Multiscale thermomechanical analysis of multiphase materials



Sourena Yadegari Varnamkhasti

10 mm Multiscale thermomechanical analysis of multiphase materials

Sourena Yadegari Varnamkhasti



Invitation

You are cordially invited to the defense of my PhD thesis:

Multiscale thermomechanical analysis of multiphase materials

on Friday November 6, 2015 from 10:00 to 11:00 in the Senaatszaal of the Aula of Delft University of Technology

Prior to the defense, at 9:30 I will give a short introduction to my research



Sourena Yadegari Varnamkhasti

Propositions

appended to the dissertation Multiscale thermomechanical analysis of multiphase materials Sourena Yadegari Varnamkhasti

1- In a consistent thermomechanical formulation, a decomposition of the total deformation implies a decomposition of entropy, in a way in which the two decompositions are in a one to one correspondence with each other, i.e., for a given process there exists a unique sub-entropy that describes the thermal aspect of the same process. The converse of the proposition also holds.

2- The devil is in the details, and the details are in microstructures.

3- Adoption of multiscale methods by industry can be accelerated given than they are combined with solution methods that benefit from many-core architectures that are common in today's hardware. Example of this include usage of heterogeneous parallel schemes.

4- Mathematical objects and physical phenomena belong to two different domains. The former being abstract objects that only exist in a mathematician's mind, while the latter being 'observables' that may be measured objectively. The task of a modeler is to assign mathematical objects to a particular phenomenon that 'approximates' the best the observations.

5- "Essentially, all models are wrong, but some are useful" George E.P. Box.

A model cannot be judged to be right or wrong (based on absolute quantifiers); at best, it can approximate what has been observed. Instead, for the description of a given observable with multiple models, it can be stated that there is no right model; some just provide better approximations than others.

6- A community deprived of educational opportunities requires as much attention as a community exposed to food shortage. The negative consequences of the latter are immediate and life threatening, while the negative consequences of the former are gradual, yet could result in the latter.

7- If an activity is your intellectual habit, do not make it into your *work.

(Work is defined here as an activity that is performed for a limited amount of money in a limited amount of time.)

8- A debate ought not to be started unless at least one of the partners is willing to change his/her opinion at the end of the debate.

9- Advancements in computational technology have made the computer science courses an indispensable part of any serious graduate program that deals with numerical analysis.

Stellingen

behorende bij het proefschrift **Multiscale thermomechanical analysis of multiphase materials** Sourena Yadegari Varnamkhasti

1- In een consistente thermomechanische formulering impliceert een decompositie van de totale deformatie een decompositie van entropie, op zo'n wijze dat de twee decomposities in een één-op- één-verhouding staan tot elkaar, m.a.w., voor een bepaald proces bestaat er een unieke sub-entropie dat het thermische aspect van hetzelfde proces beschrijft. Het tegenovergestelde geldt ook.

2- De duivel schuilt in de details, en de details schuilen in microstructuren.

3- De ingebruikname van multischaalmethoden door de industrie kan versneld worden, op voorwaarde dat zij gecombineerd worden met oplossingsmethoden die profiteren van veel-kern architecturen die gangbaar zijn in de hardware van tegenwoordig. Een voorbeeld hiervan is het gebruik van heterogene parallelle schema's.

4- Wiskundige objecten en fysische fenomenen behoren tot twee verschillende domeinen. De eerstgenoemde soort bestaat uit abstracte objecten die uitsluitend in de geest van een wiskundige bestaan, terwijl de laatstgenoemde soort bestaat uit 'observabelen' die objectief gemeten kunnen worden. De taak van een modelleur bestaat eruit om wiskundige objecten toe te wijzen aan een bepaald fenomeen dat de waarnemingen het meest 'benadert'.

5- "In wezen zijn alle modellen fout, maar sommigen zijn nuttig" George EP Box.

Een model kan niet bestempeld worden goed of fout te zijn (op basis van absolute kwantoren); op zijn best kan het hetgeen dat waargenomen is, benaderen. In plaats daarvan kan voor de beschrijving van een bepaald observabele met meerdere modellen gesteld worden, dat er geen goed model is; sommige modellen verstrekken simpelweg betere benaderingen dan anderen.

6- Een gemeenschap die beroofd is van onderwijsmogelijkheden vergt evenveel aandacht als een gemeenschap die blootgesteld is aan voedselschaarste. De negatieve gevolgen van de laatstgenoemde zijn onmiddellijk en levensbedreigend, terwijl de negatieve gevolgen van de eerstgenoemde geleidelijk zijn, doch in de laatstgenoemde zouden kunnen resulteren.

