis involves several micro-scale simulations for each of the integration points of the macroscopic mesh, the Taylor's constraint (recall Section 3.3.4) has been employed in order to speed-up these computations: Taylor's boundary condition leads to a constant deformation state within the RVE, therefore, the state-update procedure only needs to be performed once for each crystal; an improved algorithm developed around this detail and included in **Links** enables a reduction of memory requirements and computational cost. Note, however, that since a first-order homogenisation scheme is employed at this stage, the second gradient of the macroscopic displacements must be indirectly computed through the third-order tensor, $\mathbf{H}$, with the second derivatives of the shape functions, succinctly given in terms of the material global shape functions, or material global interpolation matrix, $\mathbf{N}^g$, whose spatial counterpart is expressed in (2.7.11), by:

$$\mathbf{H}^g = \frac{\partial}{\partial \mathbf{p}} \left(\frac{\partial \mathbf{N}^g}{\partial \mathbf{p}} \right), \quad (5.1.1)$$

or, in index notation, by:

$$H_{i,j,k}^g = \frac{\partial N_i}{\partial p_j \partial p_k}, \quad (5.1.2)$$

such that the second gradient of the displacements, initially introduced in (2.8.1), may be rewritten as:

$$\mathbf{G} = \frac{\partial^2 \mathbf{u}}{\partial^2 \mathbf{p}} \Rightarrow \mathbf{G} = \mathbf{u} \cdot \mathbf{H}^g, \quad (5.1.3)$$

where, for clarity, $\mathbf{u}(\mathbf{p}, t)$ denotes the displacement vector field and $\mathbf{u}$ is the global vector of nodal displacements. Recall, from Equation (2.7.13), that the displacement can be approximated by a discreteised version of the displacement field given by $\mathbf{N}^g \cdot \mathbf{u}$. In addition, it must be noted that this procedure is only possible for discretisation into quadratic elements (i.e., elements with quadratic shape functions). For a more detailed description of this subject see [Rodrigues Lopes \(2019\)](#). In this context, it is worth clarifying why a first-order homogenisation scheme has been initially adopted instead of its extension, based on second-order continuum mechanics. For one, such framework would entail a significantly higher computational cost (note that in the second-order homogenisation scheme the deformation state would cease to be constant within each RVE and the aforementioned Taylor-related algorithmic simplification could no longer be employed), which is accentuated by the fact that the results would depend on the microstructural characteristic length, associated with the chosen RVE length (recall that the analysis of the dependence of the computed results with the RVE length is one of the main goals of this dissertation). Furthermore, second-order boundary conditions, which require displacement gradient boundary restrictions (in addition to the standard displacement constraints), would also need to be defined, a subject

around which there is quite some uncertainty regarding which specific condition should be employed in a given particular problem, and that is outside the scope of this work.

A convergence analysis is inherently a statistical one. Therefore, in order to determine the ideal RVE size, multi-scale simulations with RVEs containing 10 to 400 grains have been performed for each of the specimens under analysis. We will refer to each group of simulations with a specific number of grains, that is, to any series of simulations with a specific RVE size, by a *set* of simulations. Furthermore, stemming from the RVE's nature and eventual lack of representativity, an element of *randomness* can be expected in the outputted macroscopic results, particularly for the sets with smaller RVE sizes. In order to circumvent this unpredictability and minimize its influence on our convergence assessment, ten different RVEs have been considered for each set of simulations. Each RVE model has been generated with the polycrystal generation and meshing software Neper (Quey et al., 2011), in which the adjustment of a *seed* parameter leads to different, randomly generated microstructures. For a matter of clarity, each of these ten different microstructures will be designated by the term *sample*. In this context, Figure 5.1 presents two different samples generated for the set of simulations associated with an RVE size of 10 grains.

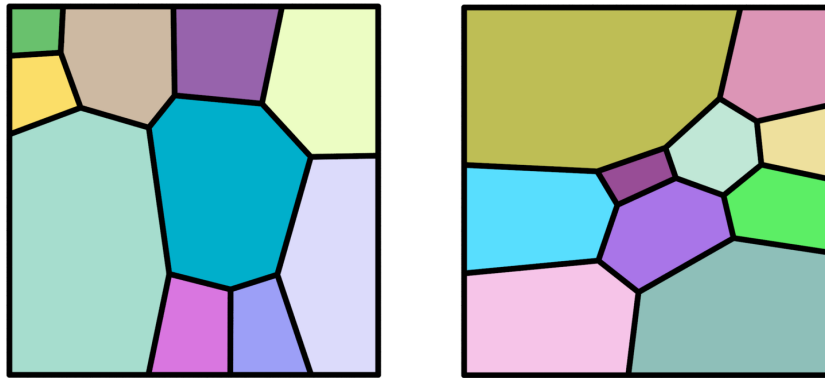


Figure 5.1: Two distinct generic representative volume elements containing ten grains each, generated with the open-source software package Neper (Quey et al., 2011).

In order to properly evaluate the convergence of the obtained macroscopic results, two different statistical parameters were considered. Firstly, we determined each set's average of the energy (work) transferred to the specimen. Secondly, recalling the element of randomness previously stated, we have also determined the standard deviation (more specifically, the coefficient of variation) relative to the transferred energies in each set. A Python script that reads the relevant data from the macroscopic results' files of the multi-scale analyses carried out through *Links* and presented in this Chapter was implemented in order to obtain both these statistical parameters in an immediate manner. To compute the work transferred to the specimen in each simulation, the reaction curve was numerically integrated with respect to the prescribed displacement by means of the *Simpson's rule* (which constitutes a particular case of the *Closed Newton-Cotes* rules), that approximates each

subinterval n comprised of three adjacent points of the reaction curve as a parabola, such that for each midpoint x_i of a given subinterval n the Simpson's rule reads:

$$\int_{x_{i-1}}^{x_{i+1}} f(x) \approx \frac{\Delta x}{3} [f(x_{i-1}) + 4f(x_i) + f(x_{i+1})], \quad (5.1.4)$$

in which Δx is, in this case, equal to $(x_{i+1} - x_{i-1}) / 2$. From here, the coefficient of variation between the transferred work values of the samples in each set can be directly obtained. Note that to employ both these mathematical procedures, rather than coding their respective algorithms, readily available Python packages, namely SciPy and NumPy, were used. On this topic, it is also worth mentioning that in order to automate the execution of these simulations, as well as to reduce the probability of any eventual human errors, Bash scripts were also implemented for the generation of the input files and subsequent submission to `Links`.

The results displayed in this Chapter can be divided into two major Sections (see Figure 5.2). Initially, martensitic transformation (MT) is not considered, that is, solely the crystal slip plasticity mechanism is included in the admitted constitutive model (besides, naturally, the initial elastic domain), and the results for each of the three stated macroscopic problems are presented. This is our first assessment of the required RVE size. Subsequently, we admit the MT phenomenon and its resulting TRIP effect and repeat the ten samples of the previously adopted RVE size. One of the main purposes of this Chapter is to collect the histories of the first and second deformation gradients at the selected points of interest, which will be then studied in the decoupled micro-scale simulations discussed in Chapter 6. Nevertheless, the analysis of the homogenised response convergence with the increase in the RVE size is required to obtain representative results and, consequently, an accurate homogenised depiction of the macroscopic material behaviour. This initial assessment of the influence of MT on the macroscopic response is also of great significance as it not only validates (and complements) the initially expected outcomes based on the general martensitic transformation theory but also allows a more curated selection of the interest points analysed in Chapter 6.

5.2 Numerical Results without Martensitic Transformation

In this Section, the results regarding the convergence analysis for increasing RVE sizes for each of the considered macroscopic specimens are presented. In each case, the macroscopic distributions of relevant quantities obtained from the analysis of a specific sample from the selected RVE size are also shown. To present these results we selected the sample with the closest response to the computed average of its corresponding set. Each crystal is modelled by the single crystal slip plasticity constitutive model presented in Section 4.2. The material properties and constitutive model's parameters are consistent for all the numerical analyses carried out in this stage and are presented in Table 5.1. The former correspond to an ASTM A-564 alloy (also known as Sandvik Nanoflex®), a meta-stable austenitic stainless steel,

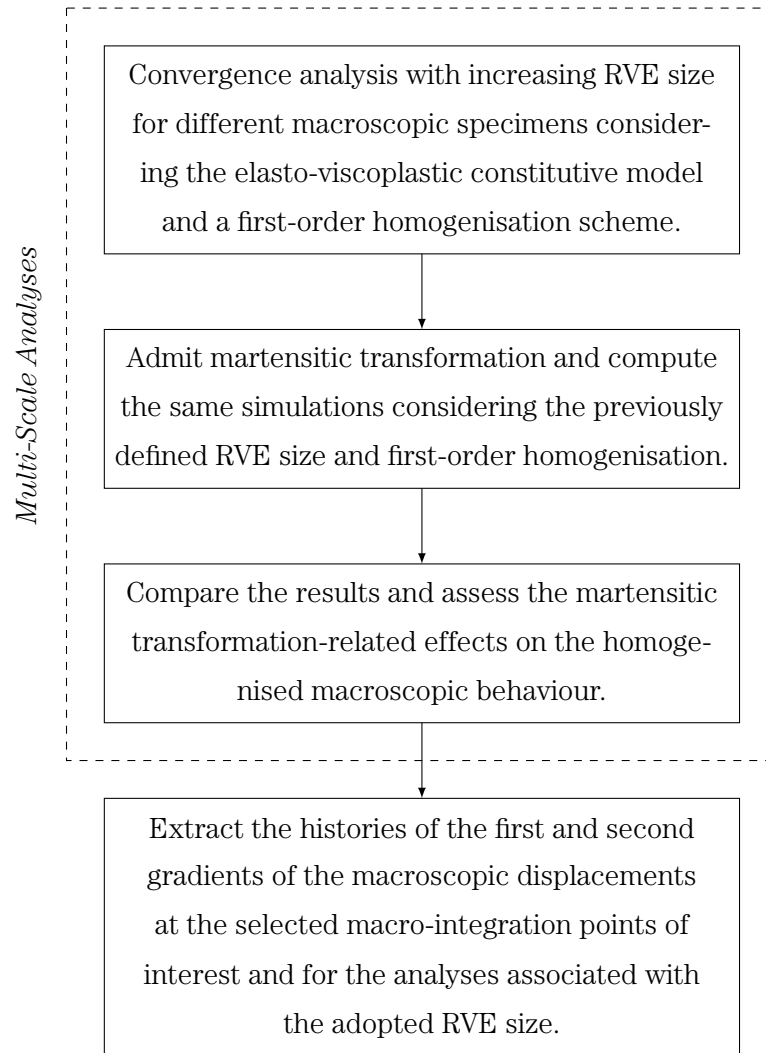


Figure 5.2: Schematic representation detailing each of the steps and decisions that outline this first stage of numerical analyses for each specimen.

Table 5.1: Material properties and elasto-viscoplastic constitutive model's parameters.

Austenite Phase's Elastic Properties [GPa]	D_{11}^A	282.69
	D_{12}^A	121.15
	D_{44}^A	80.769
Peric's Law - Expression (4.4.1) (Viscoplastic Parameters)	ϵ_p	0.01
	μ_p	— ¹
Nadai-Ludwik Hardening Law - - Expression (4.2.30) (Hardening Parameters)	$\tilde{\tau}_y$ / GPa	0.088
	K / GPa	0.195
	γ_0	0.01
	m	0.6
	q	1.4

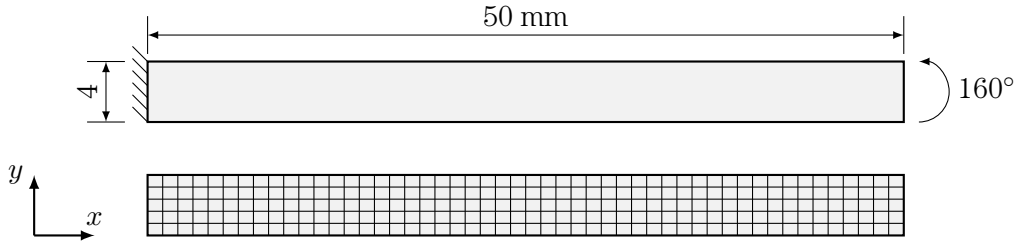


Figure 5.3: Geometry and finite element model of the 2D beam subjected to a bending rotation of 160°.

whose austenite's elastic properties were initially calibrated by [de Bortoli et al. \(2018\)](#). Note that Bortoli's model constitutes an initial version of the model adopted in this dissertation.

5.2.1 Beam Subjected to Bending Rotation

The 2D beam model studied in this first series of coupled multi-scale analyses, whose macroscopic results are here presented, is schematically presented in Figure 5.3 and is subjected to a bending rotation of 160° applied in 80 increments of 2° each. The macro-scale finite element model contains 250 8-noded quadrilateral elements with reduced integration, resulting in a total of 861 nodes and 1000 RVEs.

The statistical results are explicitly shown in Figure 5.4, where, as expected, we can immediately observe that the computed average work is converging with the increase in RVE size. However, it is worth noting that this observation is far more expressive in the right-hand side plot, where the evolution of the coefficient of variation with the increasing RVE size is presented, thus supporting the importance of this second statistical parameter on our convergence assessment. Furthermore, it must be pointed out that neither of the parameters is constantly converging with the increase in the size of the RVE, which can, to

¹ Note that the *rate-insensitivity technique* is employed, such that neither μ_p nor μ_{tr} (Table 5.2) need to be used; for more information on this topic refer to [Vieira de Carvalho et al. \(in submission\)](#).

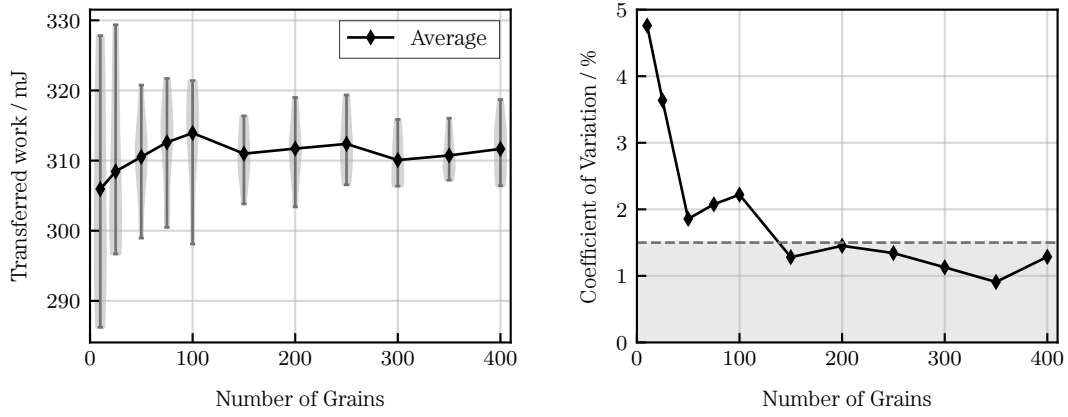


Figure 5.4: Statistical results from the multi-scale analyses of the bending beam specimen with increasing RVE's size: distribution of the work associated to the samples from each set along with its respective averages (left), and evolution of the coefficient of variation relative to the computed work values found in each set (right).

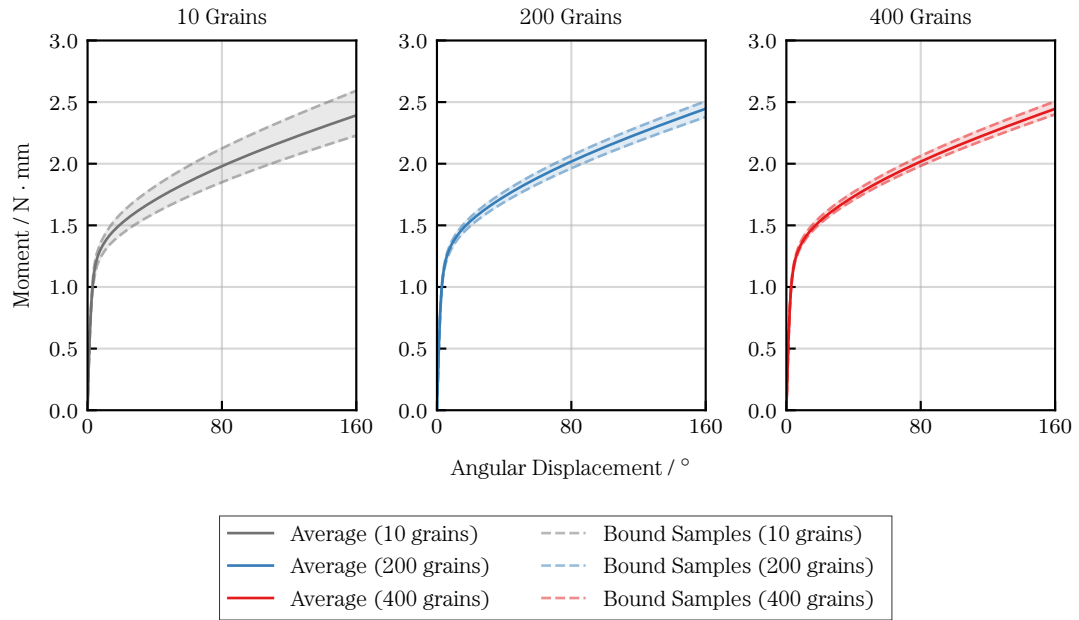


Figure 5.5: Plot of the curves of the average momentum and the upper and lower momentum bounds associated with the analyses of the bending beam specimen, for the 10, 200 and 400 grains' sets.

some extent, be attributed to the element of randomness previously stated but, more importantly, to the relatively short sample size (ten) in each set. Moreover, the right-hand side plot also includes the established convergence criteria of a coefficient of variation equal to 1.5%, for which any RVE containing 150 or more grains may then be considered representative. To further emphasise the notion of convergence and the importance of this exercise, Figure 5.5 shows the average curves of the moment for the sets with 10, 200 and 400 grains, along with lower and upper bounds associated with the two samples with the furthest results from the average curve. We can observe that this range (delimited by the lower and upper bounds) is significantly smaller for the RVEs of larger size, and that any discrepancies between the results from the 200 and 400 grains' sets, particularly their averages, are practically negligible.

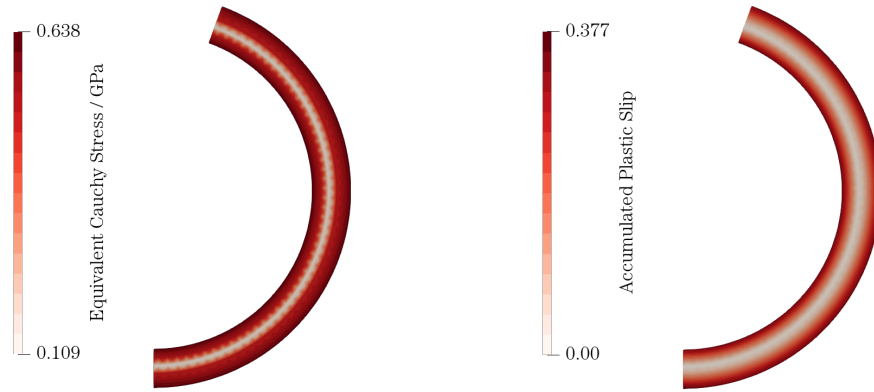


Figure 5.6: Contour plots of the equivalent Cauchy stress and accumulated plastic slip γ at the macro-scale of the bending beam at the final angular displacement of 160° and for an RVE containing 200 grains.

Figure 5.6 shows the macro-scale distributions of the equivalent Cauchy stress and the accumulated plastic slip γ at the end of the simulation, that is, for the final angular displacement of $\theta = 160^\circ$. Several observations can be immediately made. Firstly, we can observe that the stresses are most significant at the bottom and upper faces of the bending beam with the bottom face exhibiting mostly tensile stresses and the upper face plastic compressive stresses. As expected, both these regions exhibit the largest amount of plastic behaviour (slip plasticity). The neutral axis, which splits these two regions, and inherent to bending deformation, is also clearly noticeable. Due to the high curvature involved in the prescribed angular displacement we may also notice its vertical displacement (i.e., along the beam's thickness) during deformation, specifically, towards the curvature center, or, equivalently, towards the compressive stress region. While the equivalent strain measure is not implicitly shown in the aforementioned Figure, its results are directly related to the equivalent Cauchy stress, from which we may infer that the gradient of the macroscopic displacements (measure analogous to the equivalent strain) at both faces are much more significant than in the neighbourhood of the neutral axis. These differences and, particularly, the distinct nature

of the material behaviour between both faces, are quite convenient for the macroscopic analyses involving MT, as they allow to assess the relative importance of these two distinct deformation modes (tensile and compressive).

5.2.2 Double-Notched Under Plane Strain

The 2D double-notched specimen subjected to the prescribed vertical displacement $u_2 = 1.0$ mm employed in its upper face, is schematically presented in Figure 5.7, along with its macro-scale finite element mesh of 984 8-noded elements with reduced integration, resulting in a total of 3097 nodes and 3936 RVEs.

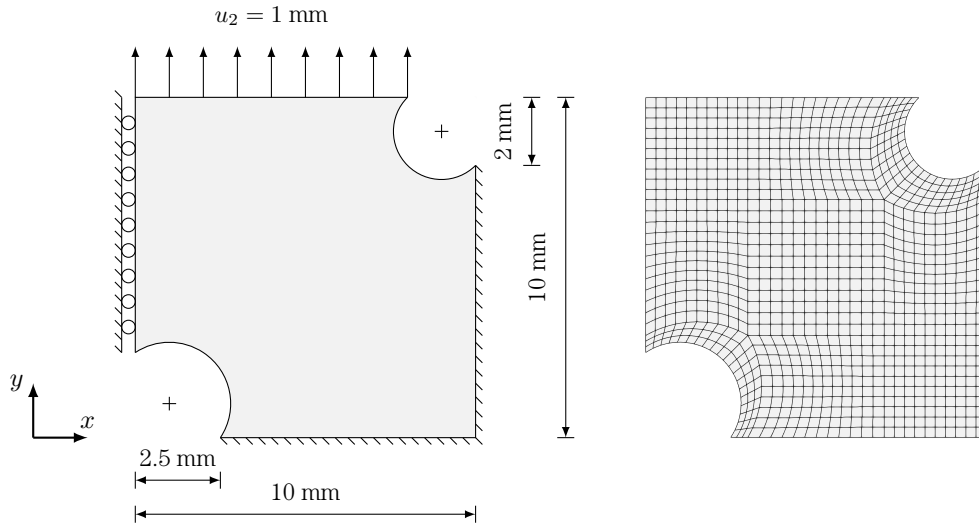


Figure 5.7: Geometry and finite element model of the 2D double-notched specimen subjected to the prescribed vertical displacement $u_2 = 1.0$ mm.

The statistical convergence parameters obtained from the macroscopic results of the double-notched multi-scale simulations and the corresponding bounds are presented in Figures 5.8 and 5.9, respectively. As we can observe, relatively to the results previously presented for the bending beam, the convergence is far more immediate. In fact, in this case, following the initially established coefficient of variation tolerance of 1.5%, we should expect representativity and, consequently, reliable homogenised results for RVEs with 50 or more grains. However, it should be noted that, despite meeting our criteria, the transferred work average value shows significant fluctuation for the range below 100 grains, which contrasts with the practically flattened evolution for RVEs containing 150 or more grains. In this context, the contour plots presented in Figure 5.10 display the equivalent Cauchy stress, the Cauchy stress σ_{xy} and the accumulated plastic slip γ , respectively, highlighting the importance of this convergence exercise, since, as shown, both measures exhibit significantly fewer discrepancies between the 200 and 400 than in between 10 and 200 grains' sets.

Regarding the stresses associated with the double-notched specimen subjected to vertical displacement, it should be remarked the development of a shear band between the two

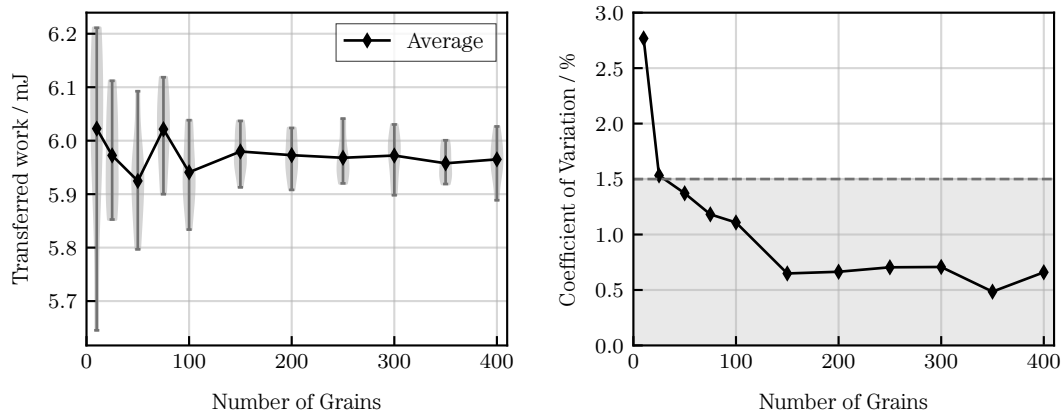


Figure 5.8: Statistical results from the multi-scale analyses of the double-notched specimen with increasing RVE's size: distribution of the work associated to the samples from each set along with its respective averages (left), and evolution of the coefficient of variation relative to the computed work values found in each set (right).

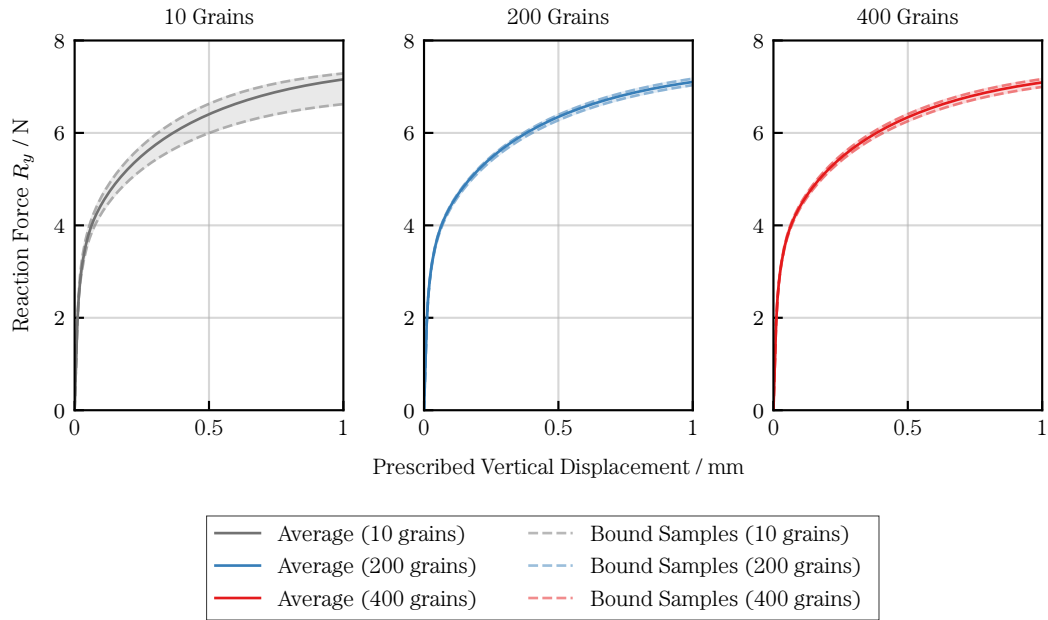


Figure 5.9: Plot of the curves of the average reaction force and the upper and lower reaction force bounds associated with the analyses of the double-notched specimen, for the 10, 200 and 400 grains' sets.