7- Indien een activiteit uw intellectuele gewoonte is, maak er dan niet uw *werk van. ('Werk' wordt hier gedefinieerd als een activiteit die uitgevoerd wordt voor een beperkte hoeveelheid geld in een beperkte hoeveelheid tijd.)

8- Een debat behoort niet aangevangen te worden totdat ten minste één van de partijen bereid is om zijn/haar mening aan het einde van het debat te herzien.

9- De vooruitgang in computationele technologie heeft de informatica-opleidingen tot een onmisbaar onderdeel gemaakt van ieder serieus promotieprogramma dat zich bezighoudt met numerieke analyse.

Deze stellingen worden opponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotoren Prof.dr.ir. R Benedictus, Prof.dr.ir. ASJ Suiker en copromotor Dr. S Turteltaub

These propositions are considered opposable and defendable and as such have been approved by promotors Prof.dr.ir. R Benedictus, Prof.dr.ir. ASJ Suiker and co-promotor Dr. S Turteltaub

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PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universtiteit Delft, op gezag van de Rector Magnificus Prof. ir. K.C.A.M. Luyben, voorzitter van het College voor Promoties, in het openbaar te verdedigen op vrijdag 6 November 2015 om 10.00 uur door

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To My Parents

Foreword

This thesis summarizes the research I have done during my PhD study on different aspects of multiscale analysis in multiphase materials at the faculty of Aerospace Engineering at Delft University of Technology. The research was funded by STW (Stichting Technische Wetenschappen) through the Multiscale Simulation Techniques (MuST) project.

I would like to acknowledge my co-promotor Sergio Turteltaub and second promotor Akke Suiker for providing me the opportunity to do research in the field of numerical analysis. I have benefited greatly by their support, attention to details and thorough analysis of problems I encountered while doing research. Our long and engaging discussions were very pleasant and often provided me with stimulating and rich ideas to tackle problems at hand. I am greatful for their assistance on grammatical corrections of the manuscript. I am also grateful for the support of Rinze Benedictus in his role as first promotor.

Next, I thank Piet Kok (Tata Steel) for providing the geometrical microstructures of multiphase steels, which are used extensively through this manuscript. I also thank Gertjan Kloosterman (Dassault Systemes) and Eric van der Giessen for many useful suggestions and discussions we had during the user committee meetings. My thanks also go to Anke Hans for her constructive feedback on the propositions and the Dutch translation of the summary. Gratitude goes to Jan Hol and Laura Chant for their assistance in providing the computational resources and administrative support, as well as my former officemates Pooria Pahlavan, Ke Liang, Weiling Zheng, Sathiskumar Ponnusami and Daniël Peeters for creating a pleasant atmosphere and interesting discussions.

Summary

The thermomechanical simulation of materials with evolving, multiphase microstructures poses various modeling and numerical challenges. For example, the separate phases in a multiphase microstructure can interact with each other during thermal and/or mechanical loading, the effect of which is significantly more complicated than the individual behavior of the phases. The interactive behavior also depends on the specific volume fractions and spatial distribution of the individual phases. An accurate modeling of the phases requires a thermodynamically consistent formulation and a robust numerical implementation of the evolution of the corresponding observable and internal variables. The complex nonlinear characteristics of these micromechanical models introduce substantial challenges with respect to their upscaling towards higher levels of observation, as necessary for analyzing large-scale engineering problems in a computationally efficient way. The work presented in this thesis addresses these aspects in detail by focusing on a class of multiphase steels, which are the so-called transformation-induced plasticity (TRIP) steels. This class of structural steels shows an excellent combination of strength and ductility. The transformation-induced plasticity effect can be ascribed to the presence of grains of metastable austenite that are surrounded by ferritic grains. The austenite can undergo a phase transformation when subjected to thermal and/or mechanical loading, thereby introducing an increase in the effective material strength. In addition, both the austenite and the ferritic matrix may deform plastically, which increases the overall ductility of the material. In order to explore the complex micromechanical characteristics and the practical application of this material in more detail, three main research questions were identified, of which the first one is: (1) How can a TRIP steel microstructure be modelled in a fully thermodynamically consistent way? The thermomechanical coupling is particularly relevant since in TRIP steels the phase transformation occurring during mechanical loading is accompanied by the release of a substantial amount of energy (latent heat) that, in turn, affects the mechanical response of the material. The second research question formulated is: (2) How does the response of a TRIP steel microstructure depend on the spatial distribution of the austenitic phase within the ferritic matrix? From the viewpoint of practical applications, the attention here is focused on comparing the response of a TRIP steel sample with a banded austenitic microstructure to that of a sample with randomly distributed austenitic grains. Considering the large number of degrees of freedom of these and other engineering problems, a computationally efficient implementation of the micromechanical model is necessary. This issue is reflected by the third research question, which reads: (3) Is it possible to include the micromechanical constitutive behavior and geometry of the individual phases within an computationally efficient multiscale formulation?