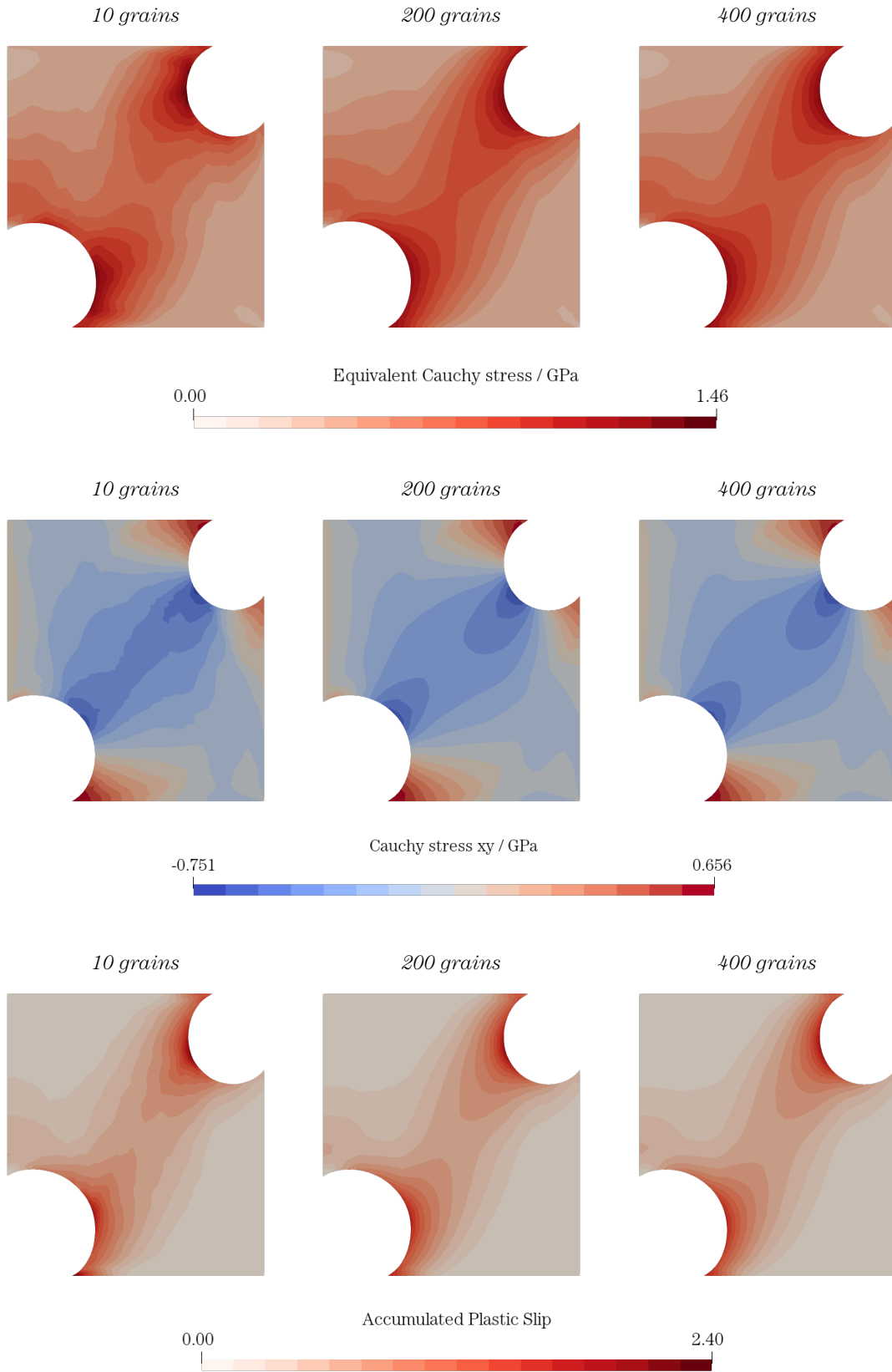


Figure 5.10: Contour plots of the equivalent Cauchy stress, Cauchy stress σ_{xy} and accumulated plastic slip γ obtained at the macro-scale of the double-notched specimen at the final displacement $u_2 = 1.0$ mm and for the bound samples in the 10, 200 and 400 grains' sets.

notches located at the upper-right and bottom-left corners of the specimen, which naturally arises from its geometry and prescribed loading condition. Since the principal mechanism behind plastic deformation is shear, it is with no surprise that the resulting accumulated plastic slip depicts an analogous distribution to that of the above-mentioned shear-band noticeable both in the equivalent Cauchy stress and Cauchy stress σ_{xy} countour plots. However, the most significant accumulated plastic slip values are present at the center region of the edges of both notches, where, specifically, the shear stress values, but also the remaining stresses associated with other deformation modes are predominant. This is also be observed in the contour plot of the equivalent Cauchy stress.

5.2.3 Butterfly Specimen Subjected to Shear

The last series of simulations discussed in this Section involves the numerical analysis of the butterfly specimen presented in Figure 5.11. Similarly to the previous double-notched specimen, this problem also constitutes a shear dominant loading scenario, imposed through the application of a horizontal displacement of magnitude $u_1 = 1.0$ mm on the specimen's upper face. The macro-scale finite element mesh (also shown in the aforementioned Figure) consists of 2080 20-noded hexahedral elements with reduced integration, which results in a total of 10785 nodes and 16640 RVEs.

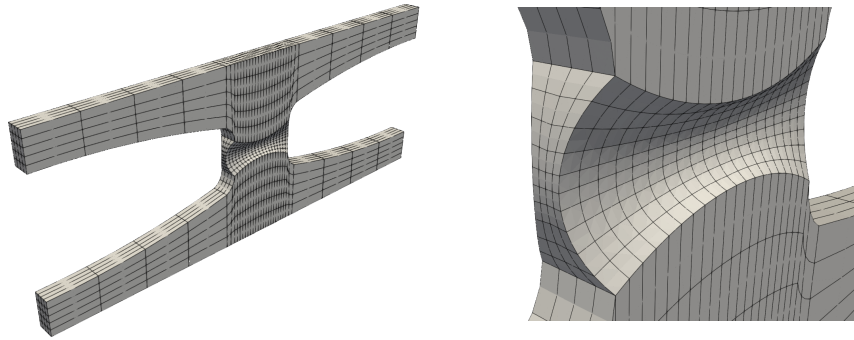


Figure 5.11: Geometry and finite element model for the butterfly specimen subjected to the horizontal displacement $u_1 = 1.0$ mm, with detail on the necking zone.

The statistical convergence parameters obtained from the macroscopic results of the butterfly multi-scale simulations are presented in Figure 5.12 and the plot of the average reaction curve along with the upper and lower reaction bounds for the sets of 10, 200 and 400 grains are shown in Figure 5.13. The stabilization of the obtained results is equivalent to that of the two previously discussed problems, with the only apparent difference being the more regular decrease of the coefficient of variation with the increase in the RVE size, which would presumably be the observed trend in all cases had more samples been admitted for each of the considered RVE sizes (sets).

Similarly to the previous case, the loading scenario here considered leads to a constitutive response mainly driven by shear. This can be observed in Figure 5.14, where the

significance of the shear stresses along the xy plane at the center of the specimen's necking zone is manifestably clear, while the normal stresses are more predominant in the surrounding regions, particularly at the two lateral edges of the specimen's neck. Again, the distribution of the accumulated plastic slip is practically analogous to that of the shear stresses. At this stage, the conclusions to draw from the analysis of the butterfly specimen are nearly identical to the ones presented in the discussion of the double-notched. Indeed, the incentive for the execution of these numerical analyses in particular is mostly the study of these phenomena in the three-dimensional space.

5.3 Numerical Results with Martensitic Transformation

From the results presented in the previous Section, we may conclude that any RVE containing more than 150 grains satisfies the pre-established coefficient of variation tolerance of 1.5%. That being said, we opted for the RVE size of 200 grains, since, relatively to the 150 grains' set, it does not pose a significant increase of the required computational power. The histories of the deformation gradient, $\mathbf{F}$, and second gradient, $\mathbf{G}$, are then captured, for each specimen, from the multi-scale analysis of the microstructural sample (RVE) containing 200 grains and that produces the closest homogenised macroscopic response to the computed average of its corresponding set. Following the steps outlined in Figure 5.2, we may proceed to the multi-scale analyses of each of the three specimens under the constitutive model that simultaneously admits mechanically-induced MT. The properties and parameters regarding the martensitic phase and its transformation are presented in Table 5.2. All of the properties involved in the austenite's elasto-viscoplastic behaviour (listed in Table 5.1) remain valid. Moreover, it must be emphasised that the mechanical energy ΔG_{mech} required for MT were calibrated in order to obtain evident, but still adequate, levels of transformation and different evolutions of phase transformation along the prescribed displacement in each specimen, which enrich our analyses and overall discussion.

Table 5.2: Transformed martensite elastic properties and rate of transformation's parameters.

Martensite Phase's Elastic Properties [GPa]	D_{11}^M	282.69
	D_{12}^M	121.15
	D_{44}^M	80.769
Rate of Transformation	ϵ_{tr}	0.01
Parameters - Expression (4.4.1)	μ_{tr}	—
Transformation's Required Mechanical Energy ΔG_{mech} / GPa	Bending	0.015
	Double-Notched	0.05
	Butterfly	0.3

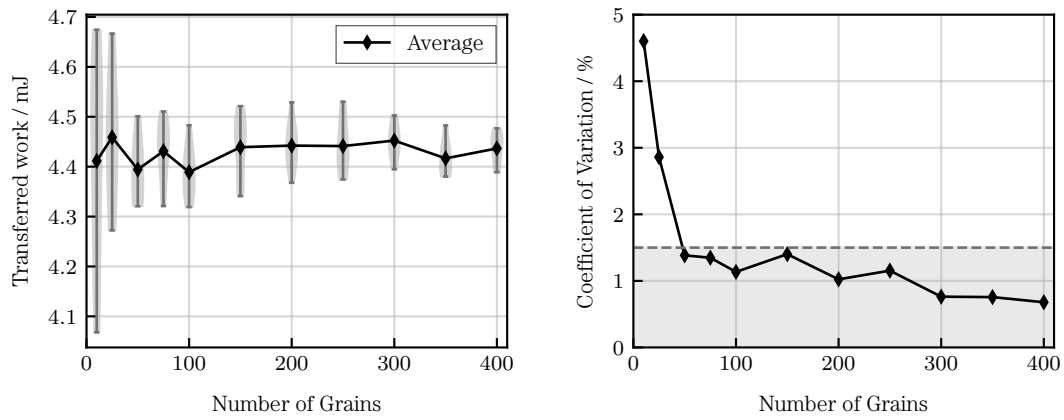


Figure 5.12: Statistical results from the multi-scale analyses of the butterfly specimen with increasing RVE's size: distribution of the work associated to the samples from each set along with its respective averages (left), and evolution of the coefficient of variation relative to the computed work values found in each set (right).

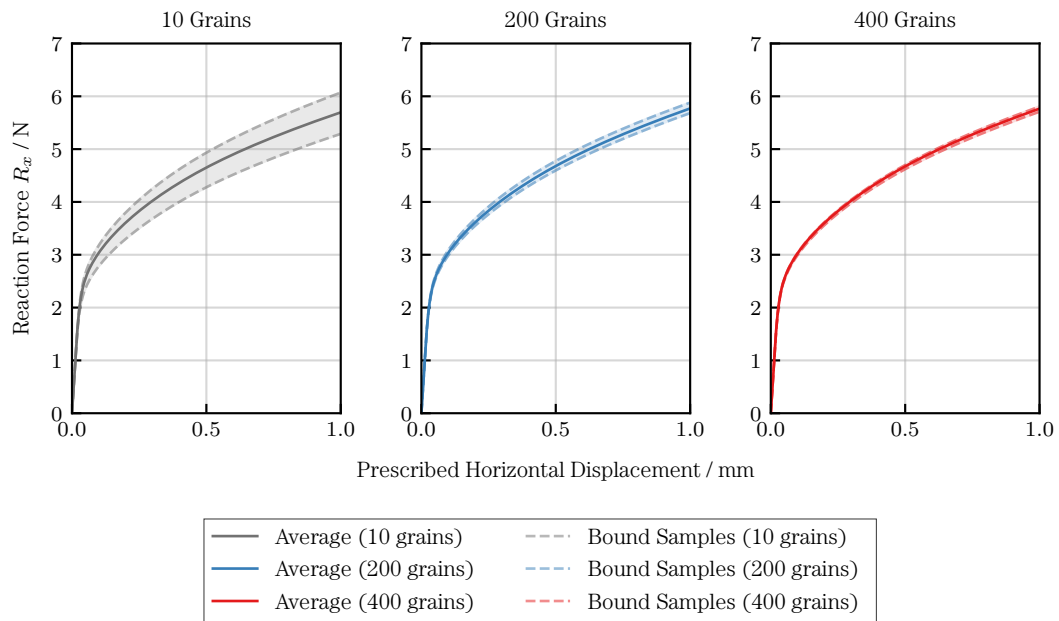


Figure 5.13: Plot of the curves of the average reaction force and the upper and lower reaction bounds associated with the analyses of the butterfly specimen, for the 10, 200 and 400 grains' sets.

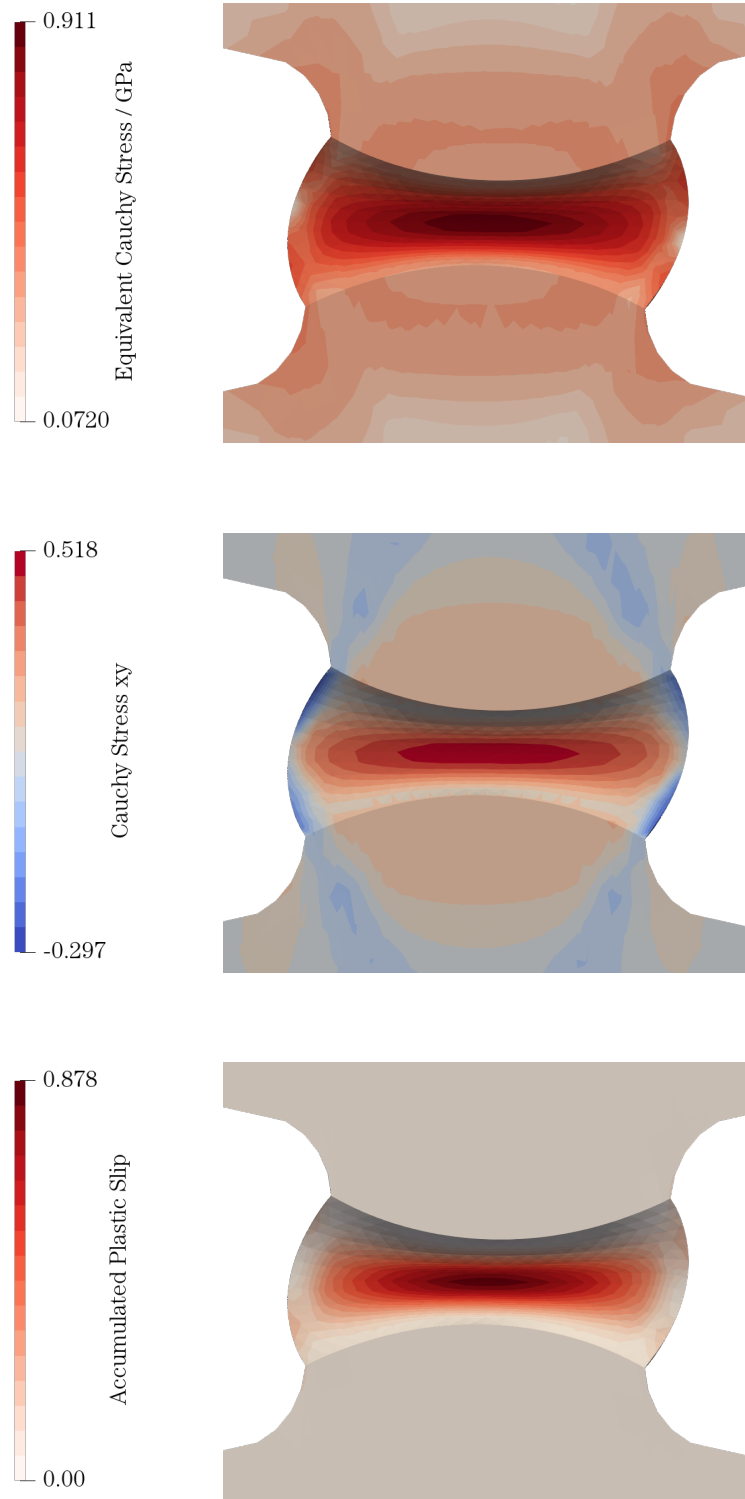


Figure 5.14: Contour plots of the equivalent Cauchy stress, Cauchy stress σ_{xy} and accumulated plastic slip γ obtained at the macro-scale of the butterfly specimen at the final displacement of $u_1 = 1.0$ mm and for an RVE containing 200 grains.

Naturally, the homogenised responses obtained from these simulations will be substantially different from those discussed in the previous Section, in which MT was not admitted. Thus, for the results discussed in Chapter 6 to provide any valuable information, the deformation histories enforced in the micro-scale analyses of any given specimen must be consistent. That being said, we chose to capture the histories of $\mathbf{F}$ and $\mathbf{G}$ during the prescribed displacement solely from the analyses with the elasto-viscoplastic crystal slip plasticity-based constitutive model, without martensitic transformation. This explains why the convergence study and subsequent adoption of the RVE size was centered on the results from Section 5.2. Nevertheless, for the sake of consistency, and to assess any potential convergence inhibiting MT-related effects, the statistical analysis of the variation found in the results obtained from the adopted RVE size when considering MT is also presented. Following the framework of the previous Section, ten multi-scale simulations (for the ten samples containing 200 grains) are carried out for each of the three specimens. The coefficients of variation computed for each specimen are presented in Table 5.3. As we can observe from these results, the presence of MT leads to a generalised increase in the coefficients of variation of each specimen, even violating, in the case of the bending beam, our initially established convergence criteria. The exact role of the martensitic phase in this delay of the homogenised convergence is better understood with the analysis and comparison of the homogenised macroscopic responses obtained under both the considered constitutive models (see, for instance, Figure 5.15).

Table 5.3: Coefficients of variation relative to the work associated with the prescribed displacements in each specimen for RVEs of 200 grains, with and without plasticity-induced MT.

	Bending	Double-Notched	Butterfly
without MT	1.44	0.66	1.02
with MT	2.10	1.09	1.10

Following these results, it must be emphasised that all stages of both constitutive models are formulated under the assumption of material anisotropy. In the elastic domain, this detail is not relevant given the isotropic nature of the material properties (the austenite phase is elastically isotropic - see Table 5.1). Conversely, when non-linear effects become present, for instance when the yield threshold is surpassed and the material begins to deform plastically, the macroscopic response may become greatly dependent on the material microstructure or, more accurately, on the RVE size. Indeed, as the number of grains included in the RVE increases, the response of the material gradually becomes isotropic (or less anisotropic). This is clear in the convergence results presented in Section 5.2, in which the larger RVEs showed significantly less variations within the plastic domain. That being said, when MT, which in itself is highly dependent on crystallographic orientation, is considered, the anisotropic effects are further exalted.

With the possibility of mechanically-induced MT, the material response depends on an

intricate play between crystal slip plasticity and phase transformation. Hence, to fully grasp the interactions between both phenomena and how their individual and simultaneous evolutions impact, not only the macroscopic material behaviour, but also each other, a rigorous study must be carried out. Accordingly, the following discussion focuses on two main measures directly related to the non-linear phenomena at play: the accumulated plastic slip and the volume fraction of the martensitic phase. Moreover, due to the aforementioned obtained decrease of the convergence of the homogenised response, caused by the inherently anisotropic nature of these phenomena, we chose to devote the analysis of these measures to a single sample, instead of to the set's average (as we have done until this point). This also applies to the equivalent Cauchy stress, equally addressed.

5.3.1 Beam Subjected to Bending Rotation

Regarding the bending beam specimen, the plots of the set's average moment curve and corresponding bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction are presented in Figure 5.15. Immediately, we can infer that the response is instantly met with some degree of MT, albeit of minuscule magnitude at the early stages of deformation (and thus, not perceptible in either of the presented Figures), which is mostly due to the small critical transformation energy barrier, in this case, $\Delta G_{mech} = 0.015$ GPa. Since for this specimen and enforced loading scenario phase transformation begins at stresses much lower than the austenite's yield stress, this constitutes what may be referred to as *stress-assisted transformation* and leads to several noticeable differences when compared with the simulations that did not admit phase-transformation.

As phase transformation begins prior to plastic slip, and considering the fact that transformation occurs at a constant stress², the yield plateau in the responses with phase transformation appears at stress values far inferior than those found in the simulations solely subject to plastic slip. Moreover, MT naturally implies that the transformation deformation gradient, $\mathbf{F}^{tr}$, is non-null, which, according to the multiplicative decomposition of the deformation gradient expressed in (4.3.9), necessarily leads to the decrease of the elastic deformation gradient, $\mathbf{F}^e$, that, in turn, is directly associated with the resulting stress state.

As we have exhaustively underlined, the considered constitutive model is fully coupled, meaning that phase transformation and plastic slip may occur in a simultaneous manner. However, in these circumstances, perfect transformation implies that once any given transformation system is formed, it will not reach the yield stress required for plastic slip to occur. That being said, any transformation system established before plastic slip has commenced may only continuously transform until it becomes fully martensitic, thus ceasing the transformation mechanism and recovering the elastic behaviour under the elastic properties of the developed martensitic phase (which, in our analyses, are identical to those of the parent austenite phase). This concept is clearly perceived in Figure 5.15, in which the

² Note that the critical energy ΔG_{mech} remains unchanged during transformation, a feature that resembles the *perfect plasticity* phenomenon, in which the hardening effect does not occur, and may then be analogously referred to as *perfect transformation*.

analyses where MT is admitted exhibit substantially less accumulated plastic slip than the analyses where solely plastic slip is considered. Again, the multiplicative decomposition of the deformation gradient also renders this detail.

Recalling that MT is intimately related to a volumetric growth of the material, one would expect that significant differences would be observed when that growth is promoted or, in contrast, inhibited. To assess this behavioural features of the MT phenomenon, Figures 5.16 and 5.17 present the same information as Figure 5.15, but with regard to the three³ nodes of the bottom left finite element mesh's element (see Figure 5.3) and the three upper nodes of the upper left element, respectively, as opposed to the entire specimen. Immediately, we may observe that the degree of phase transformation is indeed much more considerable in the nodes mainly exposed to a tensile loading scenario (bottom left element), which actually promotes the volumetric expansion required for MT. Accordingly, one may also observe that this more pronounced phase transformation, directly translates to an equally less pronounced increase of the local accumulated plastic slip, compared to that of the nodes enclosed in the upper left element. At the angular displacement $\theta \approx 116^\circ$, the material defined by the three bottom nodes becomes fully martensitic (as shown in both Figure 5.16 and by the specimen's global fully-martensitic volume fraction measure included in Figure 5.15) and the elastic domain is partially recovered. This is depicted by the sample's equivalent Cauchy stress, which promptly surpasses that of the equivalent analysis without MT, and from the overall moment curves. Once the elastic domain is recovered, several response mechanisms unfold. Firstly, one may observe that the onset of the recovered elastic domain is followed by the gradual decrease of the plastic strain rate (and consequent stabilisation of the accumulated plastic slip⁴) in the bottom face of the bending beam (three bottom nodes). Indeed, while transformation is immediately present in the initial stages of the deformation, in a local sense, so is plastic slip - recall that both mechanisms are heavily dependent on the crystallographic orientation. Furthermore, contrarily to MT, the material under plastic slip may eventually reach the transformation critical value, resulting in a simultaneous evolution of plasticity (in the austenite phase) and transformation until the fully martensitic configuration is locally attained and plastic slip can no longer exist (since the constitutive model does not encompass plasticity in the martensitic phase phase). From this point, the material behaves elastically and, thus, the evolution of this region until the conclusion of the prescribed displacement is rather clear.

On the other hand, the compressive region embodied by the three upper nodes of the upper left element seems to be greatly affected (albeit, not necessarily through a direct cause-effect relation) by the restored overall elastic behaviour and several unique observations can be made. In what respects the observed phase transformation, no significant

³ These three nodes allow us to effectively assess the two extremes (tensile and compressive deformation) of the material behaviour under the particular loading scenario at hand.

⁴ Note that the apparent slight decrease of the accumulated plastic slip is due to the extrapolation from the integration points to the considered nodes. What should be understood is that once the elastic domain is recovered and the local plastic strain rate begins to decrease until it actually becomes null, at which point the accumulated plastic slip remains constant for the remainder of the simulation.

differences are apparent, with MT progressing at a relatively constant rate. Meanwhile, the plastic behaviour increase considerably, with the accumulated plastic slip showing an exponential growth in the martensitic elastic domain interval. Moreover, at the later stages of the simulation, the equivalent Cauchy stress also abruptly increases in a similar fashion to the stress state increase in the bottom face of the beam once the elastic behaviour is initially restored, which explains the concurrent, subtle slope shift of the moment curves. However, this increase is much more assertive and, contrarily to the previous instant, does not match any noticeable achievement in what regards MT, which difficulties any attempt at establishing a conclusive correlation between the observable phenomena. In fact, it must be emphasised that, to some extent, these observations are accompanied by the development of rather unfeasible stresses within the tensile region of the bending beam (obtained due to the model's disregard of the martensite plastic behaviour), thus limiting the legitimacy of some of these observed behavioural features.

Nevertheless, a phenomenon that may shed some light on these events is the evolution of the beam's neutral axis throughout deformation. This aspect was already briefly addressed in our first discussion of the results from the analyses of the bending beam specimen (Section 5.2.1). However, when MT is involved, and, specifically, when the elastic domain is partially recovered up to the extent observed in our simulations, significant, counter-intuitive differences can be found. In this regard, Figure 5.18, presents the evolution of the position of the neutral axis along the beam's thickness by means of the axial Cauchy stress σ_{xx} captured from the left nodes of the five elements of the beam's left side - since this side of the beam is geometrically constrained to remain normal to the x axis, σ_{xx} constitutes an equivalent measure to the circumferential stress $\sigma_{\theta\theta}$ (more adequately associated with the assessment of the position of the neutral axis in curved beams). Each line in the aforementioned Figure corresponds to a specific angular displacement and a total of 80 evenly-spaced increments of the prescribed displacement are included (hence, 80 lines in each plot). Moreover, the line transparency aims to depict the evolution of this data over time, with increasing transparency translating to more advanced stages of the deformation.

In this Figure, the upper plot contains the evolution of the neutral axis in the analysis solely under plastic slip and the typical neutral axis' behaviour can be recognized. Indeed, as the deformation progresses, one may observe the gradual shift of the neutral axis' position towards the curvature center. Furthermore, this plot also allows us to distinguish the geometrical domains along the beam's thickness still elastically defined from those in which the austenite's yield stress has been surpassed and, thus, some degree of plastic deformation is necessarily present. Initially, the beam is practically straight and, thus, the stress distribution is mostly linear along its thickness; however, as deformation advances and plastic slip inevitably occurs, this linear evolution becomes confined to the beam's domain not yet plastically affected. Note as well that the observed dislocation of the neutral axis would eventually lead to the typical elastic, curved beam hyperbolic stress distribution, had plastic deformation been neglected.

In turn, the bottom plot of the aforementioned Figure depicts the evolution of the neu-

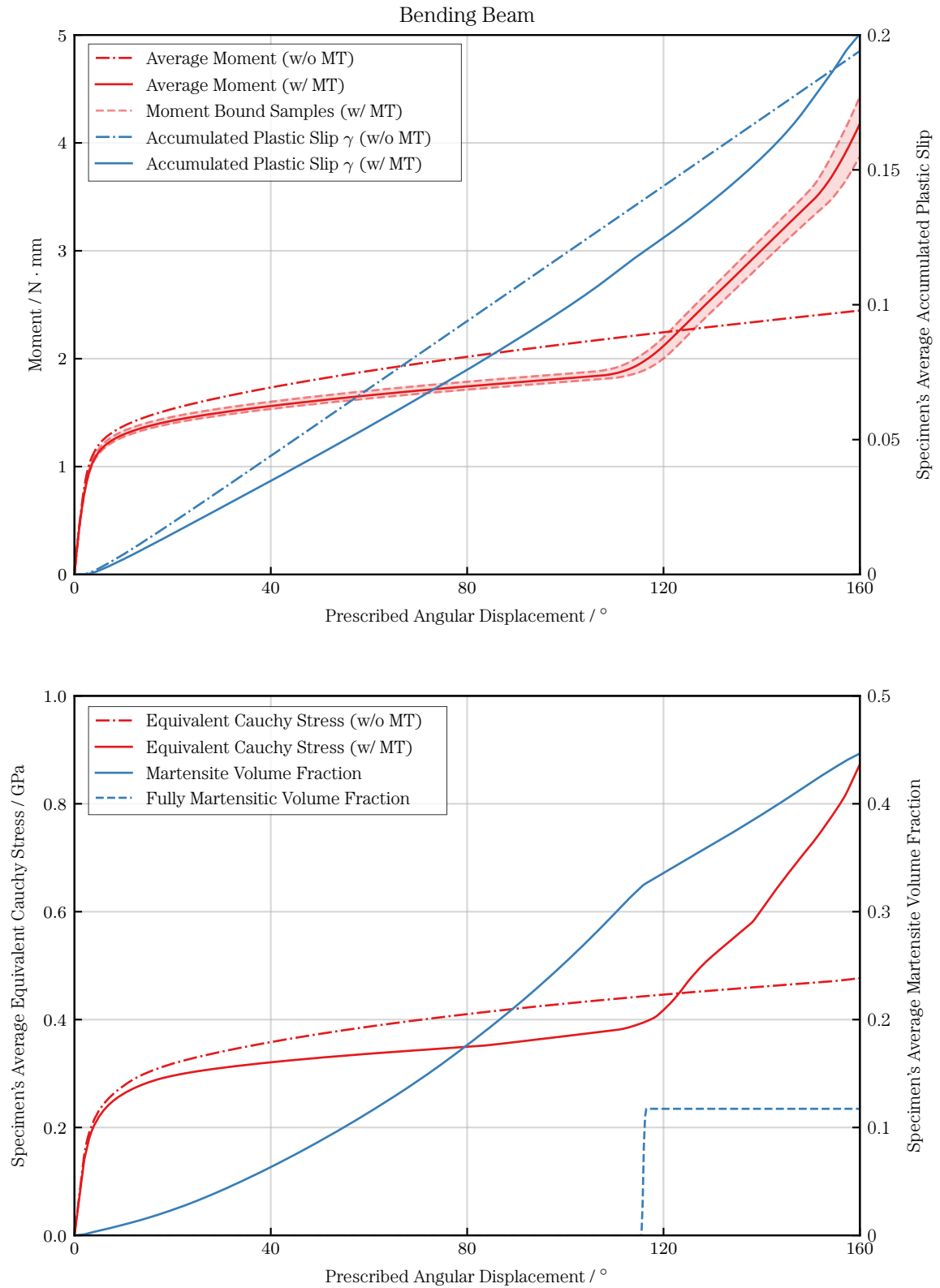


Figure 5.15: Evolution of set's average moment curve and corresponding bottom and upper bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction from the bending beam analyses without and with martensitic transformation.

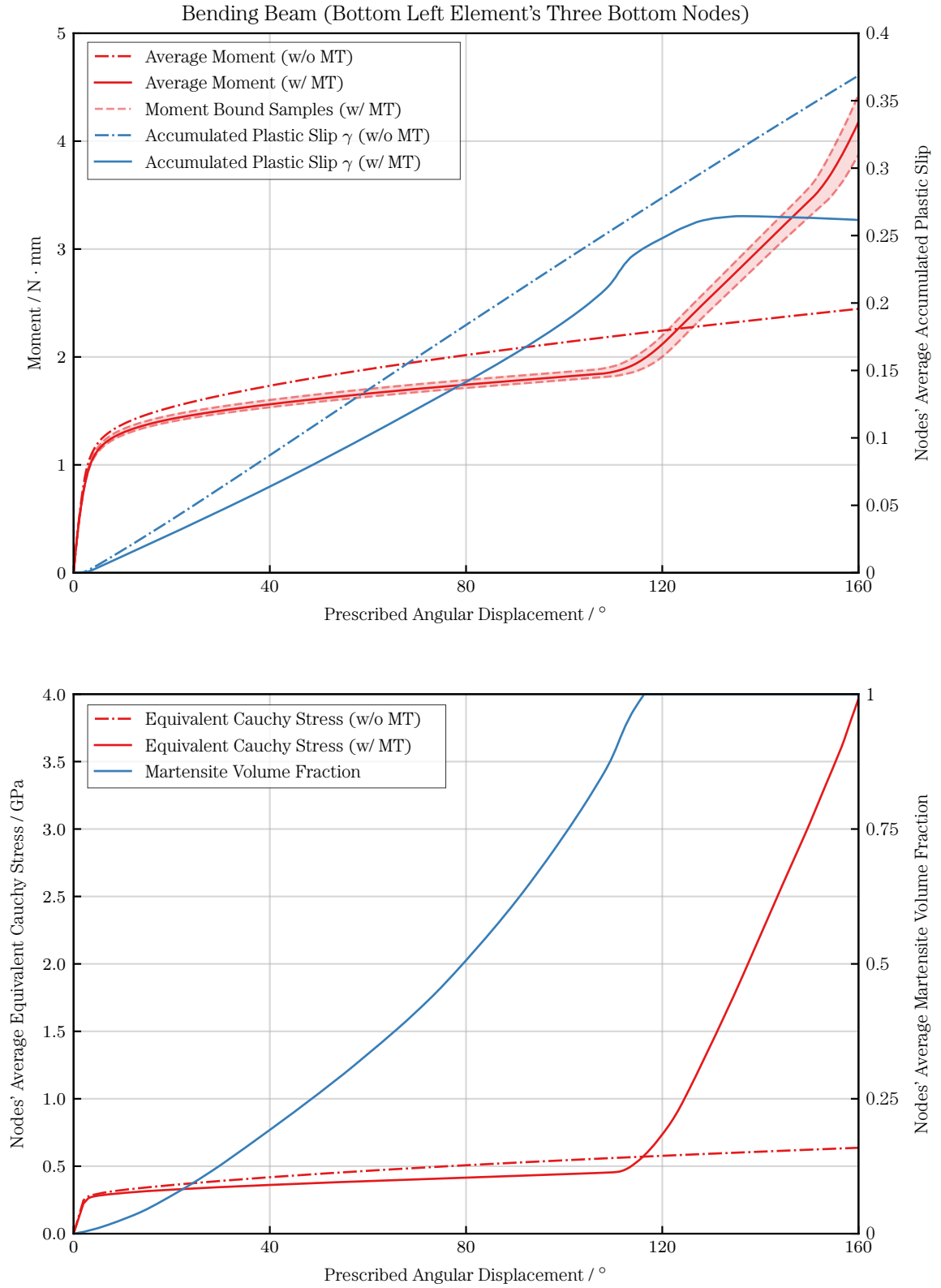


Figure 5.16: Evolution of set's average moment curve and corresponding bottom and upper bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction from the bottom left element's three bottom nodes without and with martensitic transformation.

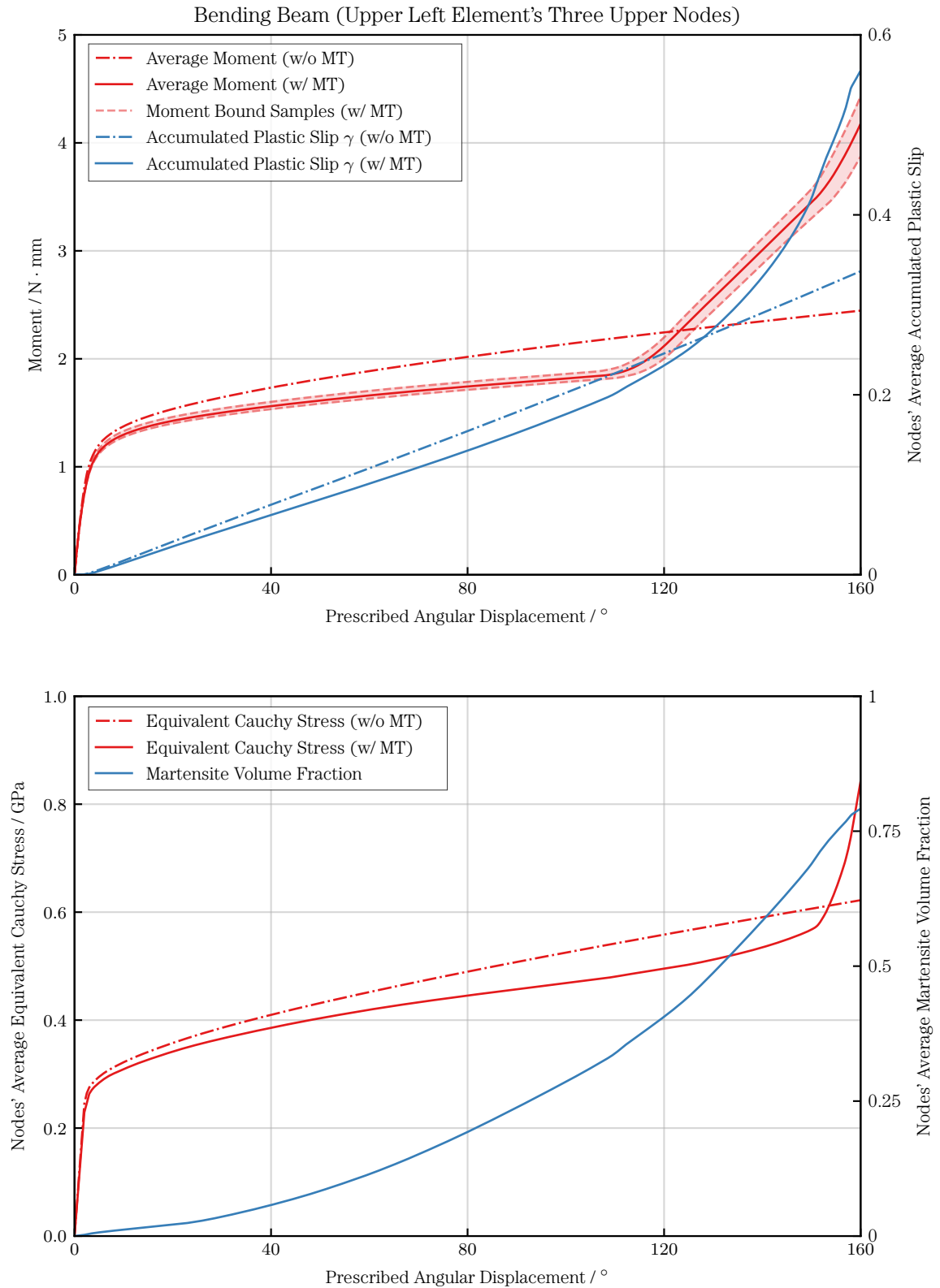


Figure 5.17: Evolution of set's average moment curve and corresponding bottom and upper bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction from the upper left element's three upper nodes without and with martensitic transformation.

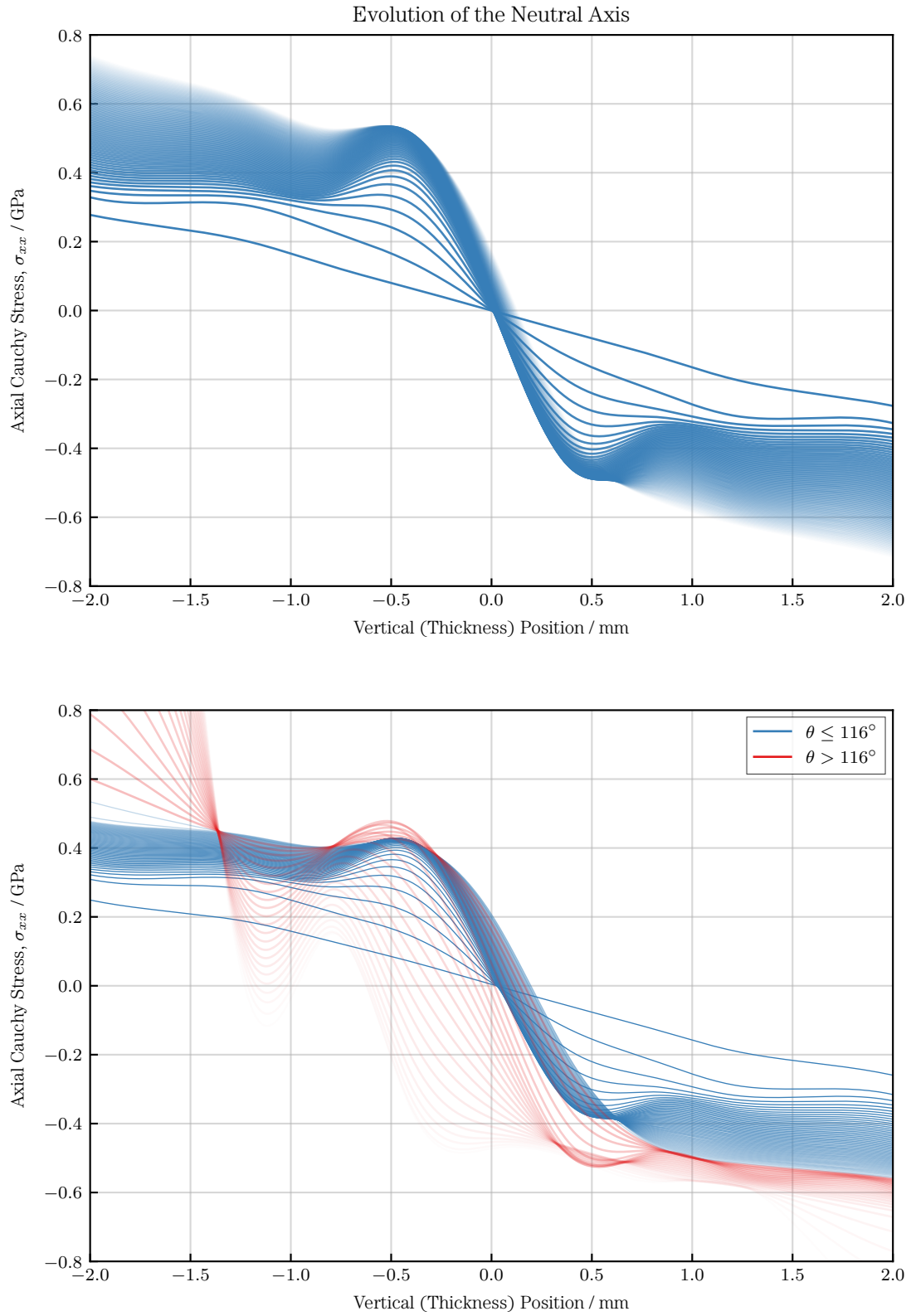


Figure 5.18: Evolution of the vertical position of the bending beam's neutral axis during deformation.

tral axis in the analyses where MT is admitted. In this case, two main differences can be immediately outlined. Firstly, and perhaps not as conspicuous, the momentarily larger shift of the position of the neutral axis towards the compressive side (curvature center) must be remarked. Indeed, in the analysis solely under plastic slip, both halves of the beam depict axial Cauchy stress distributions of mostly the same magnitude. Nevertheless, the equivalent Cauchy stress is slightly more pronounced in the compressive side, which is tied to the equally slight movement of the neutral axis. On the contrary, in the analysis in which MT is admitted, prior to the partial return of the overall elastic behaviour, both the axial and the equivalent Cauchy stresses become increasingly more pronounced in the compressive side of the beam throughout the course of the prescribed displacement, which explains the larger movement of the neutral axis in these circumstances. Subsequently, the recovered elastic behaviour aligns with the gradual reversal of the neutral axis' position towards not only the centroid of the beam's cross section, but far beyond it, into the region subjected to the tensile load. This behaviour is depicted by the red lines in Figure 5.18, which also provide a sense of the sheer increase of the stress state in the tensile region from the instant the bottom face of the beam becomes fully martensitic. In fact, the correspondence between these overwhelming stresses and the counter-intuitive shift of the neutral axis in the opposite direction to the center of curvature is difficult to overlook. To some degree, the resulting stress distribution resembles the hyperbolic distribution typically observed in the bending load of elastic, curved beams. Evidently, in such distribution the neutral axis is within the geometrical domain initially subjected to compression, which is not the case of the presented results. Moreover, the material at hand is obviously not restricted to elastic behaviour; however, the single recovery of the elastic domain in the bottom half of the beam, and the consequent increase of the respective stresses seems to artificially impose the transfer of the neutral axis to the vicinity of this region. Notably, at the final stages of the simulation, the neutral axis slowly converges to the interface delimiting the outer, plastically deformed tensile region and the central region still within the elastic domain. Simultaneously, the stresses in the former only continue to rapidly increase, as one would expect since it is elastically deforming. With this in mind, it becomes clear that in order for the static balance to be maintained (in detail, for the sum of normal forces acting on the section defined by the neutral axis to be null and the moment associated with these forces to be equal to the applied bending moment), stresses at the opposite end of the cross section (in this case, the upper face of the beam, subjected to compressive loads) must necessarily also rapidly increase. This can be easily observed in the bottom plot of Figure 5.17. The rapid increase of the strain rate in the compressive region can also be explained by this phenomenon.

Lastly, it must be emphasised that, while to some extent this mechanism may indeed be observed and is well-founded, the degree to which we are discussing it is simply a product of our disregard for plastic slip in the martensitic phase and, as a result, simply a hypothetical scenario. Nevertheless, these observations are of incredible interest and must be discussed to fully understand the computed material response. For the sake of completeness, Figure

5.19 presents the distributions of the accumulated plastic slip and volume fraction of the martensitic phase associated with the sample considered in this discussion.

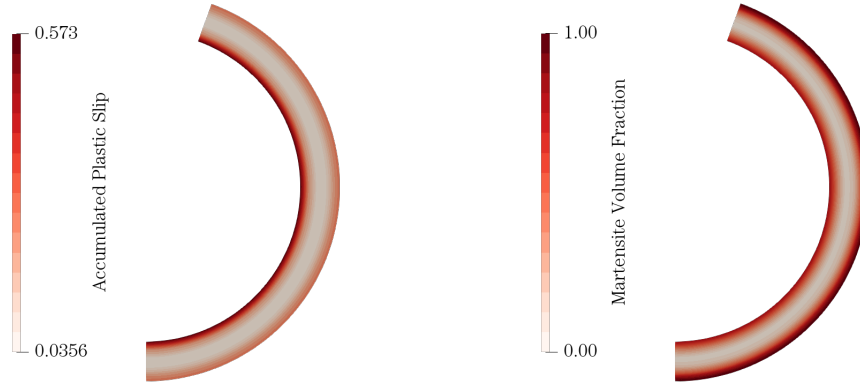


Figure 5.19: Contour plots of the homogenised accumulated plastic slip γ and martensite volume fraction obtained from the analysis of the bending beam specimen with MT, at the final angular displacement of 160° and for an RVE containing 200 grains.

5.3.2 Double-Notched and Butterfly Specimens

The plots of the set's average reaction curve and corresponding bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction of the analyses of double-notched and butterfly specimens are presented in Figures 5.20 and 5.21, respectively. As most relevant details involved in the coupling of plastic slip and MT phenomenon were already presented and discussed in the analysis of the bending beam specimen, and since both double-notched and butterfly specimens are subjected to shear-dominant loading scenarios, it is opportune to address these results at once. In addition, as we will observe, both cases depict similar MT evolutions and resulting effects. Indeed, relatively to the bending beam case, the MT onset is slightly delayed, which can be attributed to the larger imposed critical transformation energy barrier, ΔG_{mech} . In fact, in both cases, martensitic transformation is only firstly observed when already within the plastic domain, meaning that, in a general sense, the yield stress value is reached first and the resulting yield plateau remains identical to that of the corresponding analyses in which MT is not admitted. Accordingly, the accumulated plastic slip observed in the early stages of the simulations are also identical, regardless of the constitutive model. Since the material is not modelled under perfect plasticity (hardening is admitted), the stress levels continue to escalate as plastic deformation evolves. Accordingly, the transformation stresses (projection of the stresses in the transformation systems) also increase until they eventually reach the transformation critical value, which leads to the increase of MT. As we initially reported, in Section 1.2.3, a possible explanation for this type of martensitic nucleation could be the austenite's plastic slip and resulting shear band intersections; however, such mechanism is not captured by the adopted constitutive model, such that, in these circumstances, the main promoter of

MT is indeed the eventual reach of the required mechanical energy, made possible by the hardening phenomenon.

Contrarily to the results from the bending beam specimen, in which the MT-related partial recovery of the elastic domain and consequent increase of the reaction force and stresses happened very quickly, in both the double-notched and butterfly results, these quantities increase in a much more gradual manner and not in the precise instant a region of the specimen becomes fully martensitic. This may be due to the loading scenario in each case. Indeed, in the bending beam, a significant portion of the specimen's domain is driven by a tensile loading, which promotes MT. This, coupled with the fact that the corresponding transformation begins prior to plastic slip, and, thus, at a constant stress level (perfect transformation) explains why the stresses only begin to increase once transformation ceases. Meanwhile, both the double-notched and butterfly specimens contain the onset of MT after the plastic yield stress has already been reached, which, coupled with the shear-dominant loading scenarios, results in a much more complex coupling of phenomena.

Lastly, it may also be observed (in these two sets of results, but also in the previous plots associated with the bending beam problem, albeit not previously referred in its discussion) that, while initially the presence of MT leads to the decrease of the plastic strain rate and, consequently, to a less pronounced homogenised accumulated plastic slip, eventually, the accumulated plastic slip developed in parallel with MT actually becomes superior than that exhibited in the results associated with analyses in which MT is not admitted. This could be explained by the inherent volumetric growth of the material during transformation - caused by crystallographic differences between the austenite and martensitic phases (Fahr, 1971) - which must then be accommodated by the surrounding parent matrix through the development of dislocations and subsequent local surpassing of austenite's yield stress (hence the often used, and equally valid, *transformation-induced plasticity* designation). However, due to use of the first-order homogenisation scheme and the previously introduced algorithmic simplification, this is again not the case and is simply a numerical artifact. In detail, this arises from the admitted slip plasticity flow rule (expression 4.3.22), in which with the approach of the fully-martensitic configuration, ξ^a decreases and, consequently, $\dot{\gamma}^a$ must increase in order to maintain the same level of plastic deformation. This detail renders the illusion of a larger amount of plastic deformation, but is simply the product of how these mechanics are formulated in the considered constitutive model.

For reference, Figures 5.22 and 5.23 present the distributions of the accumulated plastic slip and martensite volume fraction obtained from the analyses of the respective samples considered in this discussion.

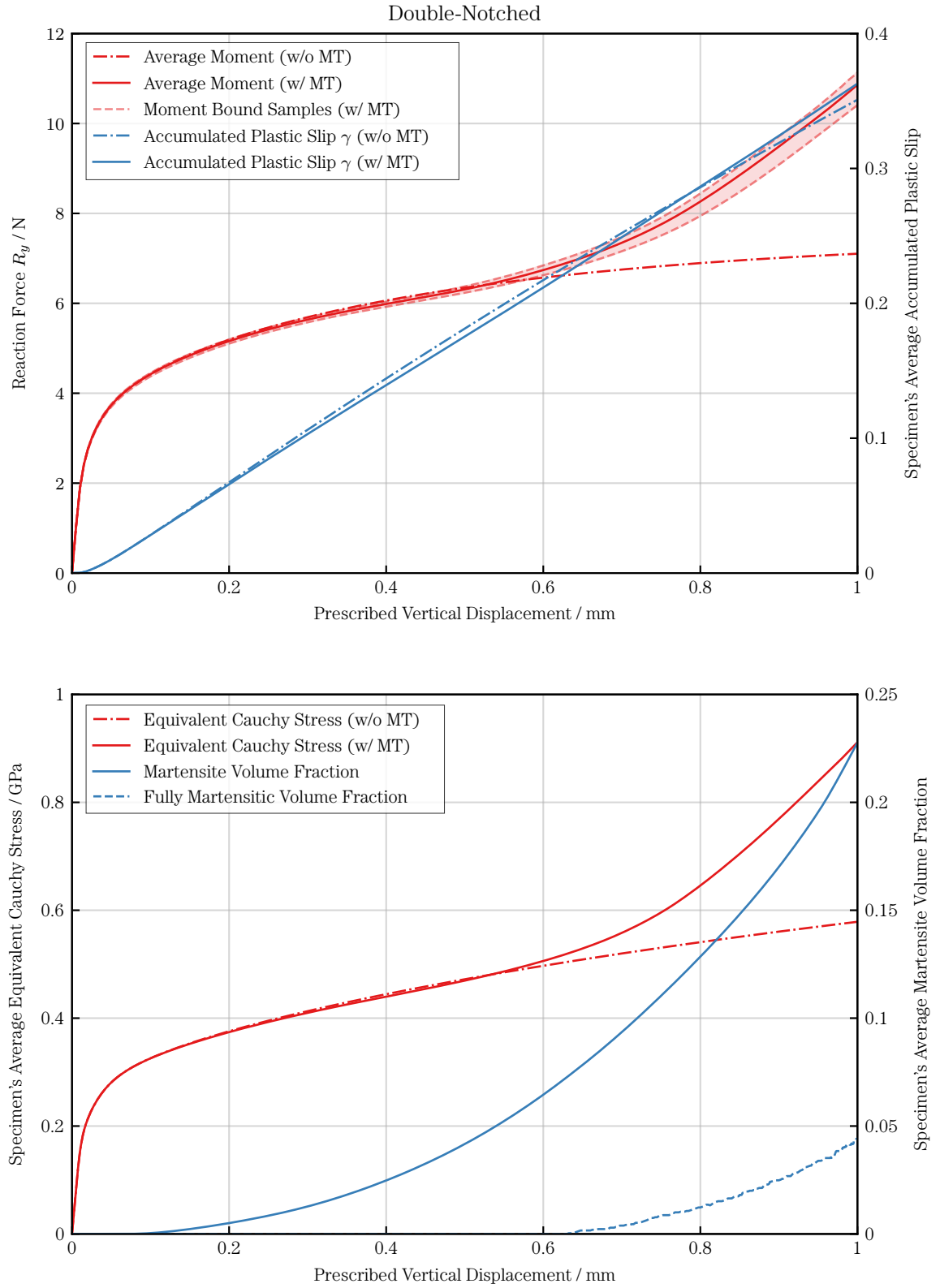


Figure 5.20: Evolution of set's average moment curve and corresponding bottom and upper bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction from the double-notched analyses without and with martensitic transformation.