For answering the three research questions above, the thermomechanical behavior of the TRIP steel phases is modelled in a fully coupled way, where the generation of heat associated to the martensitic phase transformation and the plastic deformation are accounted for explicitly in the thermodynamic formulation. In analogy with the decomposition of the deformation, the entropy density is separated in a reversible contribution, a transformation contribution, a plasticity contribution and a thermal-mechanical coupling contribution. The last term follows from combining mechanical and thermal constitutive information of the individual phases with basic thermodynamical requirements. One of the observations resulting from this approach is that for a single crystal of austenite the increase in temperature associated with the latent heat of transformation reduces the transformation rate and significantly reduces the transformation-induced plasticity effect. However, for an aggregate of austenitic and ferritic grains, which is representative of a TRIP steel, the delay in the transformation-induced plasticity effect due to latent heat is relatively small, since the ferric matrix absorbs the latent heat generated in the austenite and thus effectively acts as a thermal sink. To evaluate the influence of the spatial distribution of the austenitic (secondary) phase within the ferritic matrix, the effective responses for banded and dispersed austenitic microstructures are computed by means of numerical homogenization. A comparison of these microstructures shows that banded microstructures may allow for plastic localization in the ferritic matrix, which, in comparison to dispersed microstructures, diminishes the strengthening effect provided by the austenitic phase. For the performance of more demanding computational simulations at higher (macroscopic) scales of observation, an efficient multiscale approach termed the generalized grain cluster method (GGCM) was developed. The method is suitable for the prediction of the effective macroscopic behavior of an aggregate of single-crystal grains composing a multiphase steel. The GGCM is based on the minimization of a functional that depends on the microscopic deformation gradients in the grains through the equilibrium requirements of the grains as well as kinematic compatibility between grains. By means of the specification of weighting factors it is possible to mimic responses falling between the Taylor and Sachs bounds. The numerical computation is carried out with an incremental-iterative algorithm based on a constrained gradient descent method. For a multiscale analysis, the GCCM can be included at integration points of a standard finite element code to simulate macroscopic problems. A comparison with FEM direct numerical simulations illustrates that the computational time of the GGCM may be up to about an order of magnitude lower. In large-scale FEM models for structural applications, the responses at material point level thus may either follow from the GGCM alone, or from combining this method with fully-resolved FEM modeling at the level of individual grains (i.e., a combined GGCM - FE^2 approach), depending on the required resolution.

Samenvatting

De thermomechanische simulatie van materialen met evoluerende, meerfasige microstructuren poneert diverse modelmatige en numerieke uitdagingen. Zo kunnen bijvoorbeeld de afzonderlijke fasen in een meerfasige microstructuur tijdens thermische en/of mechanische belasting met elkaar interacteren, waarvan het effect significant gecompliceerder is dan het individuele gedrag van de fasen. Het interactieve gedrag hangt ook af van de specifieke volumefracties en de ruimtelijke verdeling van de afzonderlijke fasen. Een nauwkeurige modellering van de fasen vereist een thermodynamisch consistente formulering en een robuuste numerieke implementatie van de evolutie van de overeenkomstige waarneembare en interne variabelen. De complexe non-lineaire eigenschappen van deze micromechanische modellen introduceren aanzienlijke uitdagingen inzake de opschaling naar hogere niveaus van observatie, hetgeen vereist is voor de rekentechnisch-efficiënte analyse van grootschalige ingenieursproblemen. Het werk dat in dit proefschrift gepresenteerd is adresseert deze aspecten in detail door te focussen op een klasse van meerfasige staalsoorten, de zogeheten transformatie-geïnduceerde plasticiteit (TRIP) stalen. Deze klasse van constructiestaal vertoont een excellente combinatie van sterkte en ductiliteit. Het transformatie-geïnduceerde plasticiteitseffect kan worden toegeschreven aan de aanwezigheid van korrels van metastabiel austeniet die omringd zijn door ferritische korrels. Het austeniet kan een fasetransformatie ondergaan wanneer deze onderworpen wordt aan thermische en/of mechanische belasting, welk een verhoging in de effectieve materiaalsterkte veroorzaakt. Bovendien kunnen zowel het austeniet als de ferritische matrix plastisch vervormen, hetgeen de totale ductiliteit van het materiaal doet toenemen. Om de complexe micromechanische eigenschappen en de praktische toepassing van dit materiaal in meer detail te onderzoeken werden drie hoofdonderzoeksvragen geïdentificeerd, waarvan de eerste luidt: (1) Hoe kan een TRIP-staal microstructuur op een volledig thermodynamisch consistente manier gemodelleerd worden? Het thermomechanisch koppelen is in het bijzonder relevant omdat in TRIP-stalen de fasetransformatie die optreedt tijdens mechanische belasting gepaard gaat met de afgifte van een aanzienlijke hoeveelheid energie (latente warmte) die op zijn beurt invloed heeft op de mechanische respons van het materiaal. De tweede onderzoeksvraag die geformuleerd is luidt: (2) Hoe hangt de reactie van een TRIP-staal microstructuur af van de ruimtelijke verdeling van de austenitische fase binnen de ferritische matrix? Beschouwd vanuit het oogpunt van praktische toepassingen wordt de aandacht hier gericht op het vergelijken van