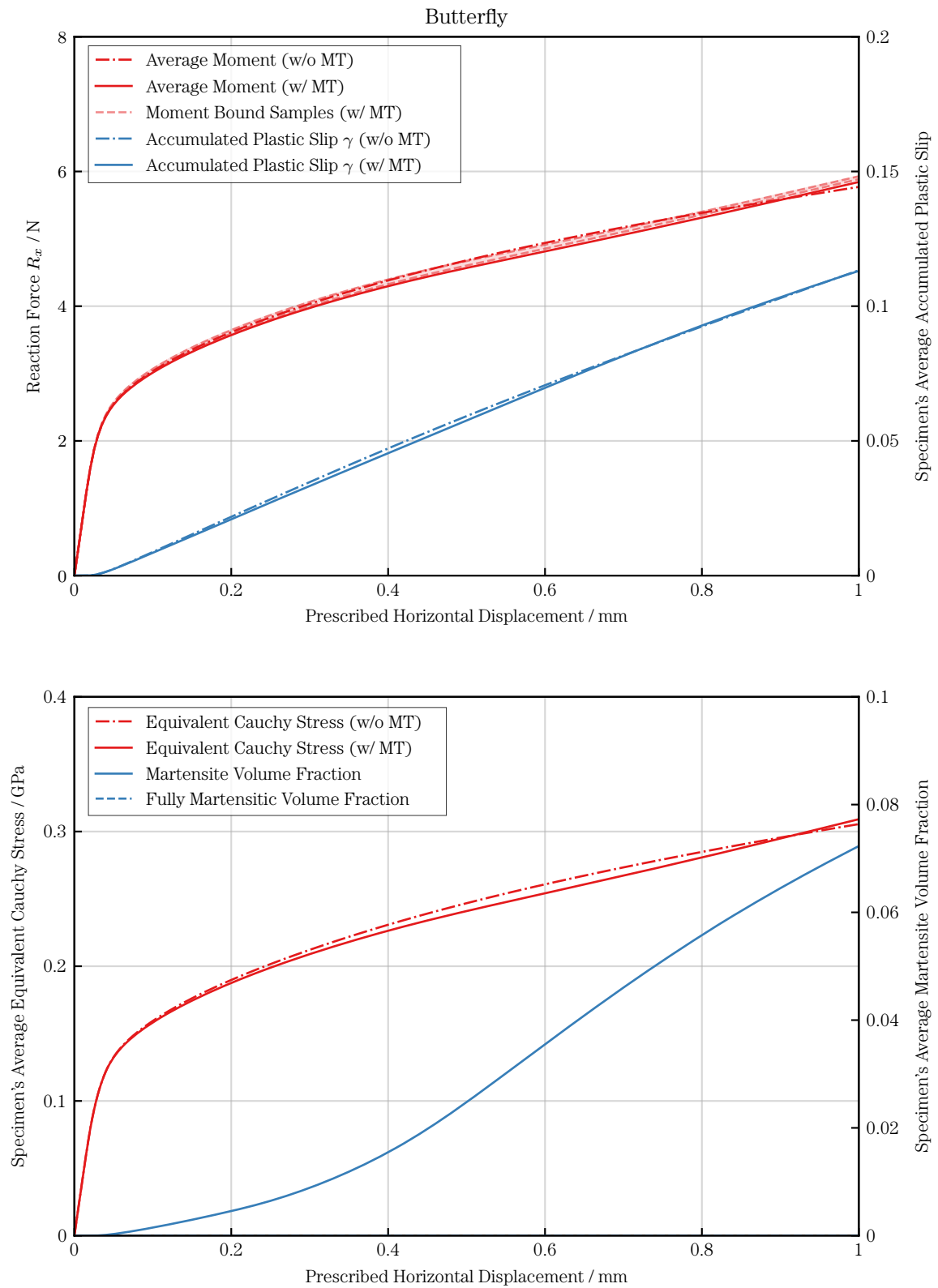


Figure 5.21: Evolution of set's average moment curve and corresponding bottom and upper bounds, equivalent Cauchy stress, accumulated plastic slip and martensite volume fraction from the butterfly analyses without and with martensitic transformation.

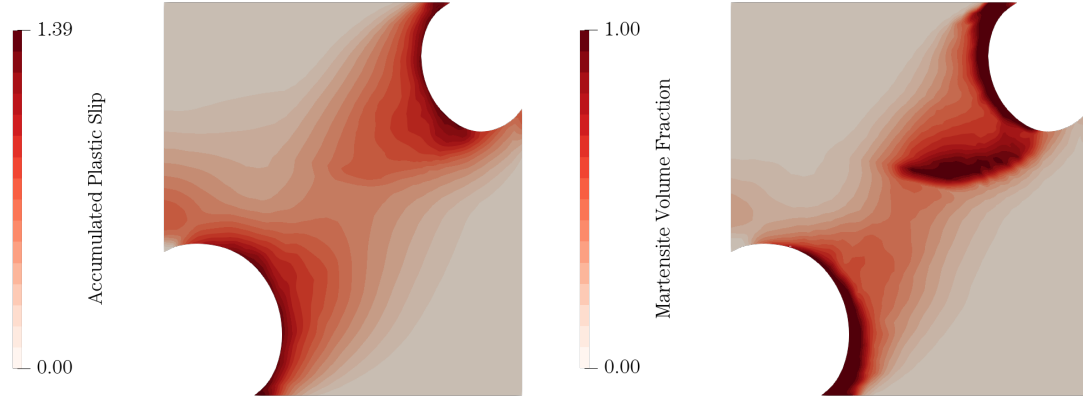


Figure 5.22: Contour plots of the homogenised accumulated plastic slip γ and martensite volume fraction obtained from the analysis of the double-notched specimen with MT, at the final vertical displacement of 1 mm and for an RVE containing 200 grains.

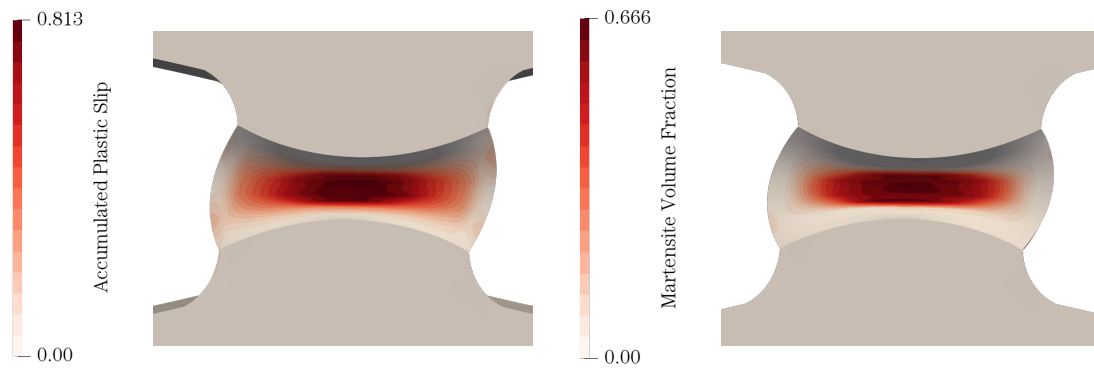


Figure 5.23: Contour plots of the homogenised accumulated plastic slip γ and martensite volume fraction obtained from the analysis of the butterfly specimen with MT, at the final horizontal displacement of 1 mm and for an RVE containing 200 grains.

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6

Micro-Scale Comparison Between First and Second-Order Homogenisation and Influence on Martensitic Transformation

In the previous Chapter, we thoroughly studied the effects from MT on the overall material behaviour by means of multi-scale analyses of different macroscopic specimens, subjected to distinct loading scenarios, and under a first-order homogenisation scheme, in which the Taylor's boundary condition was considered for the micro-scale equilibrium problem. Admittedly, until this point, second-order homogenisation and its eventual impact on the characterisation of MT has been mostly overlooked. This analysis is the focal point of the present Chapter. Following the selection of the RVE size also performed in Chapter 5, the ensuing Sections are dedicated to the micro-scale analyses of RVEs subjected to the local histories of the first and second deformation gradients at the selected points of interest, under both the first-order homogenisation scheme, with the standard periodic boundary condition (see Section 3.3.4), and the second-order homogenisation approach, with the multi-scale virtual power-based periodic constraint (Section 3.4.3), having multiple RVE lengths been considered for the latter. Comparing the results obtained with each homogenisation scheme, we expect to assess the relative importance of each of the macroscopic deformation gradients and of the RVE length in the mechanically-induced MT phenomenon at the micro-scale. The main steps involved in this second stage of numerical analyses are schematically presented in Figure 6.1.

6.1 Selection of the Macroscopic Interest Points

In order to properly assess the eventual importance of each of the macroscopic deformation gradients and, as such, the importance of the second-order homogenisation scheme on the micro-scale characterisation of the mechanically-induced MT, an adequate range of

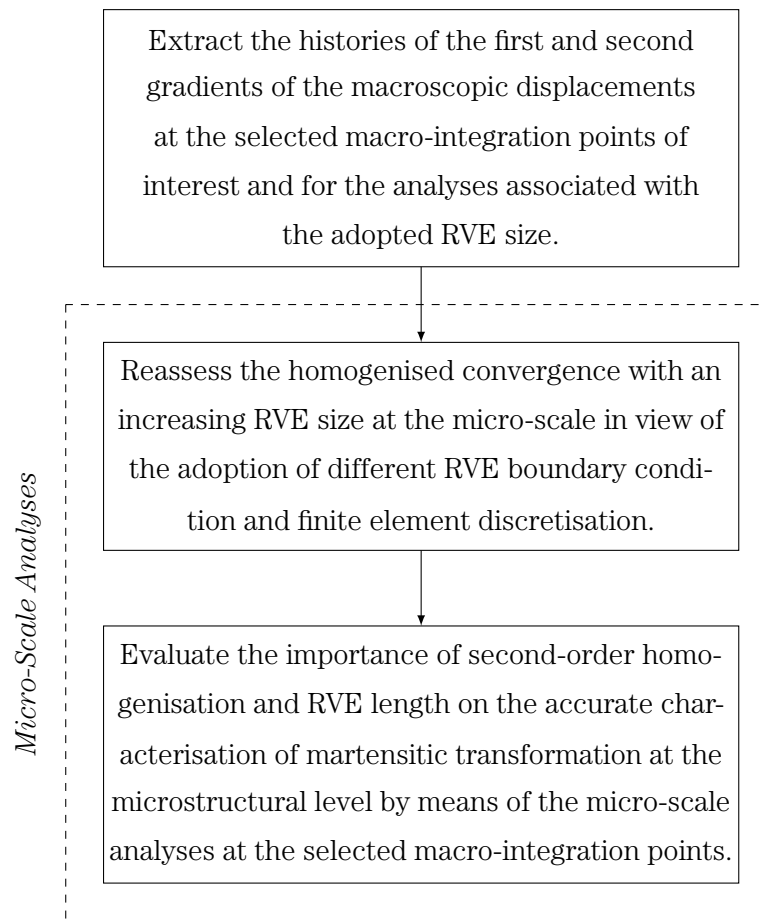


Figure 6.1: Schematic representation detailing the steps that outline the stage of the micro-scale analyses.

first and second deformation gradients must be thoughtfully selected. This selection is thus based on two main macroscopic strain measures: (i) the equivalent strain provides an analogous measure to the deformation gradient, $\mathbf{F}$, while (ii) the norm of the second gradient of the displacements, $\|\mathbf{G}\|$, numerically computed through the second derivatives of the shape functions (recall equation 5.1.3), allows a quantitative estimate of the magnitude of second-order deformation modes. In this context, the macroscopic distributions of the equivalent strain and of the norm of the second gradient of the displacements of the bending beam at the angular displacement $\theta = 160^\circ$ are presented in Figure 6.2 and the selected macro-integration points are schematically shown in Figure 6.3. Immediately, we may infer that a significant magnitude of first-order deformation is present in Point A, while, in Point B, located within the upward vicinity of the beam's neutral axis, first-order deformation modes are much more inferior, which leads us to assume that the microstructural response in Point B should, under the second-order homogenisation scheme, and compared to that from Point A, be more affected by the second gradient of the displacements. In this context, Table 6.1 compiles the norms of the first and second gradients of the macroscopic displacements captured at the four selected interest points from both the bending beam and double-notched specimens. It should be noted that the first gradient of the macroscopic displacements is indeed far inferior in Point B, while the second gradient is virtually identical. In fact, in the latter, the second gradient is much more significant, which leads us to assume that the corresponding micro-scale response is mostly governed by second-order deformation modes. As for the double-notched specimen, the respective macroscopic distributions of the equivalent strain and norm of the second gradient at the final vertical displacement $u_2 = 1.0$ mm are presented in Figure 6.4, along with the selected points of interest, C and D. This selection followed basically the same criterion as the bending beam; indeed, we may notice that in Point C the first-order deformation component is more dominant, while, similarly to Point B, albeit to a much shorter extent (due to the significantly larger magnitude of the first-order deformation) Point D is also governed by second-order deformation modes.

Table 6.1: Computed norms of the first and second gradients of the macroscopic displacements in each of the four selected points of interest.

	$\ \mathbf{F} - \mathbf{I}\ = \ \nabla \mathbf{u}\ $	$\ \mathbf{G}\ $	$\ \mathbf{G}\ / \ \nabla \mathbf{u}\ $
Point A	0.1534	0.1177	0.7673
Point B	0.0168	0.1098	6.5186
Point C	0.2882	0.0363	0.1260
Point D	0.5937	0.7834	1.3194

Having selected the relevant points of interest, we may now advance to the micro-scale analyses with the corresponding histories of the macroscopic deformation gradients. Performing these analyses with both first and second-order homogenisation schemes, and comparing the obtained results, we expect to further our understanding of how the macroscopic deformation impacts the martensitic phase transformation. Lastly, it should be emphasised

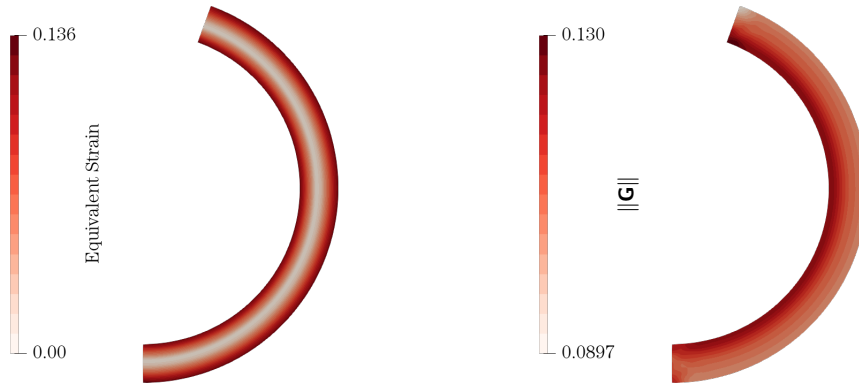


Figure 6.2: Contour plots of the equivalent strain and norm of the second gradient of the displacements of the bending beam at the final angular displacement of 160° and for a RVE containing 200 grains.

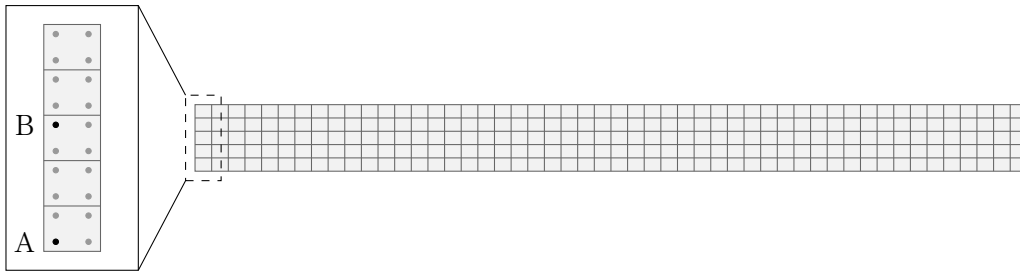


Figure 6.3: Schematic representation of macro-integration points of the bending beam, A and B, selected for the micro-scale analyses.

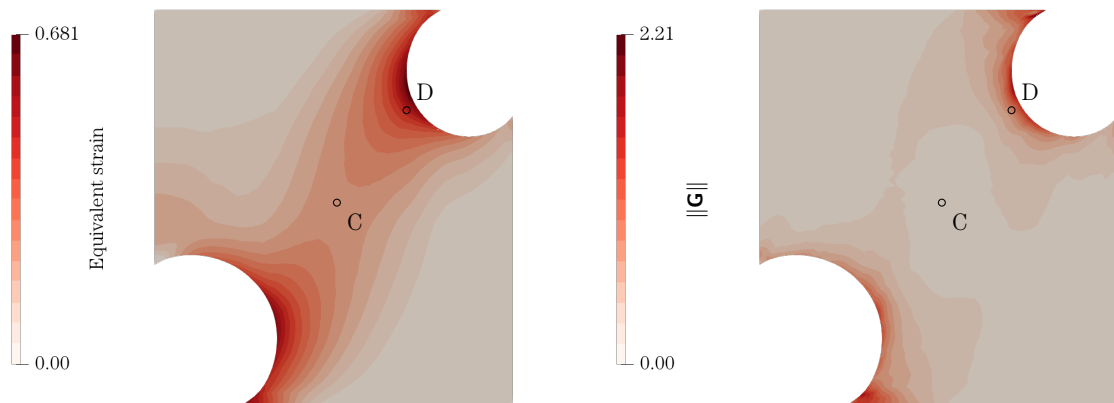


Figure 6.4: Contour plots of the equivalent strain and norm of the second gradient of the displacements of the double-notched specimen at the final vertical displacement $u_2 = 1.0$ mm and for a RVE containing 200 grains; points C and D denote the macro-integration points selected for the micro-scale analyses.

that no micro-scale studies concerning the butterfly specimen are going to be performed in the present Chapter, as they would entail unreasonable computing cost and time. The shear-dominant problem is still adequately assessed with the double-notched specimen. Furthermore, both the beam and double-notched specimens allow to directly target the initially established goals and to perform rewarding, complementary studies in a feasible manner.

6.2 Convergence Analysis at the Micro-Scale

Following the steps outlined in Figure 6.1, and before proceeding to the discussion of the results obtained from the micro-scale analyses, we must re-evaluate the convergence with increasing RVE size of the homogenised micro-scale results associated with the selected points of interest, considering the adoption of both a different RVE boundary condition and finite element discretisation. The statistical convergence parameters are mostly identical to those presented in the initial convergence study, carried out in Chapter 5, with the only major difference being that these are now computed with respect to the norm of the homogenised first Piola-Kirchhoff stress tensor (more accurately, its integral with respect to the applied displacement, which we will denote as E_P), instead of the previously considered transferred energy to the specimen (work) - note that this measure was computed by means of the integral of the macroscopic reaction force or moment, which, in this case, where each micro-scale analysis relates to a single macro-integration point, is evidently not applicable. Furthermore, it must also be remarked that this study was, again, performed purely under a first-order homogenisation scheme without MT, albeit now admitting the standard periodic boundary condition. Indeed, had we considered the second-order homogenisation approach, these results and, as such, the convergence evaluation, would also depend on the selected RVE length (and not uniquely on the RVE size).

The convergence results obtained from the micro-scale analyses with the deformation histories of points A (bending beam) and C (double-notched specimen) are presented in Figure 6.5. As we may infer from the Table 6.1, among the selected points of interest, Points A and D suffer the most significant deformations in each of the respective specimens, therefore, these should constitute the pair under analysis and the eventual evidence of convergence in these points for a given RVE size would allow us to confidently assume that the results are equally or more consistent in the remaining macro-integration points, in this case, B and C. Indeed, Point A was selected for this study; however, Point D entails a particularly severe deformation, which lead to recurrent convergence problems in the corresponding micro-scale simulations, such that Point C was alternatively selected. From the aforementioned Figure, it can be observed that in both points, A and C, the homogenised micro-scale response is far more reliable than the macroscopic responses, previously addressed, regardless of the adopted RVE size. This detail was somewhat expected and can be mostly attributed to the adoption of the standard periodic boundary condition, which, as depicted in Figure 3.5, leads to a faster convergence of the homogenised quantities in comparison to other constraint models (recall that in Chapter 5 we adopted the Taylor bound-

ary condition). Given the practically insignificant magnitude of the computed coefficients of variation, and for the sake of consistency, we will once again admit a RVE containing 200 grains. Furthermore, this results also assure us that sufficiently reliable results can be expected from the analyses of Point D.

6.3 Micro-Scale Results at the Selected Points of Interest

In this Section, the results obtained from the micro-scale simulations of the adopted RVE subjected to the deformation histories collected from points A, B, C and D are presented. The employed RVE model is shown in Figure 6.6 and contains 200 grains discretised with 4770 6-noded triangular elements with reduced integration, which leads to a finite element mesh with a total of 9719 nodes. In order to enforce a periodic displacement fluctuation field on the boundary of RVEs with non-conform finite element meshes, such as the one depicted in the above-mentioned Figure, the *mortar method* is employed to enforce the periodicity constraint (for a detailed account on this issue, see Reis and Andrade Pires (2014)).

6.3.1 Beam Subjected to Bending Rotation

Each element from the macroscopic mesh of the beam specimen has an average length of 0.8 mm, meaning that integration point is associated with an area of approximately 0.4 mm^2 . Thus, to assess the influence of the RVE length, l_{RVE} , on the micro-scale results, three different lengths are considered for the micro-scale analyses under the second-order homogenisation scheme: (i) $l_{RVE} = 0.2 \text{ mm}$, (ii) $l_{RVE} = 0.4 \text{ mm}$, (iii) $l_{RVE} = 0.8 \text{ mm}$. Before proceeding, however, it must be understood that, in the standard second-order homogenisation scheme, the concept of RVE length is entirely independent from the generalised RVE size, which, in turn, is simply a measure of the number of micro-constituents included in the RVE model and, thus, translates to the representativeness of the RVE and consequent convergence of the homogenised results. In fact, the size effects captured by the second-order homogenisation approach are solely influenced by the RVE length, with the size of the micro-constituents bearing absolutely no impact on the computed homogenised response. In this context, the appropriate length of the RVE, intrinsically associated with the macroscopic characteristic length, is particularly important and must be carefully defined so to obtain a sensible non-local character of the macroscopic response.

The homogenised equivalent stress with respect to both angular displacement and homogenised equivalent strain and the norms of the homogenised first Piola-Kirchhoff stress tensor and homogenised higher-order stress tensor obtained from the analyses associated to the bending beam's Point A, under both homogenisation schemes and for all the aforementioned RVE lengths are presented in Figure 6.7. The contour plots of the equivalent Cauchy stress at Point A over the deformed RVEs, under the first-order homogenisation scheme and second-order homogenisation with different RVE lengths are shown in Figure 6.8, considering the case in which MT is not admitted. Following this framework, Figures

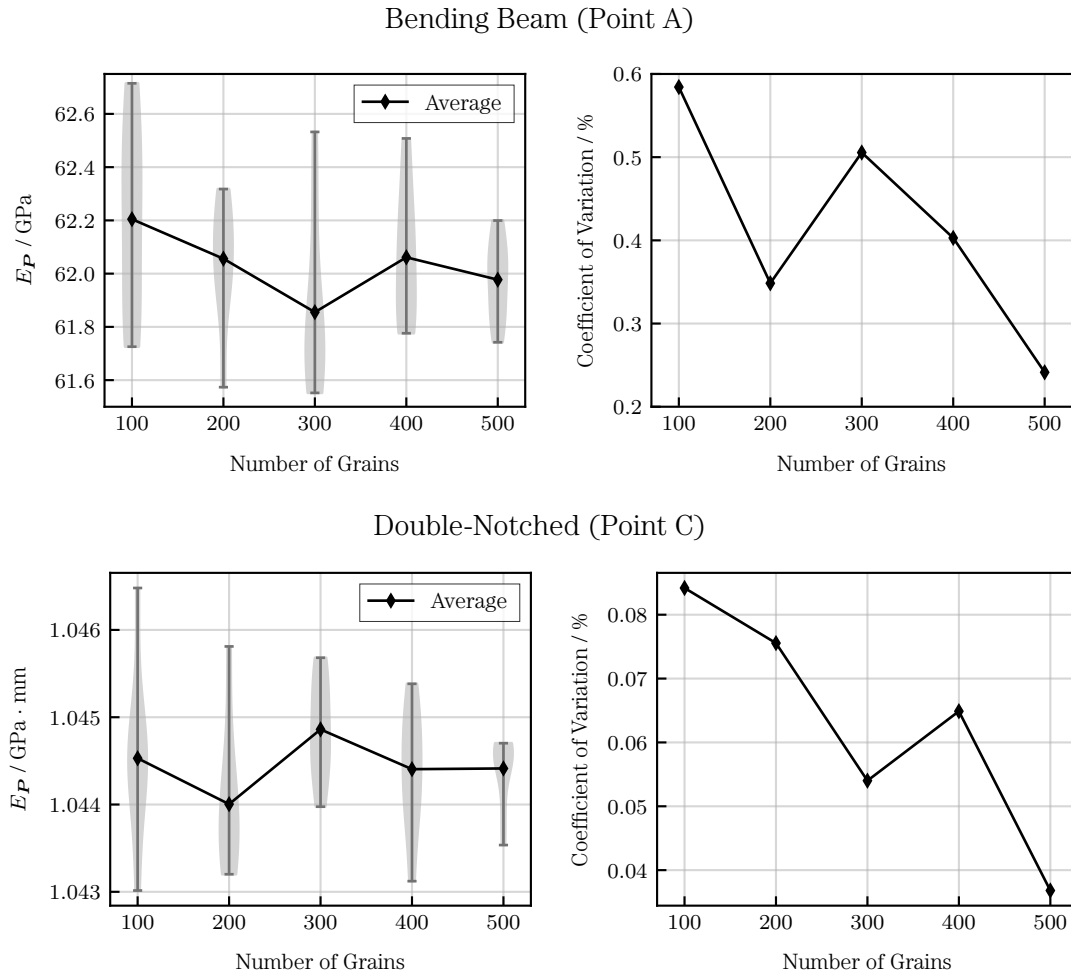


Figure 6.5: Convergence analysis with increasing RVE size of the homogenised response at the macro-integration points A (bending beam) and C (double-notched specimen): density distribution of the integral of the norm of the homogenised first Piola-Kirchhoff stress tensor with respect to the prescribed displacement (E_P) for each set and respective averages (left) and the corresponding coefficients of variation (right).

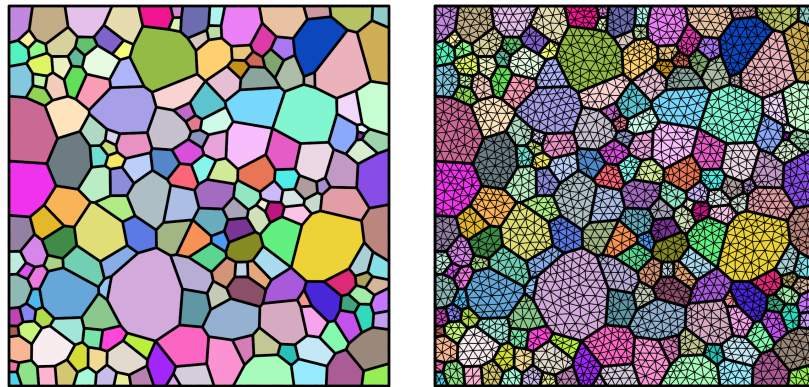


Figure 6.6: 2D representation of the RVE employed to model a polycrystalline microstructure containing 200 grains, generated with the open-source software package Neper (Quey et al., 2011).

6.9 and 6.10 display the contour plots of the equivalent Cauchy stress associated with the simulations performed under the assumption of MT and of the corresponding martensite phase volume fraction, respectively.

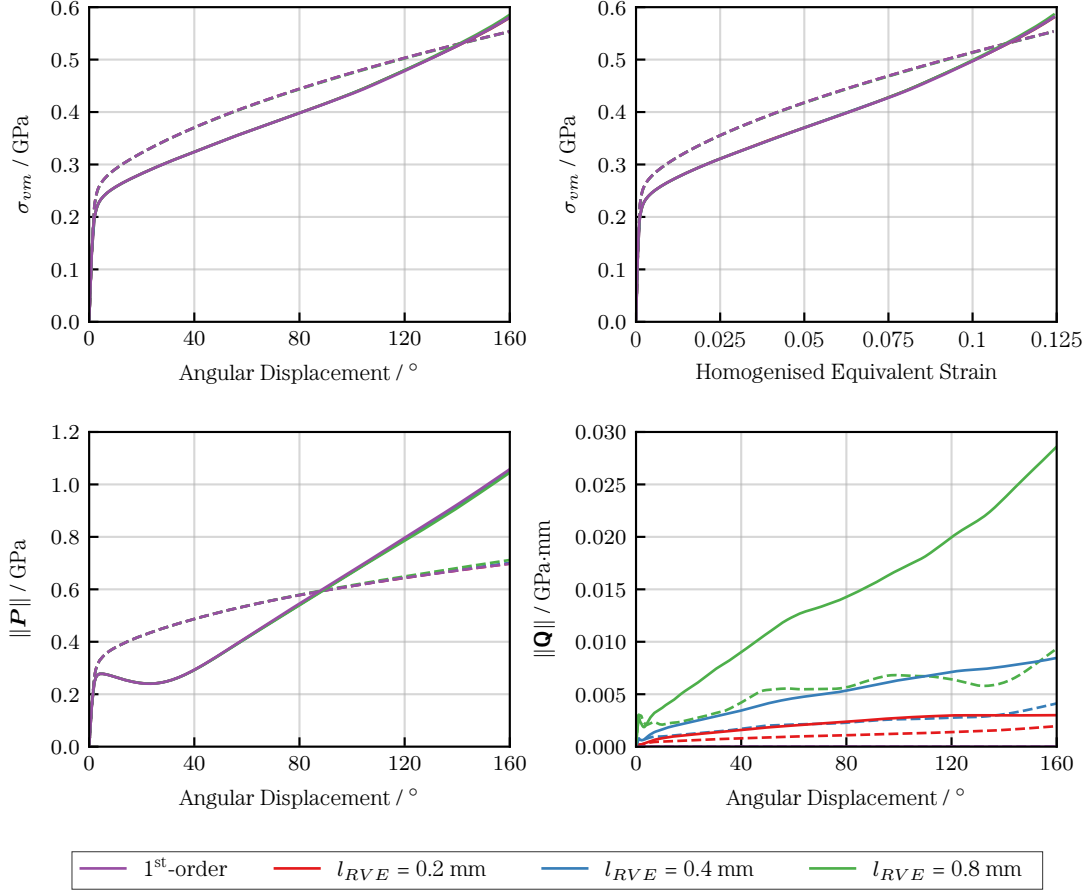


Figure 6.7: Evolution of the homogenised equivalent stress, norm of the homogenised first Piola-Kirchhoff stress tensor and norm of the homogenised higher-order stress tensor obtained from the RVEs subjected to the deformation history from Point A, without (dashed lines) and with (solid lines) mechanically-induced MT.

Moving on to the analyses associated with Point B, the corresponding homogenised equivalent stress with respect to both angular displacement and homogenised equivalent strain and the norms of the homogenised first Piola-Kirchhoff stress tensor and homogenised higher-order stress tensor are presented in Figure 6.11. Regarding the analyses without MT, the contour plots of the equivalent Cauchy stress at Point B are presented in Figure 6.12. For this Point in particular, Figure 6.13 is especially revealing, not only for the understading of the results displayed in Figure 6.11, with which the evolution of the position of the beam's neutral axis is intrinsically related, but also to trully grasp the difference between both homogenisation schemes and how it may impact the computed results. Regarding the analyses in which MT is admitted, Figures 6.14 and 6.15 present the contour plots of the equivalent Cauchy stress and corresponding martensite volume fraction, respectively, under both homogenisation schemes and distinct RVE lengths.

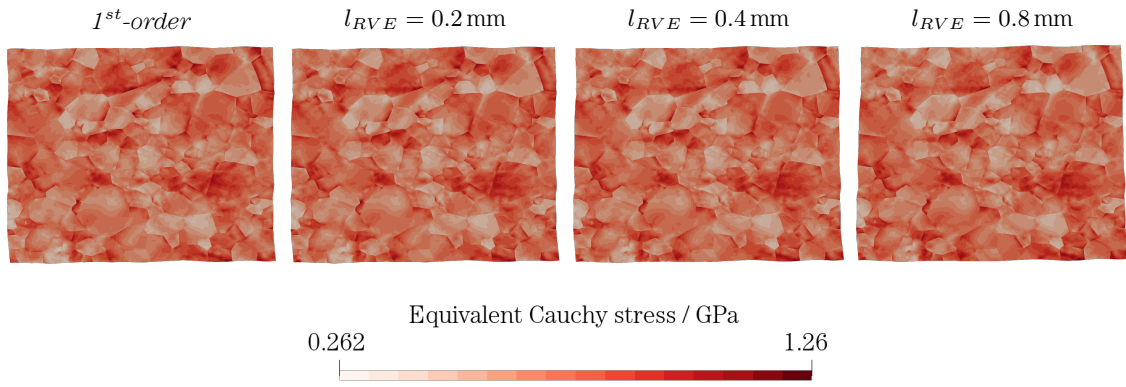


Figure 6.8: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point A, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° and for the analyses without MT.

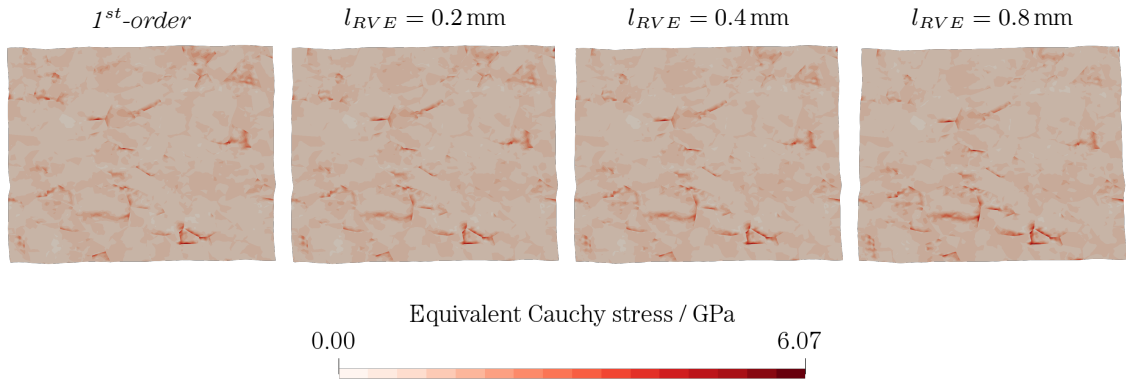


Figure 6.9: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point A, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° and for the analyses with MT.

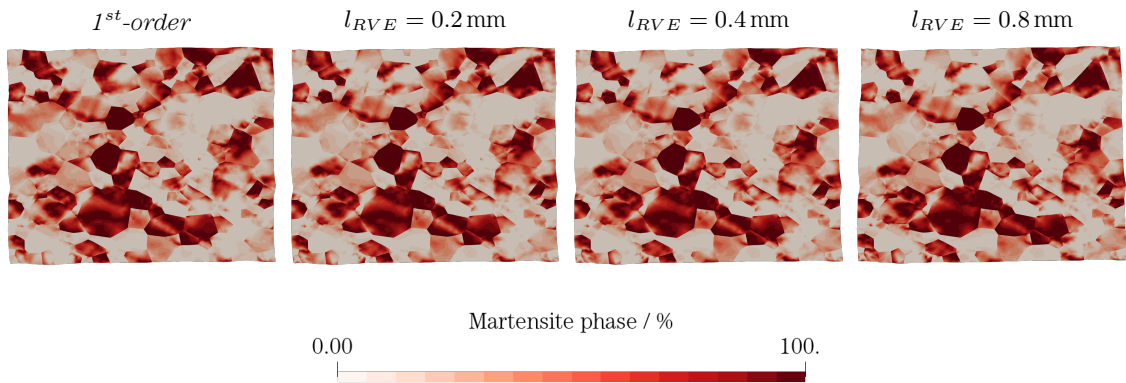


Figure 6.10: Distribution of the martensite volume fraction over the RVEs associated with the deformation history from Point A, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° .

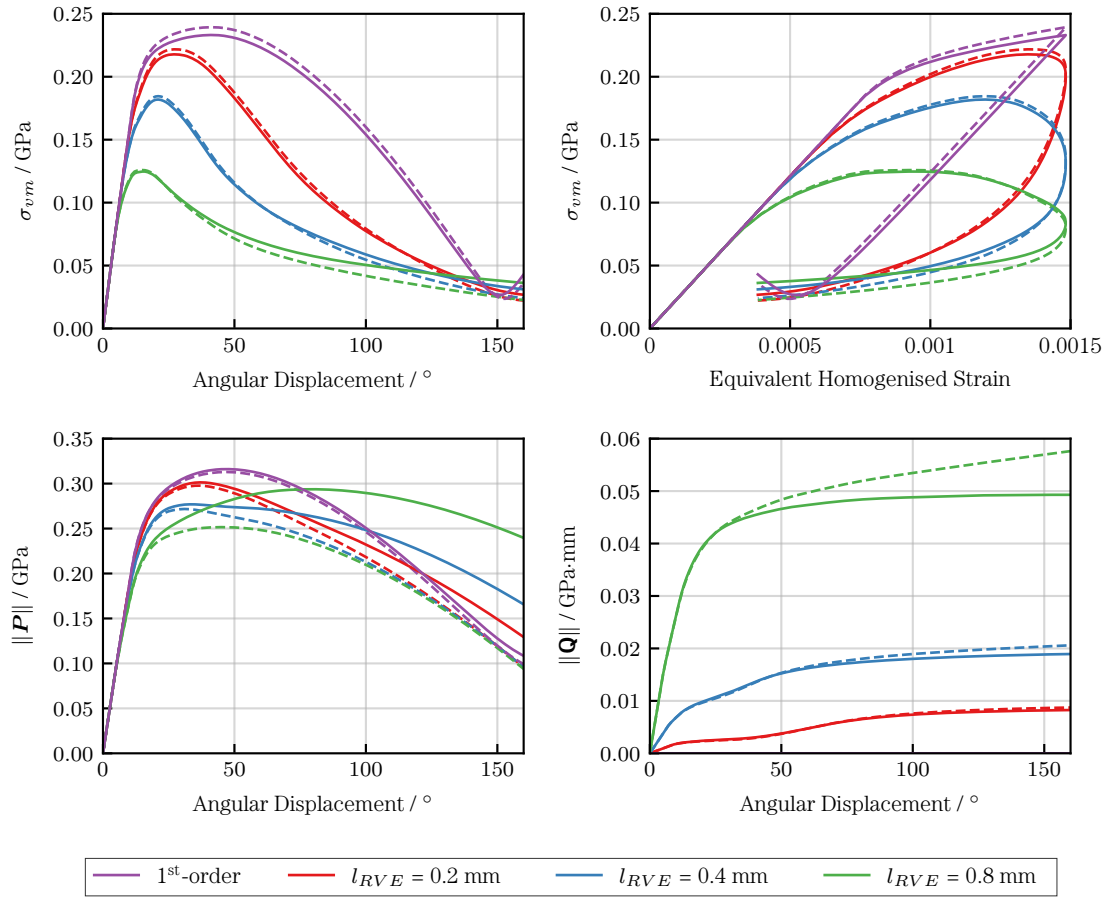


Figure 6.11: Evolution of the homogenised equivalent stress, norm of the homogenised first Piola-Kirchhoff stress tensor and norm of the homogenised higher-order stress tensor obtained from the RVEs subjected to the deformation history from Point B, without (dashed lines) and with (solid lines) mechanically-induced MT.

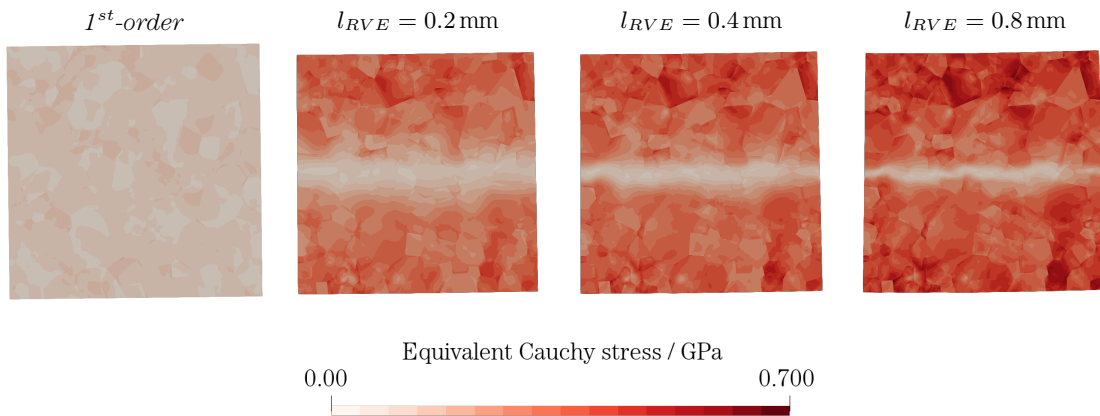


Figure 6.12: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point B, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° and for the analyses without MT.

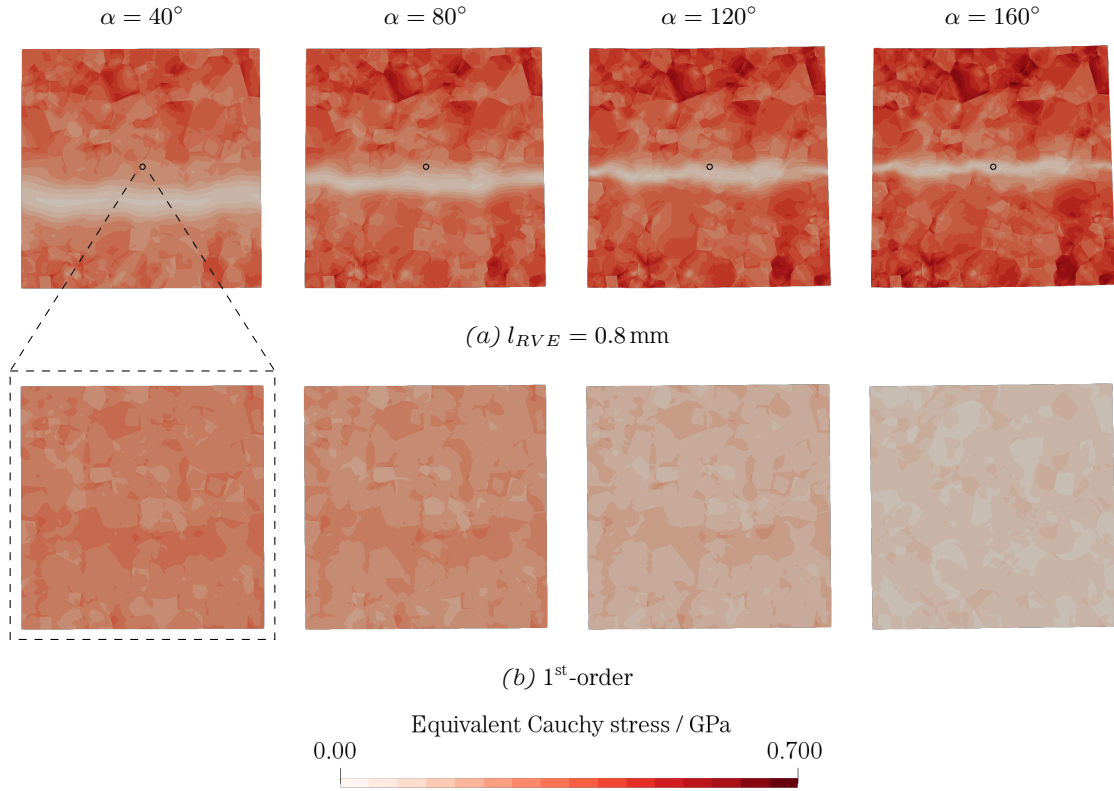


Figure 6.13: Evolution of the distribution of the equivalent Cauchy stress for an RVE length $l_{RVE} = 0.8 \text{ mm}$ associated with the deformation history from Point B, obtained from the analyses without MT.

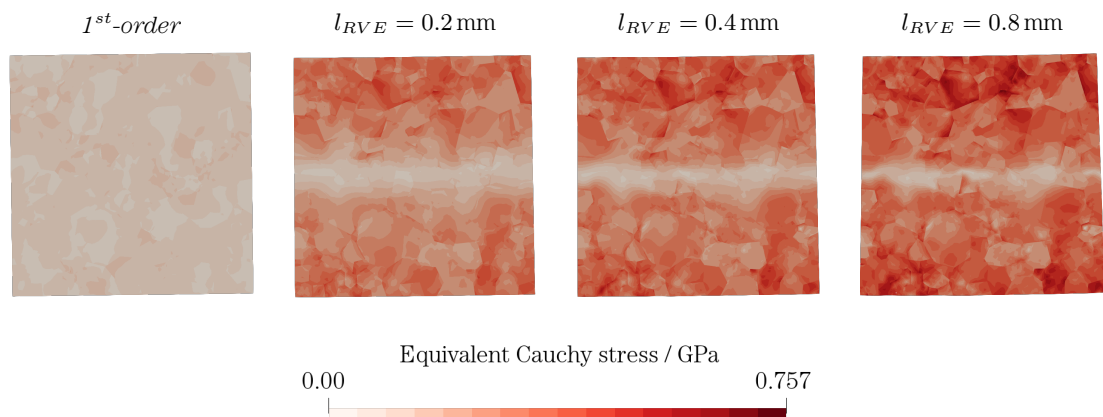


Figure 6.14: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point B, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° and for the analyses with MT.

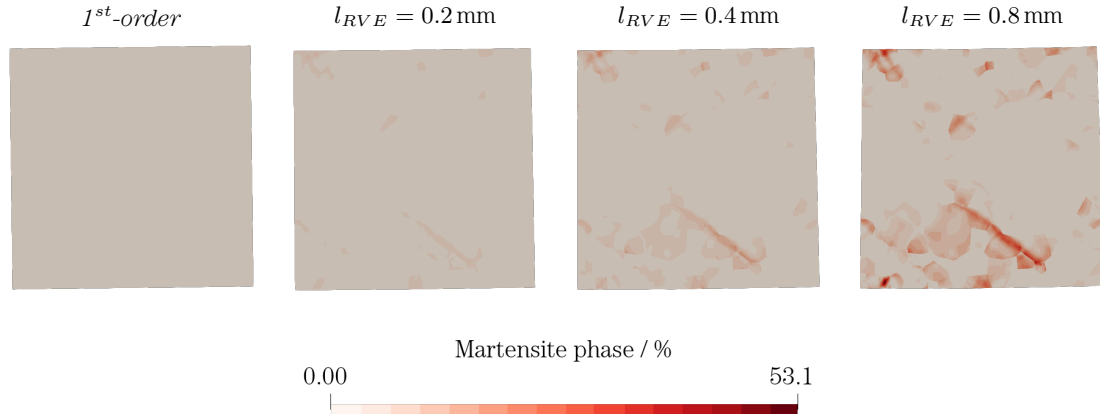


Figure 6.15: Distribution of the martensite volume fraction over the RVEs associated with the deformation history from Point B, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° .

Discussion of the Results

Regarding the bending beam problem, presented as a whole in Figures 6.2 and 6.3, two different points of interest were selected on the basis of the corresponding equivalent strain and second gradient of the macroscopic displacements, and examined under first-order and second-order homogenisation schemes, with several RVE lengths being considered for the latter. As shown in Figure 6.3, Point A is near the bottom face of the beam specimen, which, given the prescribed angular displacement, leads to it being located within the tensile region, where, as a result, the strain values are quite significant. On the other hand, Point B is located just slightly above the initial neutral axis of the undeformed beam. Due to the large curvatures involved in the prescribed bending motion, the neutral axis of the deformed beam is actually shifted upwards, in the direction of the curvature center and ceases to contain the center of gravity of the beam's cross section. For this reason, at the end of the angular displacement, Point B actually overlaps the final neutral axis, which explains its inferior strain, noticeable on the contour plot of the homogenised macroscopic equivalent strain in Figure 6.2 and sustained by the norm of the deformation gradient presented in Table 6.1. This phenomenon is particularly evident when comparing the micro-scale stress state at increasing macroscopic rotations (see Figure 6.13). Contrastingly, the second gradient magnitude is nearly constant on the entire beam at any stage of the deformation. Therefore, the response of the RVEs subjected to the deformation history from Point A is significantly more dominated by first-order deformation modes than those associated with the deformation history captured from Point B. In fact, evaluating the norms of the deformation gradient and second gradient quantitatively and computing the ratio between both, it becomes evident that the behaviour in Point B is heavily influenced by the second gradient of the displacements, $\mathbf{G}$, whereas in Point A the first deformation gradient is slightly more important.

Looking at the results related to Point A, we can observe that the response under the first-order homogenisation scheme is undistinguishable from those under second-order ho-

mogenisation for any of the considered RVE sizes. Still, if we look closely, we may notice that for the final angular displacement values the response of the RVE with $l_{RVE} = 0.8$ mm is just starting to diverge from the remaining ones. In addition, it is also worth noticing that the norm of higher-order stress tensor, $\|\mathbf{Q}\|$, increases with larger RVE lengths, that, for each length, the norm $\|\mathbf{Q}\|$ is higher for the RVE where MT is admitted, and that the discrepancy between the responses with and without MT for any given RVE length is far more pronounced for a larger l_{RVE} . This shows that, although for Point A the first deformation gradient is dominant and the impact of second-order homogenisation is seemingly insignificant, the second-order deformation modes are still being accounted for and its effect impacts the development of the martensite phase, even if minimally.

On the contrary, the homogenised response of the RVEs under the deformation history from Point B is strongly influenced by the adoption of the second-order homogenisation scheme and, consequently, by the chosen RVE length. This can be observed in the plots presented in Figure 6.11, as well as in the contour plots of the equivalent Cauchy stress shown in Figure 6.12. At first glance, two key comments can be made. Firstly, it is strikingly clear that an increase in the RVE length moves the response further away from the one obtained under first-order homogenisation. For this reason, this scheme may be regarded as the equivalent to the second-order homogenisation approach with an infinitesimal RVE length. This idea is schematically shown in Figure 6.13. Secondly, it is once again proven that the discrepancies on the overall homogenised responses between the analyses with and without MT increase for larger RVE lengths. Indeed, a larger l_{RVE} leads to a more accurate account of the second-order effects, which, in this case, imply a more advanced development of the martensite phase. However, it should be understood that the differences found in the martensite volume fraction between both homogenisation schemes do not necessarily result from the presence of second-order deformation modes in itself; rather, the second-order homogenisation scheme leads to a more detailed characterisation of the microstructural behaviour, which, in turn, may or may not favour phase-transformation. In this context, comparing the deformed state of the RVEs from Point B associated with first-order homogenisation and second-order homogenisation with $l_{RVE} = 0.8$ mm (presented in Figures 6.14 and 6.15), we can observe that the latter accurately depicts the tensile and compressive regions in the bottom and top halves of the RVE, respectively, which explains the slightly more pronounced martensite phase in the region below the beam's neutral axis (recall that MT is intrinsically related to the volumetric growth/expansion of the material, which is promoted by the nature of the displacements in this region).

Regarding the homogenised response properties depicted in Figure 6.11, it must be remarked that the difference between the results obtained with and without phase transformation is more nuanced than that of the analyses related to Point A, which is obviously due to the much more significant deformation gradient (of overall tensile nature) and consequently more advanced martensitic transformation found in the results from Point A. On this topic, it is worth pointing out the importance of evaluating not only the homogenised equivalent stress, but also the norm of the first Piola-Kirchhoff stress tensor, whose evolu-

tions, and, particularly, the differences found between the problems with and without phase transformation in each of the stress measures, may differ significantly, as we may observe from the results obtained from Point B. In short, the homogenised equivalent stress, or, alternatively, the homogenised Von Mises stress, only accounts for the deviatoric stresses, while the norm of the first Piola-Kirchhoff stress tensor, on the other hand, also considers hydrostatic stress state, which, as we have seen, is intimately related to the activation of MT (note, in Figure 6.11, that while the homogenised equivalent stress follows mostly the same evolution regardless of if transformation is being admitted or not, the evolutions of the norms of the first Piola-Kirchhoff stress tensor show increasing discrepancies for larger RVE lengths and, consequently, higher values of the homogenised martensite volume fraction). For this reason, the norm of the first Piola-Kirchhoff stress tensor actually constitutes a sound measure of impact of the second-order homogenisation and respective l_{RVE} on the martensitic transformation and corresponding microstructural behaviour (we will return to this issue later on).

Still on the results obtained from the deformation history collected from Point B, it is worth pointing out that, similarly to the results from Point A, the norm of the homogenised higher-order stress tensor increases with the RVE length, while, on the contrary, the equivalent homogenised stress, σ_{vm} , decreases for a larger l_{RVE} . The explanation for such behaviour is better understood by looking at the evolution of σ_{vm} with respect to the equivalent homogenised strain (top-right plot of Figure 6.11). Initially, the typical evolution is observed, with an initial linear part, correspondent to the elastic behaviour, and a subsequent yielding phase. However, once the equivalent homogenised strain reaches around 0.0015 an unloading-like behaviour is observed. Again, this behaviour is explained by the upwards shift of the neutral axis during the prescribed angular displacement. The RVE under the first-order homogenisation scheme only accounts for the macroscopic deformation gradient, therefore, the movement of the neutral axis is only perceived by the corresponding RVE once the onset of the strain unloading, that is, the top boundary of the neutral axis reaches the infinitesimal material Point B. On the other hand, the RVEs under second-order homogenisation actually capture the bending deformation mode and, as a result, the position and evolution of the neutral axis is adequately depicted within the RVE. This notion is neatly portrayed in Figure 6.13 and explains the difference in the smoothness of the transitions to the unloading-like state presented in the plot of the equivalent homogenised stress with respect to the equivalent homogenised strain (Figure 6.11).

As a final remark, it must be emphasised that the size of the micro-constituents is not captured by neither of the considered homogenisation schemes. Indeed, for a given RVE size, and, thus, for a fixed number of micro-constituents (in this case, grains), one would expect that a larger RVE length would entail equally larger grains, and vice-versa. Visually, that is immediately perceptible; however, this feature is not mathematically captured by the considered second-order formulation and, therefore, the presumable *Hall-Petch strengthening* effect and the overall grain size impact on the TRIP effect is clearly absent from any of the computed material responses.

6.3.2 Double-Notched Specimen Under Plane Strain

The average length of the elements from the double-notched specimen's macroscopic mesh is 0.3 mm, therefore, following the framework carried out in Section 6.3.1, the RVE lengths considered for the second-order homogenisation-based micro-scale analyses must be: (i) $l_{RVE} = 0.075$ mm, (ii) $l_{RVE} = 0.15$ mm, (iii) $l_{RVE} = 0.3$ mm. The homogenised equivalent stress with respect to both prescribed vertical displacement and homogenised equivalent strain and the norms of the homogenised first Piola-Kirchhoff stress tensor and homogenised higher-order stress tensor obtained from the micro-scale analyses associated to the double-notched specimen's Point B, under both homogenisation schemes and for all the aforementioned RVE lengths are presented in Figure 6.16.

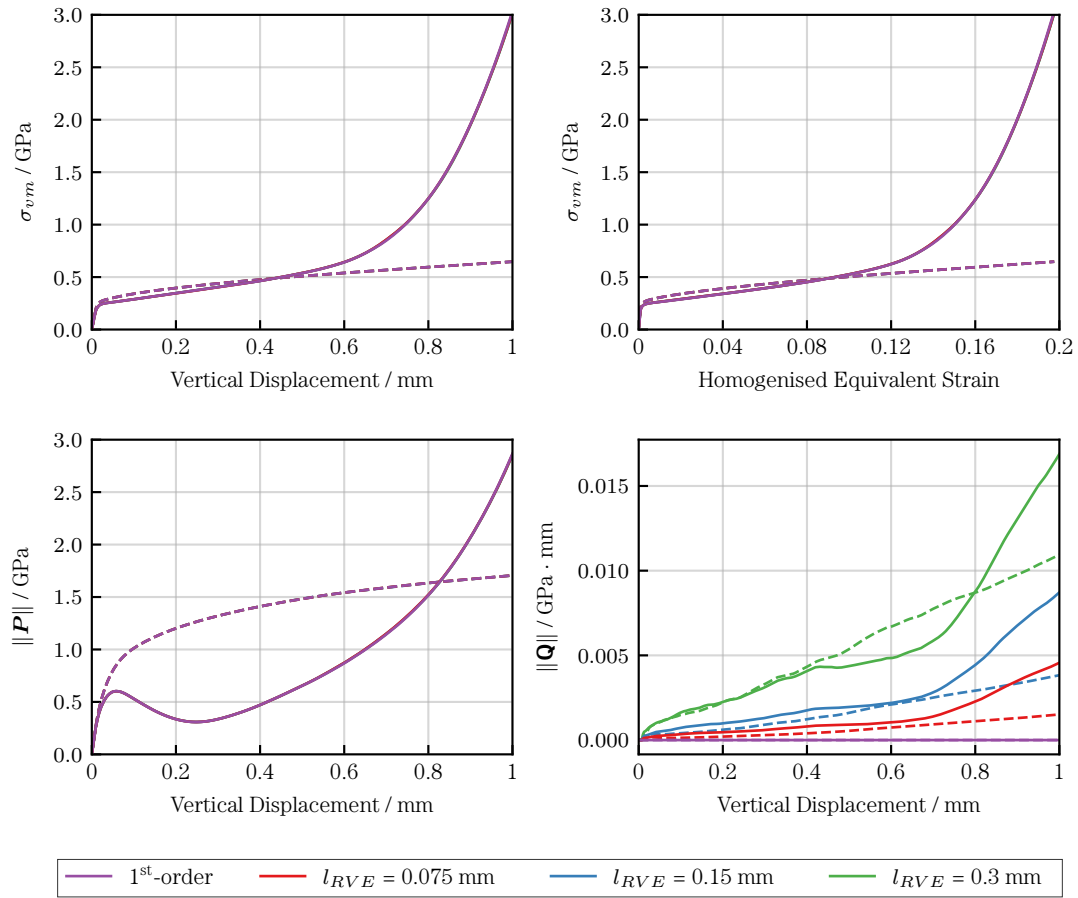


Figure 6.16: Evolution of the homogenised equivalent stress, the norm of the homogenised first Piola-Kirchhoff stress tensor and the norm of the homogenised higher-order stress tensor obtained from the RVEs subjected to the deformation history from Point C, without (dashed lines) and with (solid lines) mechanically-induced MT.

The distributions of the equivalent Cauchy stress for the final macroscopic vertical displacement of $u_2 = 1$ mm over the deformed RVEs attached to Point C are presented in Figure 6.17, for the analyses without MT, and in Figure 6.18, for the analyses in which it is admitted. The distribution of the developed martensite volume fraction over the RVEs is

shown in Figure 6.19. Regarding the magnitude of the stresses observed under the assumption of MT, displayed in Figures 6.16 and 6.18, the case could be made that such results are incorrect, which would be a fair assumption, given the unrealistical physical implications. However, this is easily explained by the constitutive model disregard of the plastic deformation in the martensite phase and resulting elastic behaviour once a given material point becomes fully martensitic. In this respect, it must be noticed that both the first and second gradients of the displacements are significantly larger for the deformation history captured from Point D, therefore, in order to obtain clear, presentable results, it is preferable if we limit the extent of the corresponding prescribed macroscopic vertical displacement. That being said, the following results associated with Point D are presented for the macroscopic displacement $u_2 = 0.5$ mm.

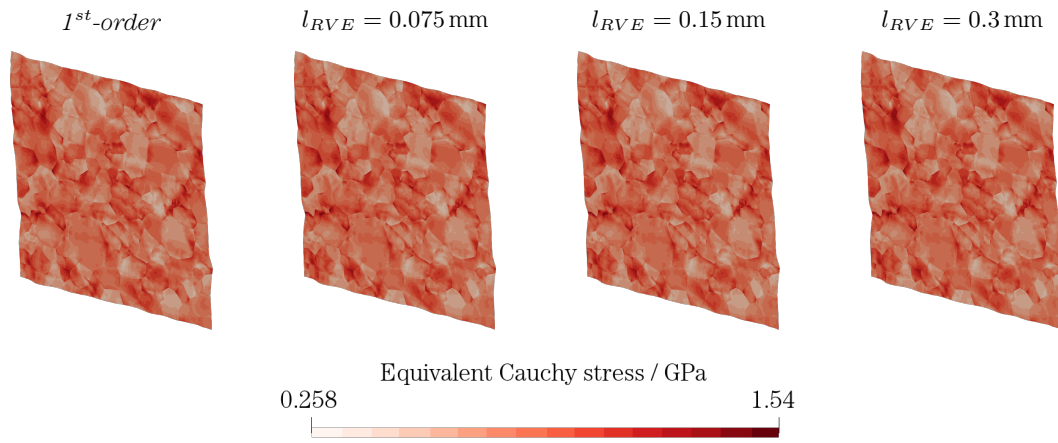


Figure 6.17: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point C, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 1 mm and for the analyses without MT.

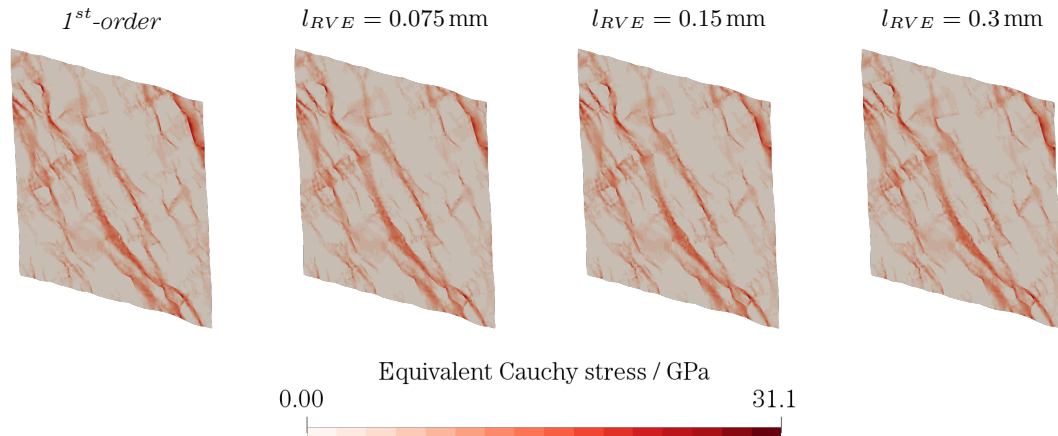


Figure 6.18: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point C, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 1 mm and for the analyses with MT.

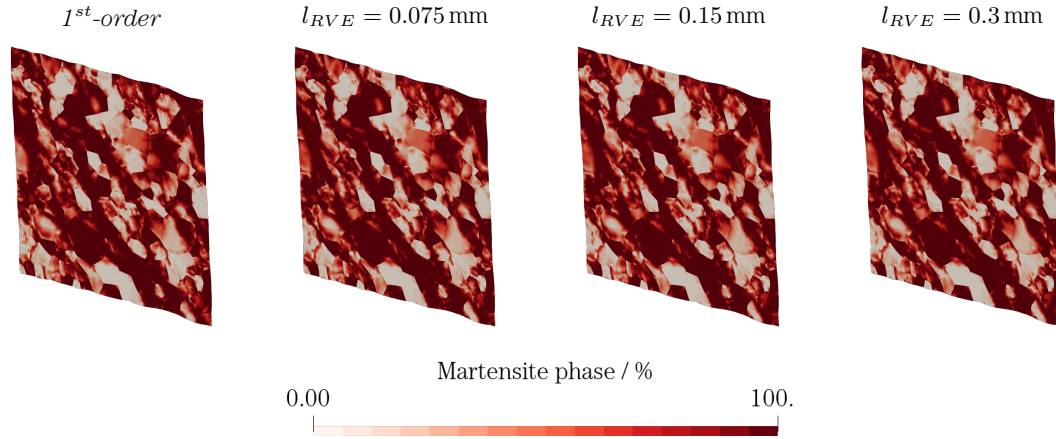


Figure 6.19: Distribution of the martensite volume fraction over the RVEs associated with the deformation history from Point C, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 1 mm.

Figure 6.20 presents the the homogenised equivalent stress with respect to both prescribed vertical displacement and corresponding homogenised equivalent strain and the norms of the homogenised first Piola-Kirchhoff stress tensor and homogenised higher-order stress tensor obtained from the analyses associated with Point D. The distribution of the equivalent Cauchy stress for the macroscopic displacement $u_2 = 0.5$ mm over the deformed RVEs subjected to the deformation history collected from Point D and without MT are presented in Figure 6.21. The distribution of the equivalent Cauchy stress for the same displacement, under the assumption of MT, and the corresponding distribution of the martensite volume fraction are respectively shown in Figures 6.22 and 6.23.

Discussion of the Results

Regarding the double-notched specimen under plane strain, briefly presented in Figure 6.4, two points were considered. For Point C, located practically at the geometric center of the specimen, the equivalent strain is quite significant, while the norm of the second gradient of the displacements is nearly non-existent. Thus, the analysis of the results associated with Point C is, at this stage, rather straightforward - again, similarly to the results obtained from the deformation history from Point A, the homogenised results are identical regardless of the adopted homogenisation scheme and RVE length.

In contrast, the deformation history retrieved from Point D, located near the edge of the upper-right notch, exhibits an extremely high strain, along with an even higher norm of the second gradient of the displacements. Although the resulting ratio $\|\mathbf{G}\| / \|\nabla \mathbf{u}\|$ is much inferior than that from Point B, it must be emphasised that the deformation history from Point D provides by far the most significant magnitude of second-order deformation modes. Still, looking at the homogenised stress measures displayed in Figure 6.20, we can observe that, while the evolution of the homogenised equivalent stress is identical for both homogenisation schemes and any l_{RVE} , some slight differences can be observed in the evo-

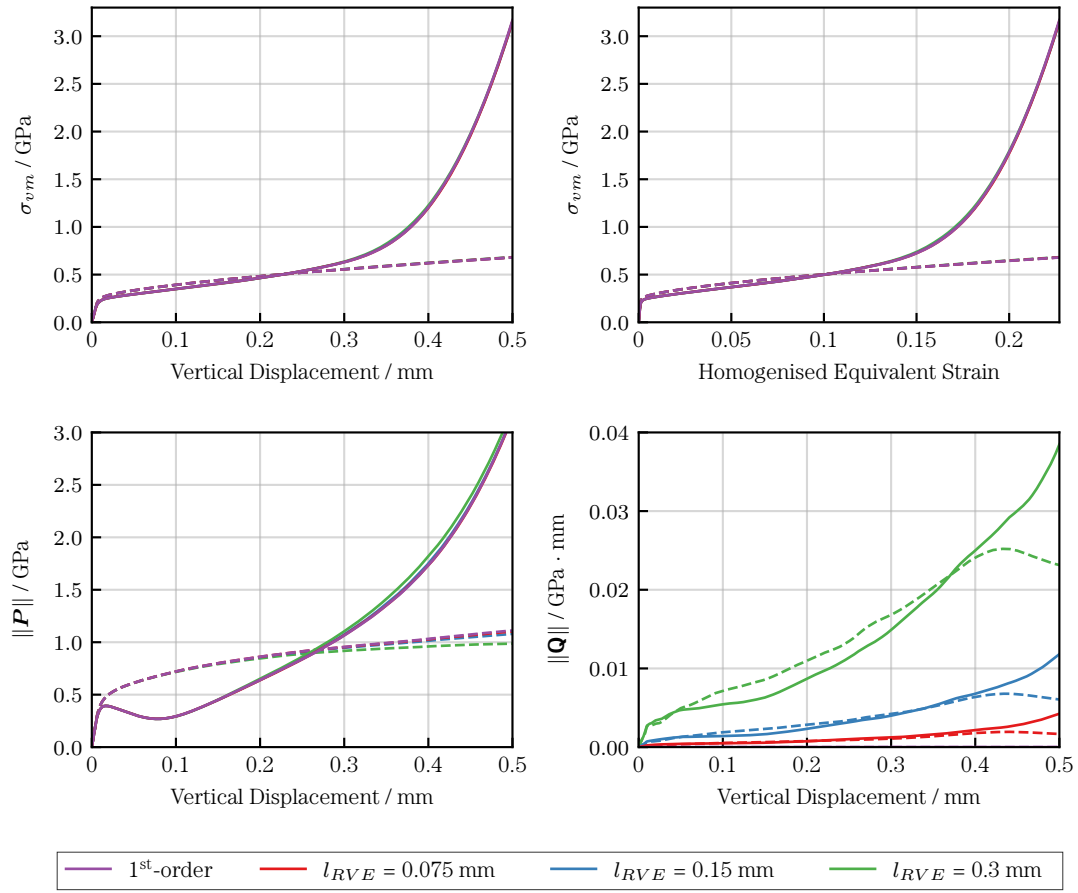


Figure 6.20: Evolution of the homogenised equivalent stress, the norm of the homogenised first Piola-Kirchhoff stress tensor and the norm of the homogenised higher-order stress tensor obtained from the RVEs subjected to the deformation history from Point D, without (dashed lines) and with (solid lines) mechanically-induced MT.

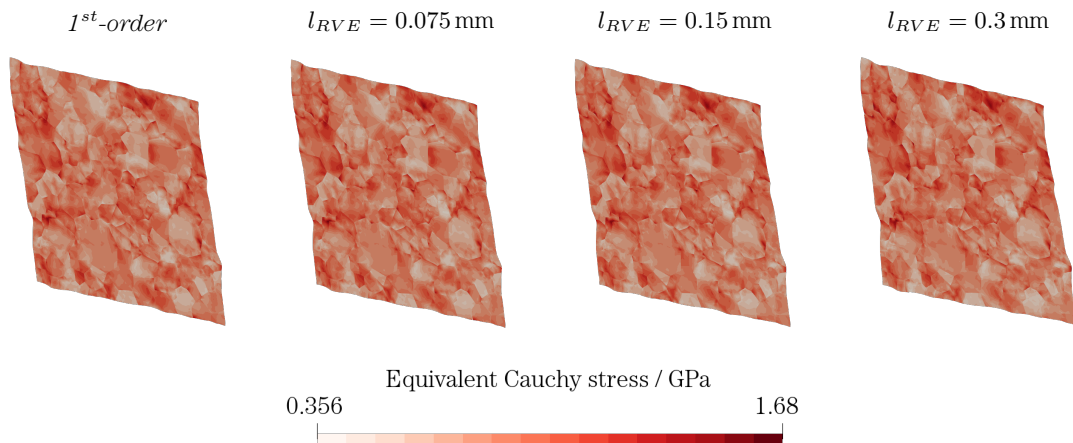


Figure 6.21: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point D, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 0.5 mm and for the analyses without MT.

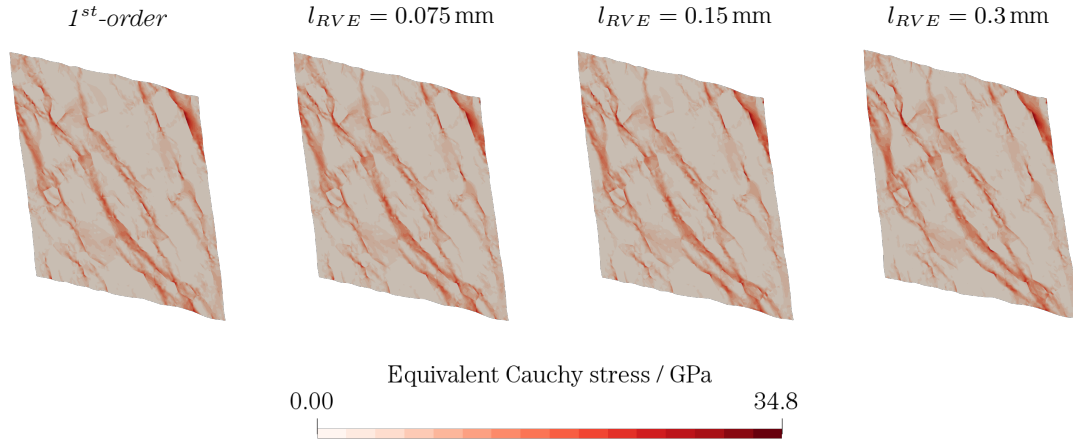


Figure 6.22: Distribution of the equivalent Cauchy stress over the RVEs associated with the deformation history from Point D, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 0.5 mm and for the analyses with MT.

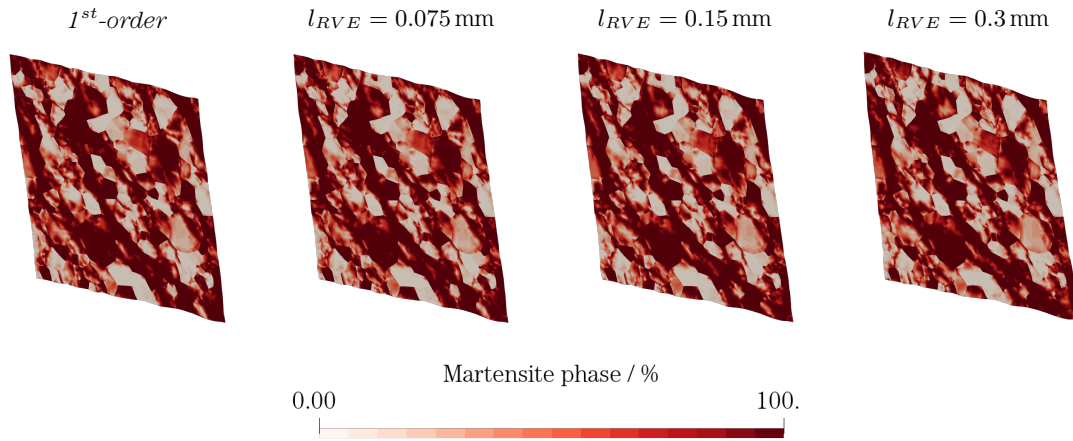


Figure 6.23: Distribution of the martensite volume fraction over the RVEs associated with the deformation history from Point D, under the first and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic vertical displacement of 0.5 mm.

lution of the first Piola-Kirchhoff stress tensor (which actually depends on the hydrostatic stress), for which the results from the RVE with $l_{RVE} = 0.3$ mm are a clear standout. The fact that such little differences are displayed by the second-order homogenisation scheme despite the sheer magnitude of the norm of the second deformation gradient allows us to confidently claim that, besides the length of the RVE, the key factor that must be met in order to witness any sizeable differences between both homogenisation schemes is the ratio $\|\mathbf{G}\| / \|\nabla \mathbf{u}\|$, rather than each of the deformation gradient's norms evaluated individually.

6.4 A Comprehensive Analysis of the Martensitic Transformation Over the Bending Beam's Thickness

In order to further understand the extent to which the RVE length and the ratio between the norms of second and first gradient of the displacements may lead to significant differences relatively to the results obtained under a first-order homogenisation scheme, or, in other words, how the macroscopic strain-gradient exactly impacts the development of MT and the RVE length required to depict such phenomena, it may be advantageous to approach the bending beam problem in a more complete manner. To do so, we adopted a finer discretisation of the bending beam's domain, whose resulting finite element mesh is constituted by 11 elements along its thickness (vertical direction) and 80 elements along the longitudinal (horizontal) direction. Contrary to the past bending beam analyses, in which we solely considered two macro-integration points, in this Section we are concerned with the behaviour of the beam over its entire thickness, such that we will consider the leftmost vertical line of 22 macro-integration points, to which we will refer as Points 1 to 22, being Point 1 the bottommost point (tensile region) and Point 22 the uppermost point (compressive region). The adopted RVE lengths are kept the same, albeit the $l_{RVE} = 0.6 \text{ mm}$ case is also admitted in order to improve the results computed from further numerical analyses. Note that since the finite element mesh is much finer, and, as a result, the macro-integration points are much closer to each other, the considered RVE lengths should also be decreased. Indeed, with these lengths, the RVE domain associated to any given point would overlap with that from its surrounding points, which, from a physical standpoint, and especially in a coupled multi-scale analysis, may seem like a questionable practice. Regardless, for the purpose of the numerical exercise we intend to perform in the present Section, this detail is not relevant and our conclusions are expected to remain valid.

On this topic, Figure 6.24 presents the evolutions of the homogenised volumetric fraction of the martensite phase and the respective ratio $\|\mathbf{G}\| / \|\nabla \mathbf{u}\|$ along the considered 22 macro-integration points. Firstly, it may be observed that the points within the bottom and upper sides of the specimen depict similar ratios of the displacements' gradients, however, the bottom side exhibits a much larger volume fraction of transformed martensite, which is simply due to the promoting nature of the respective loading scenario. Secondly, the upwards displacement of the beam's neutral axis is also noticeably pictured by both plotted measures. Lastly, and perhaps more importantly, we may observe that, besides the results associated with the points enclosed within the vicinity of the beam's neutral axis, in which the computed ratios of the gradients of the displacements are quite significant, no other points reveal any apparent differences between the results obtained from the first-order and second-order homogenisation schemes, regardless of the considered RVE length, which, in itself, may appear as quite underwhelming. In fact, even the results from the points that do depict any differences seem excessively similar, given the differences initially exposed in the analysis associated with Point B, which raises the question of if the homogenised (as in,

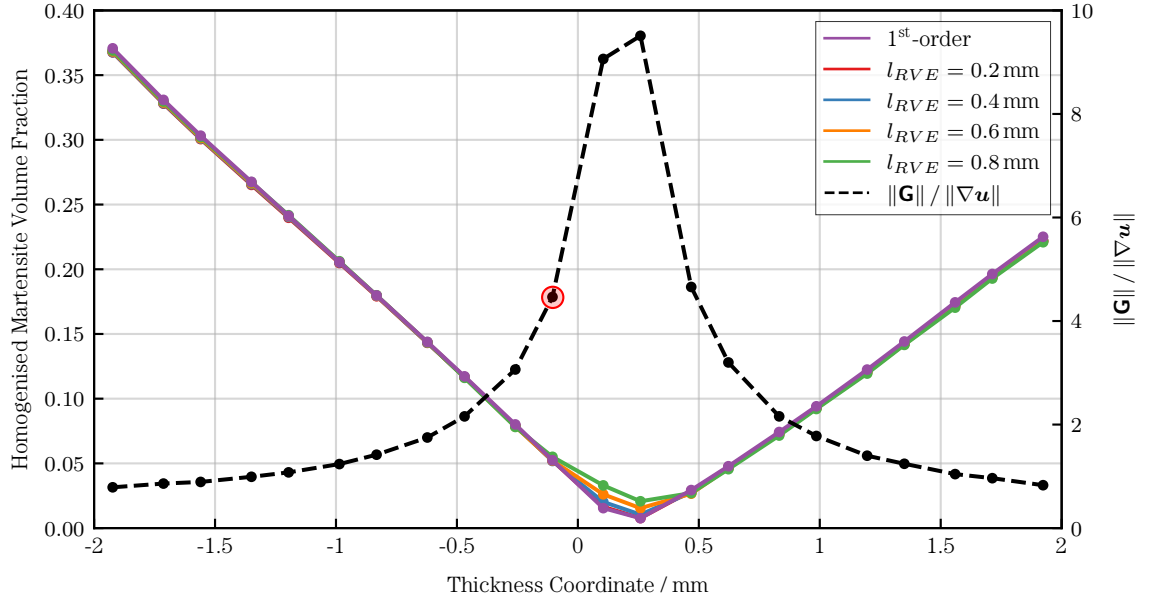


Figure 6.24: Evolution of the homogenised martensite volume fraction over the bending beam's thickness and of the corresponding ratio $\|\mathbf{G}\| / \|\nabla \mathbf{u}\|$, at the macroscopic angular displacement of 160° .

averaged) martensite volume fraction is indeed the most reliable measure of the impact of second-order effects on MT. To clarify this detail, the results from the micro-scale analyses associated with the deformation history from Point 11 (highlighted in red in Figure 6.24), for instance, can be quite revealing. In this context, Figure 6.25 presents the contour plots of the distribution of the martensite volume fraction over the deformed RVEs subjected to the deformation history collected from Point 11, while Figure 6.26 shows the corresponding evolutions of the homogenised equivalent stress with respect to both prescribed angular displacement and homogenised equivalent strain and of the norms of the homogenised first Piola-Kirchhoff stress tensor and homogenised higher-order stress tensor.

From Figure 6.25 in particular, we may observe that, analogously to the results from the analyses regarding Point B, presented in Figure 6.15, the inclusion of second-order effects has a clear impact on the microstructural behaviour and, thus, in the phase transformation phenomenon. However, contrarily to those results, in which the successive increase in the homogenised martensite volume fraction for higher lengths of the RVE might have lead to the idea that the single inclusion of said effects directly contributes to the development of MT, this analysis clearly amends that notion by showing that, in a local sense, second-order homogenisation may inhibit phase transformation (notice the top half of the RVEs exposed in Figure 6.25), which is in line with our remarks regarding the impact of second-order homogenisation on MT, presented in the Discussion of the Results in Section 6.3.1. In detail, by comparison with the deformed state of its counterpart under second-order homogenisation and $l_{RVE} = 0.8$ mm, in the RVE associated with the first-order homogenisation scheme (in

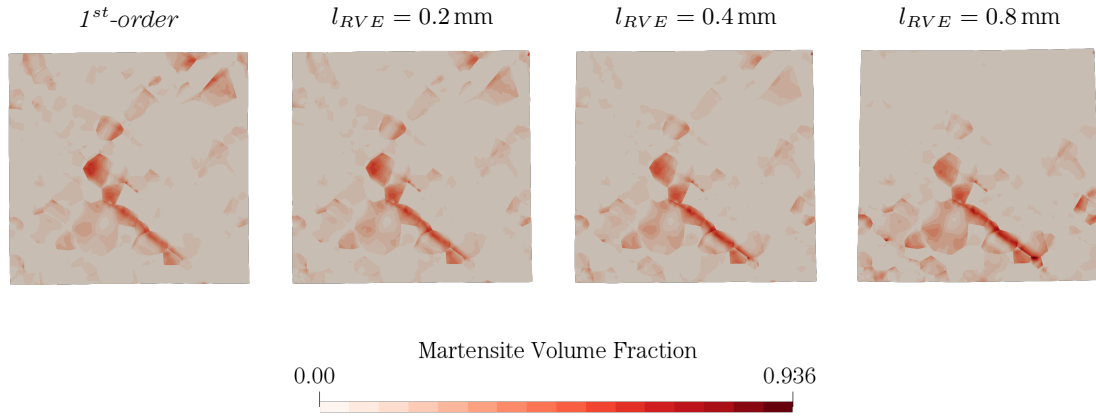


Figure 6.25: Distribution of the martensite volume fraction over the RVEs associated with the deformation history from Point 11, under the first-order homogenisation and second-order homogenisation schemes, with distinct RVE lengths, at the macroscopic angular displacement of 160° .

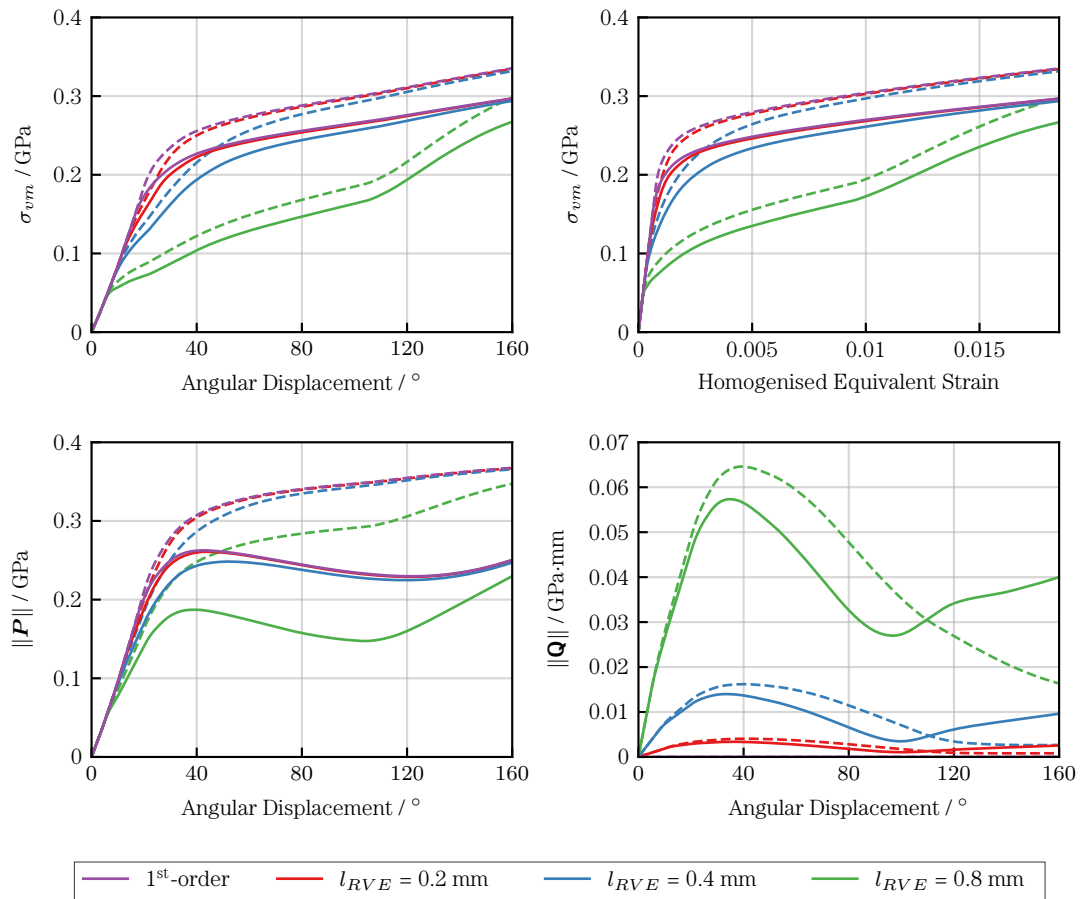


Figure 6.26: Evolution of the homogenised equivalent stress, of the norm of the homogenised first Piola-Kirchhoff stress tensor and of the norm of the homogenised higher-order stress tensor obtained from the RVEs subjected to the deformation history from Point 11, without (dashed lines) and with (solid lines) mechanically-induced MT.

which the deformation gradient is considered constant over the RVE) the tensile behaviour is overestimated in the upper half of the RVE domain, and underestimated in the bottom half. Therefore, when the second-order effects are admitted, MT is increased in the bottom half, and decreased in the upper, which, in the end, leads to a nearly identical homogenised martensite volume fraction, despite the evident differences in the observed microstructural behaviour.

Another significant difference relatively to the results associated with Point B, in which the distributions of the martensite volume fraction followed a gradual evolution from the first-order homogenisation's RVE to the one under second-order homogenisation and $l_{RVE} = 0.8\text{ mm}$, is that, in this case, the difference in these distributions only become noticeable for the latter, that is, the distributions associated with the first-order and second-order homogenisation schemes with RVE lengths equal to 0.2 mm and 0.4 mm are practically indistinguishable (to be specific, some slight differences can actually be identified in the contour plot of the martensite volume fraction associated with the RVE length equal to 0.4 mm). Again, this relationship between the differences regarding MT and the adopted homogenisation scheme (as well as the corresponding RVE length) is directly supported by the norm of the first Piola-Kirchhoff stress tensor, albeit, in this case, the homogenised equivalent stress also adequately depicts these differences. For this reason, but also considering all results previously presented, and recalling the fact that the first Piola-Kirchhoff accounts for the hydrostatic stress state, which, in turn, is intrinsically connected to the activation and development of MT, it arises as the most adequate measure of the impact of second-order effects and selected length of the RVE on MT, as opposed to the initially suggested homogenised martensite volume fraction. This subject will be explored to greater detail in the following Section.

6.4.1 A Framework for the Quantitative Assessment of the Relevance of Second-Order Homogenisation in Martensitic Transformation

As we have seen throughout this Chapter, the second-order homogenisation scheme does not always result in a more accurate description of the microstructural behaviour, regardless of the considered constitutive model (uniquely crystal plasticity or plasticity coupled with MT), often leading to the same exact response as the one obtained from the standard first-order homogenisation scheme. In short, from the results presented so far, two major takeaways are immediately clear: firstly, that a more dominant first gradient of the macroscopic displacements, or simply a strain of significant magnitude, usually hinders the relevance of the second-order homogenisation scheme and its impact on the resulting material behaviour; and, secondly, that increasing RVE lengths lead to a response more reliant on second-order effects. Fundamentally, the first-order homogenisation-based multi-scale model is adequate when the underlying RVE length satisfies the Scale Separation Principle, i.e., when the RVE length is substantially smaller than the macroscopic deformation wavelength, in such a way that the deformation gradient may be considered constant within the

RVE. On the contrary, when such conditions are not met, and complex phenomena such as phase transformation, for example, dictate the microstructural behaviour, the second-order homogenisation scheme may be required for the accurate characterisation of the material response. In this Section, we propose a numerical model for the assessment of the conditions in which a second-order homogenisation scheme is favoured over the standard first-order approach.

Temizer and Wriggers (2011) proposed that a limit based on the non-dimensional quantity $\|\mathbf{G}\| \cdot l_{RVE}$ can be defined in order to determine when a *Direct Numerical Simulation* (DNS) should be employed rather than the standard homogenisation framework. Following this idea, Rodrigues Lopes (2019) noted that the differences found between the responses under the first or second-order homogenisation schemes were also greatly dependent on the magnitude of the strain associated with the first gradient of the displacements, and tailored the aforementioned concept into the following criterion:

$$\frac{\|\mathbf{G}\| \cdot l_{RVE}}{\|\mathbf{F} - \mathbf{I}\|} > tol, \quad (6.4.1)$$

where the tolerance parameter tol establishes a measure of the differences expected between the responses under both homogenisation schemes, and above which the importance of second-order effects justifies the adoption of the second-order homogenisation approach. Since an inversely proportional relation may not accurately translate the relative weight between $\|\mathbf{G}\| \cdot l_{RVE}$ and $\|\mathbf{F} - \mathbf{I}\| = \|\nabla \mathbf{u}\|$, a more general extension of the above-mentioned criterion is also proposed and reads:

$$\frac{f_G(\|\mathbf{G}\| \cdot l_{RVE})}{f_F(\|\mathbf{F} - \mathbf{I}\|)} > tol, \quad (6.4.2)$$

where f_G and f_F denote generic scalar functions. Having established this, what follows is an attempt to develop this criterion model to more detail and, in such, arrive at an expression that allows us to evaluate when the second-order homogenisation scheme should be adopted. This means deriving an analytical function, based on the first and second gradients of the displacements and on the RVE length, that estimates the differences between the responses under both homogenisation schemes. Then, having defined the value of the tolerance parameter tol , we should obtain a closed map that delimits the applicability of the first-order homogenisation scheme. To do so, it is particularly important to study the responses of RVEs subjected to several combinations of $\mathbf{F}$ and $\mathbf{G}$, hence the usefulness of studying the full line of macro-integration points along the beam's thickness.

Firstly, we must define how to properly compute the differences between each RVE i of length $l_{RVE,i}$, subjected to second-order homogenisation, and the corresponding RVE under the standard first-order homogenisation. As we have established by now, the norm of the homogenised first Piola-Kirchhoff stress tensor provides the most complete and accurate measure of such differences, which, following the *sum of the absolute differences*,

can be determined by the following expression:

$$s_i = \frac{1}{N} \cdot \sum_{n=1}^N \left| \|\mathbf{P}\|_{i,n} - \|\mathbf{P}\|_{1st,n} \right|, \quad (6.4.3)$$

where n denotes each observation associated with a specific angular displacement θ , N is the total number of observations and $|\|\mathbf{P}\|_{i,n} - \|\mathbf{P}\|_{1st,n}|$ is the absolute difference between the norms of the homogenised first Piola-Kirchhoff stress tensor under first-order homogenisation and second-order homogenisation with RVE length equal to $l_{RVE,i}$ in each observation n . To be precise, since the overall sum of all computed differences is being averaged, i.e., divided by N , s_i is similar to the statistical concept of *variance*. In order to obtain a parameter coherent with any problem and that accounts for the magnitude of the observed range of the norm of first Piola-Kirchhoff stress tensor, the aforementioned difference must be normalised, such that the expression (6.4.3) becomes:

$$s_i = \frac{100}{N} \cdot \sum_{n=1}^N \frac{\left| \|\mathbf{P}\|_{i,n} - \|\mathbf{P}\|_{1st,n} \right|}{\|\mathbf{P}\|_{1st,n}}, \quad (6.4.4)$$

where we also multiplied by 100 in order to obtain the final s parameter as a percentage. One crucial thing to consider is that eventual convergence issues may lead to significantly different total number of increments and resulting sets of computed angular displacements between distinct analyses, therefore, in order to prevent that any specific displacement intervals (that reveal more or fewer discrepancies) are overly accounted for, only the prescribed angular displacement steps, i.e., $\theta \in [0^\circ, 2^\circ, 4^\circ, \dots, 160^\circ]$, are considered, meaning that, in this particular problem, N equals 81.

Under these conditions, Tables 6.2 and 6.3 present the parameter s_i for the analyses associated with Point A, Point B and Point 11. Note that these results, obtained with expression (6.4.4), are coherent with what we observed in Figures 6.7, 6.11 and 6.26. Accordingly, we may immediately confirm that the second-order homogenisation-based results associated with Point A, in which the first deformation gradient is the dominant component, exhibit insignificant differences relatively to the first-order homogenisation response, whereas both Points B and 11, located within the vicinity of the beam's neutral axis and, therefore, mainly driven by second-order effects, depict quite substantial differences, as portrayed by the higher magnitude of the corresponding computed s parameters. Additionally, it is also clear that a larger RVE length, and the consequent more comprehensive account of second-order effects, directly leads to the generalised increase of the observed differences between the responses obtained under both homogenisation schemes. Lastly, it must also be remarked that, at least for the aforementioned Points, the assumption of MT leads to more severe discrepancies between the homogenised results, which proves the undeniable importance of the consideration of second-order deformation modes in the characterisation of microstructural behaviour in the presence of complex phenomena such as phase transformation. Nevertheless, these discrepancies force us to study the results under both con-

Table 6.2: Parameter s_i [%] associated with the second-order homogenisation-based responses relative to the analyses of Points A, B and 11, with l_{RVE} equal to 0.2, 0.4 and 0.8 mm and without MT.

Point A (w/o MT)		Point B (w/o MT)		Point 11 (w/o MT)	
$l_{RVE,i}$	s_i	$l_{RVE,i}$	s_i	$l_{RVE,i}$	s_i
0.2	0.02480	0.2	6.35306	0.2	0.65698
0.4	0.10860	0.4	9.95141	0.4	2.98039
0.8	0.52690	0.8	13.0202	0.8	14.48096

Table 6.3: Parameter s_i [%] associated with the second-order homogenisation-based responses relative to the analyses of Points A, B and 11, with l_{RVE} equal to 0.2, 0.4 and 0.8 mm and with MT.

Point A (w/ MT)		Point B (w/ MT)		Point 11 (w/ MT)	
$l_{RVE,i}$	s_i	$l_{RVE,i}$	s_i	$l_{RVE,i}$	s_i
0.2	0.50526	0.2	6.85581	0.2	0.82112
0.4	0.59703	0.4	13.7753	0.4	4.16833
0.8	0.88275	0.8	27.8327	0.8	26.6765

stitutive models, such that the MT-related effects on the computed differences (s values) can be easily pinpointed.

Having established how to measure the observed differences arising from the adoption of the second-order homogenisation scheme, we must now infer how each of the relevant quantities included in the initially proposed model (expression 6.4.2) relate with the parameter s_i , so that the tolerance value tol is then adequately defined, based on the obtained results. That being said, we shall start by isolating the norm of the first gradient of the displacements, $\|\mathbf{F} - \mathbf{I}\|$, whose relation with the defined criterion s , computed from the analyses without MT is presented in Figure 6.27, specifically in the two upper plots. From this brief analysis, two main conclusions can be drawn: (i) firstly, it is observed that, in the general sense, a more significant first deformation gradient corresponds to lower s values, which translates to a lesser amount of observed differences between homogenisation schemes, and vice-versa, in what constitutes a relation that approximately resembles the inversely proportional relation proposed with expression (6.4.1); (ii) secondly, it is also worth noting that the results follow particularly distinct behaviours between the tensile (red points) and compressive (blue points) regions of the bending beam - note that for pairs of points of relatively similar $\|\mathbf{F} - \mathbf{I}\|$, the s parameter for a given l_{RVE} can be quite different depending on if that specific point belongs to the tensile or compressive regions of the bending beam.

When dealing with bending deformations of such high curvatures, the discussion of the upwards dislocation of the beam's neutral axis is inevitable. In this context, it must be noted that the computed first gradient of the displacements, $\|\mathbf{F} - \mathbf{I}\|$, for each point, is

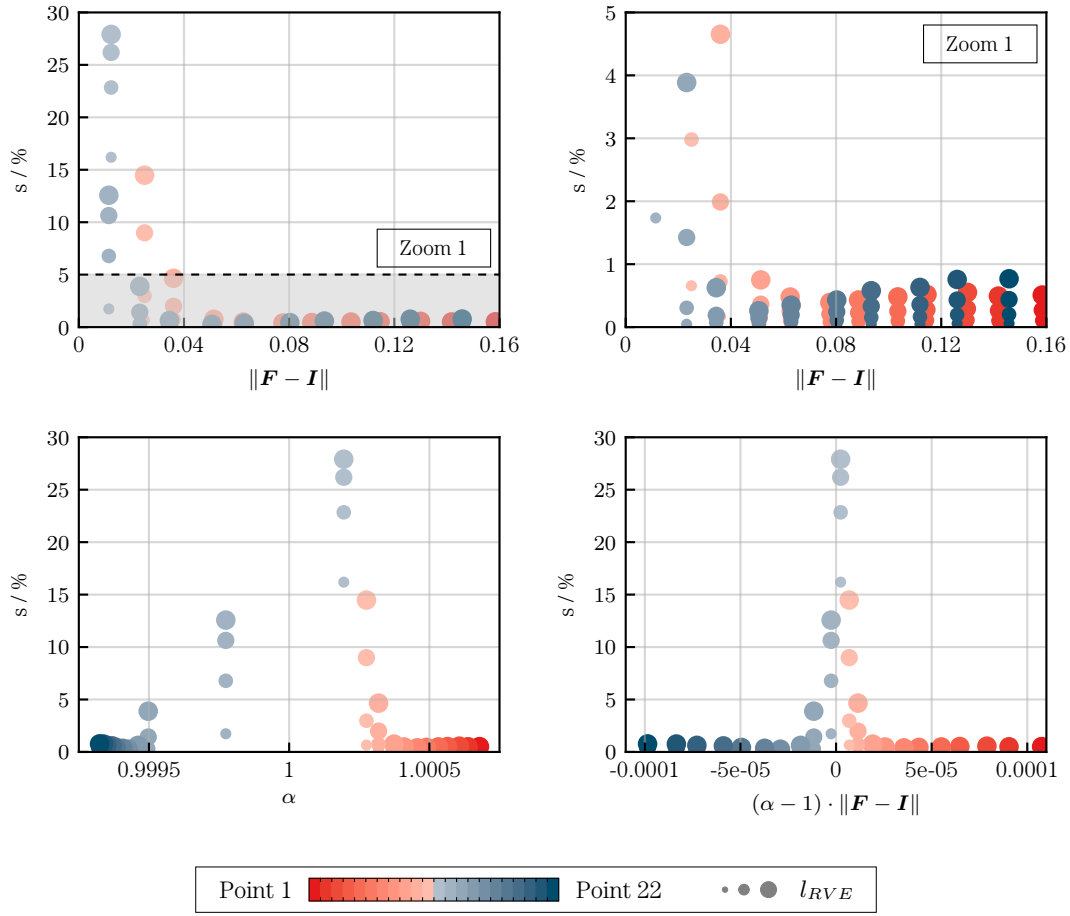


Figure 6.27: Scatter plots of parameter s associated with the second-order homogenisation-based results with RVE lengths equal to 0.2, 0.4 and 0.8 mm, with respect to different measures based on the first deformation gradient at the macroscopic angular displacement of 160° , and without MT.

associated with the final macroscopic angular displacement, i.e. $\theta = 160^\circ$, which, coupled with the neutral axis phenomenon, explains the discrepancies between the strains of pairs of directly opposing points (with respect to the longitudinal section that contains the centroid of the beam's cross section, or initial, undeformed beam's neutral axis). This asymmetry and associated behaviour of the beam's neutral axis are quite perceptible from the bottom left plot of the aforementioned Figure, in which the computed s parameters are plotted with respect to the contraction/expansion ratio α (recall Section 2.1.4), which distinctly splits the regions above and below the final beam's neutral axis.

Furthermore, it must be understood that the behaviour of the neutral axis throughout the entirety of the prescribed displacement may introduce very particular, obscure features that impair the comprehensive analysis of the presented results. Indeed, the reason for why the second-order homogenisation-based results of a given point within the compressive region (blue point) exhibits larger s values than the results with identical RVE length associated with points of similar strain and belonging to the tensile region (red point) is not

quite understood. Regardless, it must be emphasised that in the scope of the presented results, these details are rather insignificant and are, for the most part, only noticeable for larger magnitudes of the deformation gradient and, as a result, associated with very small s values.

Having addressed the results associated with the analyses without MT, we may now advance to precisely the same discussion but with regards to the analyses in which MT is, in fact, admitted. In this context, Figure 6.28 presents an identical study to that from Figure 6.27, considering the possibility of MT. As previously discussed, we may immediately observe that the computed s values suffer a generalised increase for any of the considered macro-integration points and regardless of the adopted RVE length. Indeed, when complex transformation such as MT, for instance, is present and is important for the accurate characterisation of the microstructural behaviour, the adoption of second-order homogenisation scheme becomes significantly more necessary. Nevertheless, it is also observed that the set of points belonging to the tensile region exhibits much larger differences relatively to those from the points within the compressive region of the bending beam. It is reasonable to assume that these second-order homogenisation-related discrepancies between regions are indeed caused by the equally different corresponding degrees of MT. In other words, the second-order homogenisation scheme may be regarded as more important in the material region subjected to the tensile loading scenario, which promotes the actual development of MT that, in turn, directly leads to larger differences in the second-order homogenisation-based response.

Additionally, it must also be noticed that the magnitude of the s parameter seems to be converging with the increase of the first gradient of the displacements in the points contained within the tensile-driven material region. To be precise, it is actually observed that the computed differences associated with the shorter RVE lengths become increasingly closer to those from larger RVEs, which, to some extent, corresponds to continuous decrease of the importance of the adopted RVE length. Note, however, that, again, this feature is exclusive to the points within the tensile region of the bending beam and may then be assumed as a product of the favourable nature of the respective deformation in what concerns MT. In short, we can infer that the importance of the second-order homogenisation scheme in the more accurate characterisation of the material behaviour is a subjective matter and highly dependent on the constitutive model that governs the material response. This hypothesis had already been pointed out by Rodrigues Lopes (2019), where it is stated that the overall behaviour also depends on the description of the constituents and not only on the RVE morphology, which means that either the tolerance parameter tol or the whole numerical model may have to be tailored in accordance with the constitutive model at hand. Ideally, we would be able to propose a criterion that accurately accounts for all of these specific features; however, attempting to do so may be a futile endeavour. Regardless, the overall relation between s and the norm of the first gradient of the displacements appears to be close to the initially proposed inversely proportional relation, so that we may write:

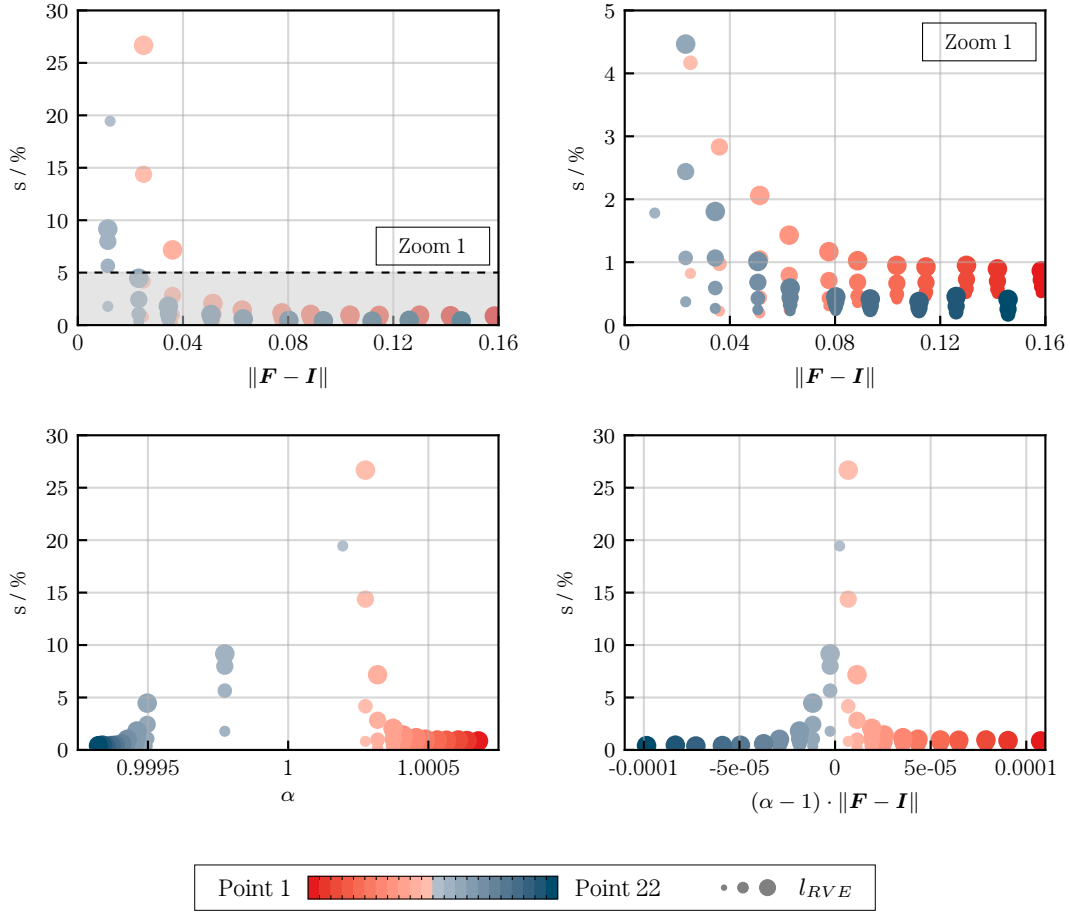


Figure 6.28: Scatter plots of parameter s associated with the second-order homogenisation-based results with RVE lengths equal to 0.2, 0.4 and 0.8 mm, with respect to different measures based on the first deformation gradient at the macroscopic angular displacement of 160° , and with MT.

$$s \propto \frac{a}{(\|F - I\|)^b}, \quad (6.4.5)$$

where the parameters a and b are to be determined by means of a *nonlinear regression analysis* and should, to some extent, encompass the effects resultant from the aforementioned undiscovered features.

Regarding the numerator of expressions (6.4.1) and (6.4.2), which includes both the norm of the second gradient of the displacements, $\|G\|$, and the RVE length, l_{RVE} , their respective relations with the parameter s are graphically represented in Figure 6.29 for the analyses without MT and in Figure 6.30 for the analyses in which MT is admitted. Immediately, we can observe that isolating the norm of the displacements' second gradient does not offer any valuable information on how s relates to it, mostly because there is no direct relation between them. While perhaps it would be expected that higher values of $\|G\|$ meant also higher values of s , it is interesting to confirm that, in fact, that is not necessarily the case, once again proving the significance of the first gradient of the displacements on the

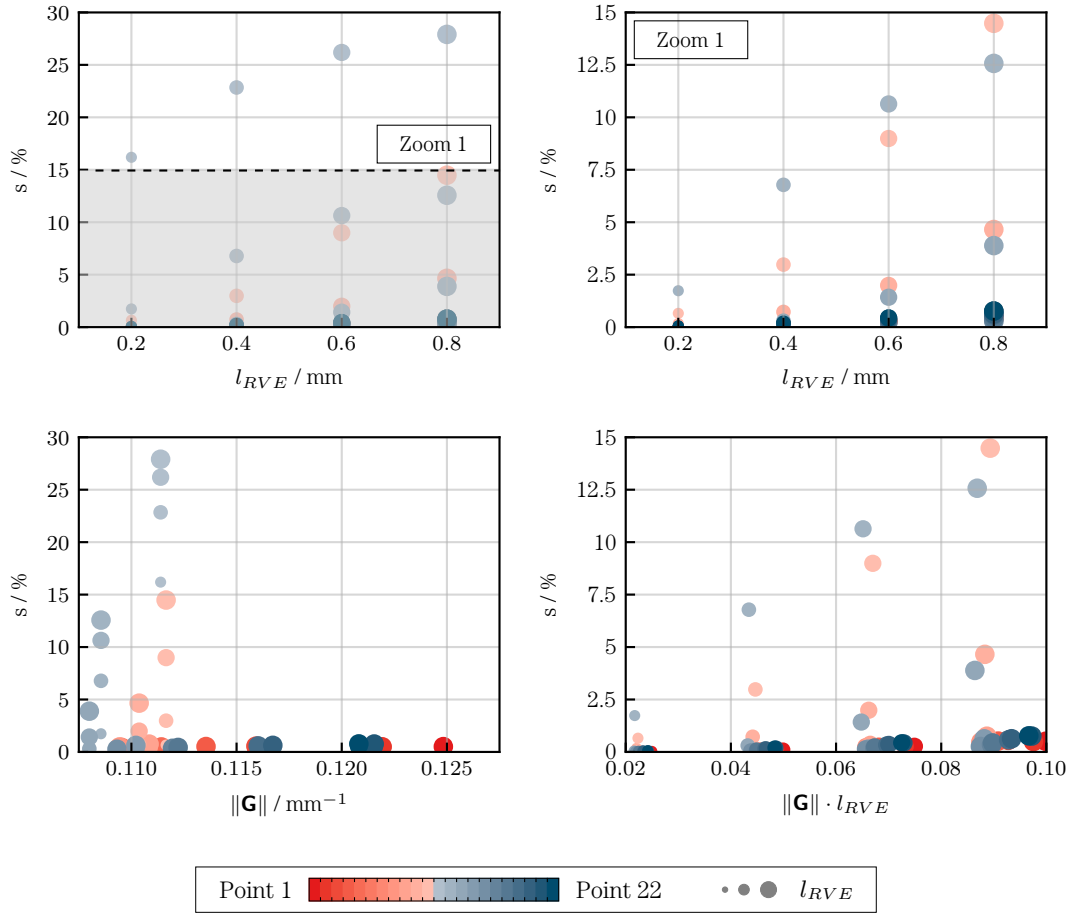


Figure 6.29: Scatter plots of parameter s associated with the second-order homogenisation-based results with RVE lengths equal to 0.2, 0.4 and 0.8 mm, with respect to the norm of second gradient of the displacements at the macroscopic angular displacement of 160° , the RVE length and the product of the two, and without MT.

material response and on the relevance of the second-order homogenisation scheme. On the other hand, the pattern of the evolution of s with respect to the length of the RVE is much more evident. However, it must be remarked that, contrarily to the initial criterion proposal, s does not seem to follow a linear evolution with l_{RVE} , but rather an exponential growth, or simply some other mathematical relation that resembles it. Regardless, it is paramount that $\|\mathbf{G}\|$ and l_{RVE} are evaluated together, by means of their product (as was initially proposed), such that the final criterion remains dimensionless, which is extremely advantageous for finding correlations. Moreover, when adequately formulated, dimensionless numbers may have a clear physical meaning, thus contributing to the understanding of the phenomenon or problem under study. With this in mind, and based on the results presented in Figures 6.29 and 6.30, the expression (6.4.5) can be extended and two final equations are established:

$$s_i \approx a \cdot \frac{(\|\mathbf{G}\| \cdot l_{RVE})_i^c}{(\|\mathbf{F} - \mathbf{I}\|)_i^b} \quad (6.4.6)$$

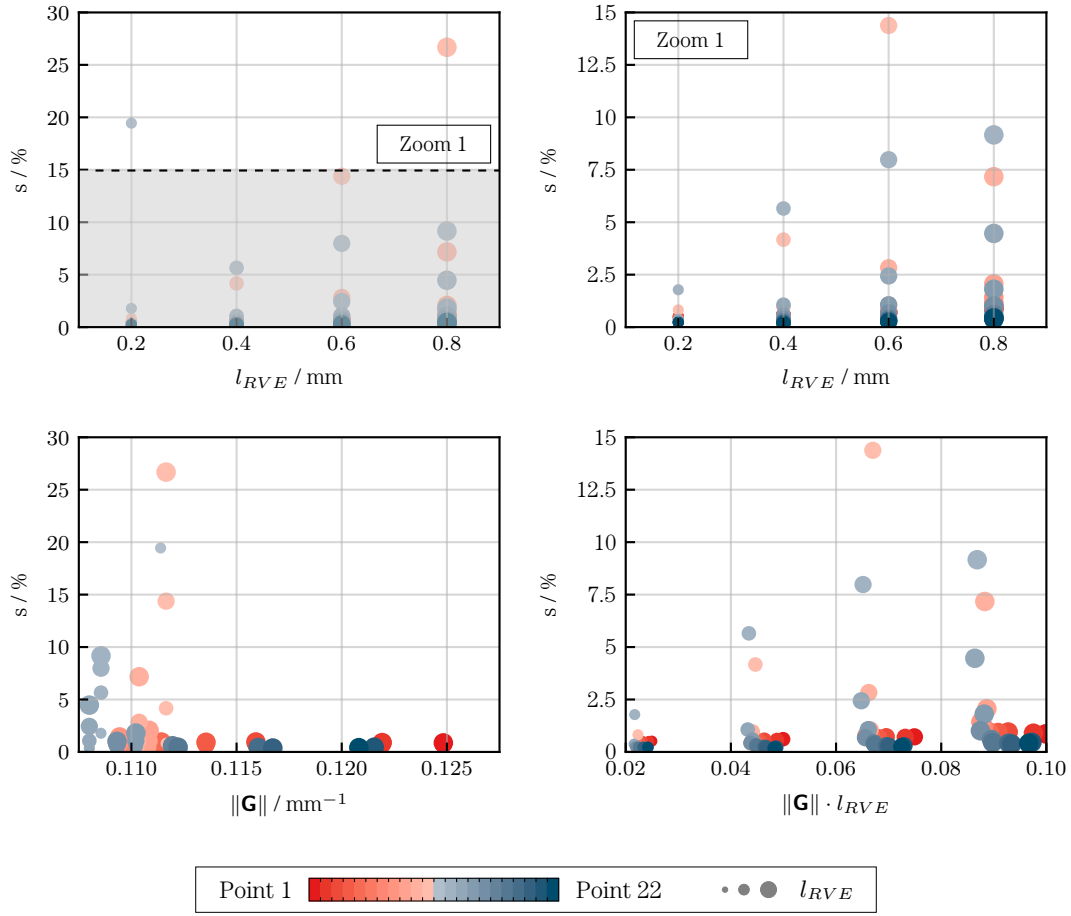


Figure 6.30: Scatter plots of parameter s associated with the second-order homogenisation-based results with RVE lengths equal to 0.2, 0.4 and 0.8 mm, with respect to the norm second gradient of the displacements at the macroscopic angular displacement of 160° , the RVE length and the product of the two, and with MT.

$$s_i \approx a \cdot \frac{e^{c \cdot (\|\mathbf{G}\| \cdot l_{RVE})_i}}{(\|\mathbf{F} - \mathbf{I}\|_i)^b} \quad (6.4.7)$$

where the additional parameter c is also to be optimised by the ensuing nonlinear¹ regression analysis. To do so, a Python script, which reads the relevant data and, by means of SciPy's optimization curve fitting procedures, computes the values of the parameters that lead to the *least squares*, or least sum of the squared residuals, was implemented.

Once determined the optimal parameters' values, we must then proceed to the evaluation of the better model, which requires us to quantify the *goodness-of-fit* of both proposed models, based on the admitted data. One of the most frequently reported goodness-of-fit measures is the *R-squared* (R^2) value, which, in short, compares the fit of a given model

¹ Here, *nonlinear* refers to the nonlinearity involved in the parameters a , b and c and not to the nonlinear nature of the measure s_i of the proposed models. Indeed, a polynomial function (where the independent variables, not the parameters, are raised by an exponent and the parameters are multiplied by said independent variables) can also model curvature, while still being considered a linear regression model.

with the horizontal line or plane of equal value to the mean of the modelled parameter, in this case s_i , in all data points, that reads:

$$\bar{s} = \frac{1}{N} \cdot \sum_{i=1}^N s_i, \quad (6.4.8)$$

where $\bar{s}$ is the above-mentioned mean and N now denotes the total number of data points. Recall that the subscript i identifies each analysis/RVE which, in turn, regards a particular macro-integration point and RVE length. From here, the sum of the squared deviations of the data points from $\bar{s}$ may then be computed as follows:

$$SS_{tot} = \sum_{i=1}^N (s_i - \bar{s})^2. \quad (6.4.9)$$

Analogously, the sum of the squared distances of the data points from the best-fit curve (determined by the nonlinear regression analysis) is also computed:

$$SS_{res} = \sum_{i=1}^N (s_i - f_i)^2, \quad (6.4.10)$$

where f_i is the predicted value obtained from either of the proposed models (expressions 6.4.6 and 6.4.7) associated with the correspondent data point of coordinates $(\|\mathbf{F} - \mathbf{I}\|)_i$ and $(\|\mathbf{G}\| \cdot l_{RVE})_i$ (x and y coordinates, respectively) and z value equal to s_i . Lastly, the R^2 measure can be written as:

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}, \quad (6.4.11)$$

or, alternatively, and perhaps more clearly, as:

$$R^2 = 1 - \frac{\text{Unexplained Variance}}{\text{Total Variance}} = \frac{\text{Variance Explained by the Model}}{\text{Total Variance}}. \quad (6.4.12)$$

Under these conditions, R^2 must be between 0.0 and 1.0 and, presumably, higher values (closer to 1.0) should mean that the considered model poses a considerably good fit of the data. While this is true in the case of a linear regression analysis, when dealing with nonlinear regression, as we are, some problems may arise, particularly if we intend to compare linear and nonlinear models (Kvålseth, 1985). Recalling the previously stated definition of a linear regression analysis (for which the model usually follows a polynomial form), comparing the deviation between the data points and the predicted values with the deviation of the data points from the mean seems quite fitting, as the horizontal line or plane essentially constitutes the simplest possible case of a linear regression. On the other hand, many nonlinear regression models cannot even reproduce that horizontal line or plane and, therefore, R^2 does not hold its mathematical meaning and may lead to misleading results of the goodness-of-fit of a given model. Spiess and Neumeyer (2010) supports this claim and

highlights that: (i) R-squared may be simultaneously high for both good and poor models and (ii) R-squared does not consistently report higher values for better models.

With this in mind, we decided for the *Standard Error of the Regression*, or residual standard error, S , as our primary goodness-of-fit measure, which, although not as objective as R-squared aims to be in what respects the fitting accuracy of a given model (in the sense that a R-squared value equal to 1.0 would mean the model precisely captures the variance of the data), S tells us, directly, and in the units of the dependent variable, s_i , how far from the data points the regression line is, on average. For this reason, the standard error of the regression provides a much more reliable and versatile tool, even allowing the evaluation of both linear and nonlinear regression models in a consistent manner. Following the already established notation, the standard error of the regression can be computed from the following expression:

$$S = \sqrt{\frac{1}{N-1} \cdot \sum_{i=1}^N (s_i - f_i)^2}. \quad (6.4.13)$$

Alternatively, the number of parameters, k , included in the regression model is also taken into account as a punitive factor, given that the adopted model should be as simple as possible:

$$S_k = \sqrt{\frac{1}{N-k} \cdot \sum_{i=1}^N (s_i - f_i)^2}. \quad (6.4.14)$$

Since the models we wish to compare include exactly the same number of parameters, this aspect is not that significant, but should, nevertheless, be considered.

Recalling the previously discussed differences of the evolution of the parameter s with respect to the norm of the first gradient of the displacements, $\|\mathbf{F} - \mathbf{I}\|$, between the tensile and compressive regions of the bending beam, it is worth performing the regression analysis for each data set, and compare any eventual differences, as well as with the analysis that includes all 22 points. That being said, Tables 6.4 and 6.6 present the fit parameters' values and corresponding R-squared and error of the regression goodness-of-fit measures of the regression analysis associated with the expression (6.4.6), considering the analyses without and with MT, respectively. The analogous results regarding the alternative model proposed in (6.4.7) are presented in Tables 6.5 and 6.7.

Immediately, we may observe that the error of the regression S_k is closely accompanied by the R-squared measure, which offers some credibility to the computed R-squared values, that, in some instances, depict magnitudes of ≈ 1.0 , and could, therefore, recalling their previously raised problems, be interpreted with some mistrust. Regarding the analyses without MT, both models capture with remarkable precision the results associated with the data points within the compressive region (Points 13-22). Curiously, these entail a more pronounced increase of s for larger norms of the first gradient of the displacements, which is not directly captured by neither of the proposed models and should, therefore,

Table 6.4: Optimal parameter values and goodness-of-fit measures of the nonlinear regression analysis with the model proposed in (6.4.6), considering the analyses without MT.

$s_i \approx a \cdot (\ \mathbf{G} \cdot l_{RVE}\)_i^c / (\ \mathbf{F} - \mathbf{I}\)_i^b$					
Data Set	a	b	c	R-squared	$S_k / \%$
Points 1 - 12	$2.007 \cdot 10^{-2}$	1.927	0.483	0.957	1.453
Points 13 - 22	$7.339 \cdot 10^{-3}$	2.300	1.137	0.969	0.496
Points 1 - 22	$5.731 \cdot 10^{-2}$	1.728	0.724	0.699	3.001

Table 6.5: Optimal parameter values and goodness-of-fit measures of the nonlinear regression analysis with the model proposed in (6.4.7), considering the analyses without MT.

$s_i \approx a \cdot \exp(c \cdot (\ \mathbf{G}\ \cdot l_{RVE})_i) / (\ \mathbf{F} - \mathbf{I}\)_i^b$					
Data Set	a	b	c	R-squared	$S_k / \%$
Points 1 - 12	$2.885 \cdot 10^{-3}$	1.924	9.066	0.953	1.511
Points 13 - 22	$9.001 \cdot 10^{-5}$	2.281	1.984	0.948	0.639
Points 1 - 22	$3.162 \cdot 10^{-3}$	1.723	1.349	0.696	3.017

Table 6.6: Optimal parameter values and goodness-of-fit measures of the nonlinear regression analysis with the model proposed in (6.4.6), considering the analyses with MT.

$s_i \approx a \cdot (\ \mathbf{G} \cdot l_{RVE}\)_i^c / (\ \mathbf{F} - \mathbf{I}\)_i^b$					
Data Set	a	b	c	R-squared	$S_k / \%$
Points 1 - 12	0.130	1.853	0.848	0.965	2.244
Points 13 - 22	0.139	1.510	1.018	0.975	0.337
Points 1 - 22	0.396	1.538	0.990	0.548	6.096

Table 6.7: Optimal parameter values and goodness-of-fit measures of the nonlinear regression analysis with the model proposed in (6.4.7), considering the analyses with MT.

$s_i \approx a \cdot \exp(c \cdot (\ \mathbf{G}\ \cdot l_{RVE})_i) / (\ \mathbf{F} - \mathbf{I}\)_i^b$					
Data Set	a	b	c	R-squared	$S_k / \%$
Points 1 - 12	$4.543 \cdot 10^{-3}$	1.847	15.211	0.960	2.397
Points 13 - 22	$2.513 \cdot 10^{-3}$	1.505	18.055	0.955	0.447
Points 1 - 22	$7.623 \cdot 10^{-3}$	1.536	18.053	0.548	6.096

be associated with a *less fit* predictive curve. Nevertheless, the differences between both regions (tensile and compressive) are quite evident and both models depict quite significant regression errors when the entirety of the data points are accounted for. Moving on to the analyses with MT, the results are quite similar, although exalted by the introduction of phase transformation and consequent amplification of the behavioural differences along the beam domain. Firstly, we may observe that, with both models, the results associated with the compressive region actually improve, which can be explained by the less pronounced increase of s for larger values of $\|\mathbf{F} - \mathbf{I}\|$. On the other hand, the goodness-of-fit results associated with the tensile data set (or the entirety of the data points) are much worse, which may be due to the overall increase of s , especially for the points subjected to larger strain, but also its stabilisation with respect to the RVE length, which, for these points, becomes less important. Indeed, neither of the proposed models seems to be able to capture these specific features with brilliant accuracy. In fact, with the exception of the compressive region of the bending beam, both models actually pose as rather underwhelming predictive tools of the importance of second-order homogenisation. From this, we may assume that such elementary, purely quantitative approach may not be sufficient to the assessment of the importance of second-order homogenisation, especially when complex phenomena that impacts the overall material behaviour to such large extent is present, in which case, additional parameters, associated with the specific constitutive model at hand, may also have to be accounted for and used for this predictive exercise. Nevertheless, the first gradient of the displacements is undoubtedly the crucial factor to take into account - note the miniscule value of the computed a parameter, which implies the larger weight of the denominator, in this case, the norm of the first gradient of the displacements.

The best-fit predictive curves for each region of the bending beam are graphically depicted in Figure 6.31, together with the corresponding data points.

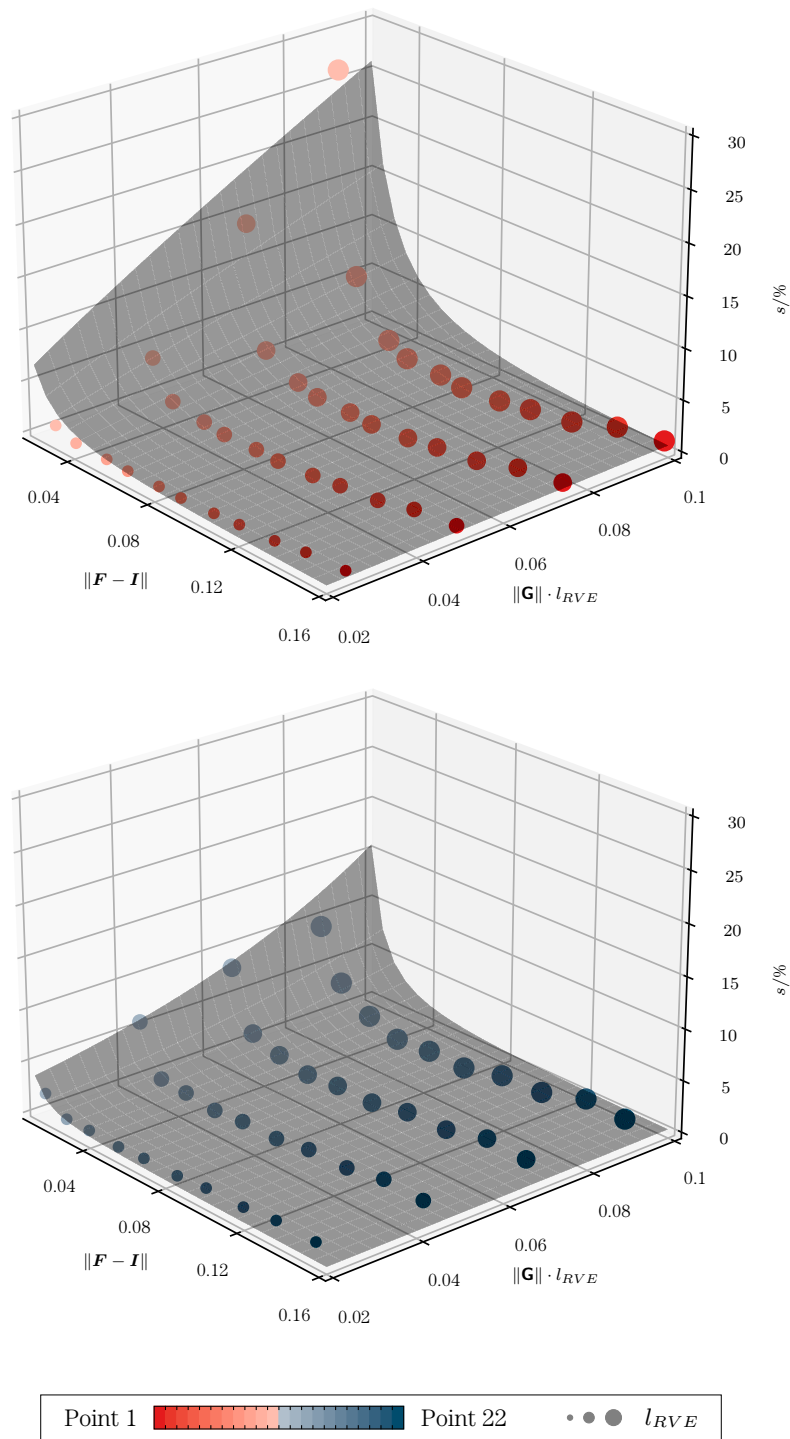


Figure 6.31: Scatter plots of the parameter s associated with the second-order homogenisation-based results of the analyses of the tensile region points (red points) and of the compressive region points (blue points), considering MT, and corresponding best-fit predictive curves.

Conclusions and Future Works

The main goal of this work consisted of studying the impact of the second-order computational homogenisation scheme and the associated RVE length on the characterisation of mechanically-induced martensitic transformation in polycrystalline austenitic steels and its consequent effects on the homogenised quantities and microstructural material behaviour. To that end, several analyses were conducted with both first and second-order homogenisation techniques. Moreover, in order to accurately assess the homogenisation scheme influence on martensitic transformation, analyses where this phenomenon is neglected were also performed.

7.1 Conclusions

Multi-scale models based on computational homogenisation provide a direct link between the overall macroscopic behaviour and the underlying microstructural features. As a result, when modelling materials that exhibit intricate phenomena at the microstructural level, their use can be incredibly beneficial. In this context, most relevant research is usually directed to standard first-order homogenisation schemes. However, these assume that the macroscopic deformation gradient is uniform within the RVE, such that solely linear deformation modes are transferred from the macro to the micro-scale. Second-order homogenisation-based multi-scale models involve the additional passing of quadratic deformation modes between scales and, therefore, constitute a more adequate tool for the analysis of complex deformations involving loadings such as bending or torsion.

Despite all the aforementioned qualities, the solution of FE^2 simulations involved in coupled multi-scale analyses may be computationally very costly, due to the large number of micro-scale problems that need to be resolved, and especially if a large number of grains and highly refined finite element meshes are admitted. In this work, several specimens and loading conditions were considered so as to gauge the relative effect of different macroscopic strain-gradients on martensitic transformation and on the second-order

homogenisation-based results. Moreover, the RVE length also plays an important role and several second-order analyses were also performed with distinct RVE lengths. For these reasons, the macroscopic, coupled multi-scale analysis with second-order homogenisation simply did not constitute a viable framework for the intended studies. Indeed, the analyses with second-order homogenisation were performed at specific material points and, thus, for a single RVE for each simulation, in what constitutes a decoupled micro-scale analysis. Nevertheless, so as to obtain these points' deformation histories, some form of preliminary coupled multi-scale analyses had to be performed. These were carried out considering the standard first-order homogenisation approach, that, coupled with the Taylor's boundary condition, leads to a constant deformation state within the RVE. Algorithmic simplifications developed around this detail enable a significant reduction of memory requirements and computational cost, and, thus, a more efficient performance of the coupled multi-scale analyses associated with the preliminary studies.

One of the key purposes of these studies is to capture the deformation histories of the points we wish to address by means of micro-scale analyses with second-order homogenisation and distinct RVE lengths. In an effort to obtain accurate results, the definition of the minimum number of grains (RVE size) is of the utmost importance. For one, the selected RVE should be representative of the whole material. Secondly, considering the anisotropic nature of the slip plasticity and martensitic transformation domains, the admitted RVE size should also represent an isotropic material, which is achieved by the increase in the number of grains contained within it. In this context, several analyses without martensitic transformation were performed for all specimens and distinct RVE sizes and the convergence of the homogenised macroscopic response for increasing number of grains was clearly observed.

While the analyses involved in the assessment of the RVE size were performed without martensitic transformation, these were subsequently repeated for the selected RVE size while admitting martensitic transformation. Comparing the results obtained under both constitutive behaviours allowed us to briefly study the main features associated with the martensitic transformation phenomenon, namely the promoting nature of deformation modes that favour the material volumetric expansion/growth, such as a tensile loading. By carefully tuning the ΔG_{mech} parameter to each specimen, we were able to address different transformation mechanisms (after and prior the onset of plastic slip), while still obtaining evident levels of transformed martensite. In either case, the complex coupling of phase transformation and slip plasticity is practically inevitable and was thoroughly discussed by means of the martensite volume fraction and accumulated plastic slip quantities. Specific features such as the displacement of the bending beam's neutral axis in the opposite direction to the center of curvature once the elastic behaviour is recovered in the bottommost, tensile-driven region of the beam are also reported and remarkable connections with specific details depicted by other quantities are also established.

Regarding the stage of the micro-scale analyses, a second convergence study was performed. Again, the first-order homogenisation scheme was considered; however, instead of the Taylor model, these analyses considered the standard periodic boundary condition,

which, as expected, lead to much faster convergence rates with respect to the increase of the RVE size.

The subsequent micro-scale analyses were performed with both first and second-order homogenisation schemes, and four points of interest were selected based on the norms of the first and second gradients of the macroscopic displacements. Here, the comparison of the results between both homogenisation approaches are quite similar regardless of if martensitic transformation is admitted or not. In detail, we observed that, besides the RVE length and the magnitude of the macroscopic second gradient, the magnitude of the first-order strain plays an important role on the divergence of the homogenised responses under the second-order framework from those obtained with the first-order homogenisation scheme. It was found that, for substantial differences to be observed, the magnitude of the second gradient of the displacements must be much larger than the norm of the first gradient of the displacements, which meets previous reports on this matter. This is the case of the points located within the vicinity of the bending beam's neutral axis, for which the introduction of the second-order scheme and corresponding consideration of quadratic deformation modes gives rise to significant differences in the homogenised microstructural responses. These differences are clearly observed with both constitutive models; however, when martensitic transformation is present, the divergence of the homogenised response is even more pronounced, thus confirming the importance of the second-order formulation on the accurate characterisation of phase transformation.

In the analyses associated with a larger magnitude of first-order strain, the homogenised responses are consistent regardless of the admitted homogenisation scheme and RVE length, which proves that size effects associated with the size of the micro-constituents are not captured by the considered standard second-order homogenisation approach, in which a first-order description is still employed at the RVE level. To render such details, a fully second-order homogenisation model, in which the micro-scale is also described by the second-order continuum mechanics theory, must be considered.

One aspect that must be emphasised is that, indeed, the direct impact of the martensitic transformation on the macroscopic material behaviour, characterised by means of the standard second-order homogenisation scheme, remains to be reviewed. As we previously referred the coupled multi-scale analyses based on second-order homogenisation simply did not pose a viable approach to the amount and sort of simulations performed in this work. Nevertheless, developments are continuously proposed to tackle this issue. One approach, for instance, may be to simply perform more approachable, preliminary analyses and, with the obtained data, carefully assess the critical points of the macroscopic specimen in which the use of the second-order homogenisation approach may be relevant and from that, perform a selective, coupled multi-scale analysis in which the determined critical points are computed with the FE^2 second-order homogenisation technique, whereas the remaining integration points still undergo the standard first-order homogenisation analysis. A first draft of this adaptive framework was initially proposed by [Rodrigues Lopes \(2019\)](#), in which a elementary criterion, based on the RVE length, the magnitude of the macroscopic

second gradient and the first-order strain, is introduced for the determination of the aforementioned critical points. In this work, an enhanced version of this criterion was proposed and calibrated with the results obtained from the refined bending beam along its thickness, which provides an adequate range of first and second-order gradients.

From this numerical study, we observed that the computed results are incredibly dependent on the constitutive behaviour of the material under analysis, which immediately poses a drawback to the eventual consistent use of such elementary numerical model. This is further confirmed by the equally different evolutions between the data points subjected to the compressive and tensile loading scenarios. While some discrepancies are already present when solely plastic slip is considered, the assumption of martensitic transformation and the associated favourable nature of the tensile deformation exalts the aforementioned differences and the consequent error of the regression. That being said, it is fair to assume that a more accurate predictive model of the required RVE length would require additional parameters related with the specific constitutive behaviour. Alternatively, it may also be the case that a purely quantitative framework is inherently limited. Indeed, if instead of the norm of the first gradient of the displacements, each of its components were accounted for and introduced in the numerical model, the prediction capabilities of the differences between the compressive and tensile regions of the bending beam would presumably be improved. Nevertheless, it is confirmed that the magnitude of the first-order strain is the most relevant factor, such that in many practical problems, the ratio between first and second gradients of the displacements may pose a sufficient tool for the eventual consideration or complete disregard of the second-order homogenisation scheme.

7.2 Future Works

In this work, the multi-scale analysis of the martensitic transformation phenomenon by means of second-order (as well as first-order) computational homogenisation has been thoroughly discussed. Nevertheless, many of the topics presented in this dissertation could be further explored. That being said, what follows are some suggestions for future research work that could help better understand the martensitic transformation and its consequent TRIP effect as a whole, but also the superior capabilities of the second-order homogenisation technique in the characterisation of martensitic transformation at the micro-scale and consequent overall material behaviour:

- Introduce the plastic domain of the martensitic phase in the constitutive model. It must be noted that any attempt at a comprehensive analysis of the impact of martensitic transformation on the macroscopic material behaviour is, to some extent, limited by the single assumption of its linear elastic behaviour, which drives the simulations to quite unrealistical results.
- Despite the computational advantages made possible by its use, the Taylor model is rather restrictive and leads to an overvalued material stiffness. Moreover, the Tay-

lor model does not consider the mechanical interactions amongst different heterogeneities of the RVE (between distinct solid phases, for instance). Thus, the Taylor model may be quite limited in circumstances in which the strain field at the interface between different solid phases may have a substantial impact on the macroscopic material behaviour. For this reason, a coupled multi-scale analysis based on first-order computational homogenisation with the standard periodic boundary condition could also be of practical interest.

- While the results of the final numerical model study and associated attempt at predicting the limited usefulness of second-order homogenisation were not as objectively satisfactory as one expected, its potential is undeniable. Therefore, with the goal of carrying out second-order homogenisation-based coupled, multi-scale analysis in a selective and efficient manner, it may be of practical interest to pursue a more accurate predictive model that would complement the second-order homogenisation adaptive framework proposed in [Rodrigues Lopes \(2019\)](#). To that end, the purely quantitative nature of the template expression considered so far may need to be disregarded and the inclusion of a larger amount and more diversified set of data points, associated with entirely different macroscopic deformations should be considered.
- Lastly, it may also be interesting to assess the resulting TRIP effect under the presence of size effects included by the size of the micro-constituents. Naturally, a purely standard second-order homogenisation scheme, as the one employed in this work, would not capture these details such that a fully second-order approach would have to be considered. However, the latter requires that the second-order continuum mechanics theory is employed at the RVE level and, therefore, the constitutive formulations followed in this work would not be applicable. Alternatively, a similar approach to that found in [Rys and Petryk \(2018\)](#) could be employed, in which the size effects associated with the size of the micro-constituents are artificially depicted by the introduction of a numerical *internal length scale* in the constitutive hardening law.

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