de respons van een TRIP-staal proefstuk met een gelaagde austenitische microstructuur met die van een proefstuk met willekeurig gedistribueerde austenitische korrels. Gezien het grote aantal vrijheidsgraden van deze en andere ingenieursproblemen, is een computationeel efficiënte implementatie van het micromechanische model noodzakelijk. Deze kwestie wordt weerspiegeld door de derde onderzoeksvraag, die luidt: (3) Is het mogelijk om het micromechanische constitutieve gedrag en de geometrie van de afzonderlijke fasen in een rekenkundig-efficiënt meerschalen-formulering te omvatten?

Om de drie bovengenoemde onderzoeksvragen te beantwoorden, wordt het thermomechanische gedrag van de TRIP-staal fasen op een volledig gekoppelde wijze gemodelleerd, waarbij de warmteontwikkeling geassocieerd met de martensitische fasetransformatie en de plastische deformatie expliciet in de thermodynamische formulering worden meegenomen. In analogie met de decompositie van de vervormingstensor is de entropiedichtheid samengesteld uit een omkeerbare bijdrage, een transformatie-bijdrage, een plasticiteits-bijdrage en een thermisch-mechanische koppelingsbijdrage. De laatste term volgt uit het combineren van de mechanische en thermische constitutieve informatie van de afzonderlijke fasen met elementaire thermodynamische condities. Een van de observaties die uit deze benadering voortkomt is dat voor een enkele austenietkristal de temperatuurstijging geassocieerd met de latente warmte van transformatie de transformatiesnelheid reduceert en het transformatie-geïnduceerde plasticiteitseffect op significante wijze vermindert. Echter, voor een aggregaat van austenitisch en ferritische korrels, welk representatief is voor een TRIP-staal, is de vertraging in het transformatiegeïnduceerde plasticiteitseffect door latente warmte relatief klein, aangezien de ferritische matrix de latente warmte gegenereerd in het austeniet absorbeert, en dus effectief als een warmteafvoer acteert. Om de invloed van de ruimtelijke verdeling van de austenitische (secundaire) fase binnen de ferritische matrix te evalueren, worden de effectieve antwoorden voor gelaagde en willekeurig verdeelde austenitische microstructuren berekend middels numerieke homogenisatie. Een vergelijking van deze microstructuren toont aan dat gelaagde microstructuren plastische lokalisatie in de ferritische matrix kunnen toestaan die, in vergelijking met willekeurig verdeelde microstructuren, vermindert het versterkende effect dat wordt veroorzaakt door de austenitische fase. Om rekenintensieve simulaties op hogere (macroscopische) schalen van observatie uit te kunnen voeren, werd een efficiënte meerschalige benadering, genaamd de Generalized Grain Cluster Method (GGCM), ontwikkeld [83]. De methode is geschikt voor de voorspelling van het effectieve macroscopische gedrag van een aggregaat van monokristallijne korrels die een meerfasig staal karakteriseren. De GGCM is gebaseerd op de minimalisatie van een functionaal die afhangt van de microscopische deformatiegradiënten in de korrels door middel van de evenwichtseisen van de korrels alsmede de kinematische compatibiliteit tussen de korrels. Door middel van de specificatie van weegfactoren is het mogelijk om de responsies na te bootsen die tussen de Taylor- en Sachs-grenzen vallen. De numerieke berekening is uitgevoerd met een incrementeel-iteratief algoritme gebaseerd op een constrained gradient descent method. Voor een multischaal-analyse kan de GGCM worden gekoppeld aan de integratiepunten van een standaard eindige-elementencode om macroscopische problemen te simuleren. Een vergelijking met directe FEM simulaties illustreert dat de berekeningstijd van de GGCM een orde van grootte lager kan liggen. In grootschalige FEM modellen voor structurele toepassingen kan de responsie op materiaalpuntniveau aldus volgen uit ofwel de GGCM alleen, ofwel vanuit een combinatie van de GGCM methode en een gedetailleerde FEM modellering op het niveau van individuele korrels (i.e., een gecombineerde GGCM-FE² benadering), afhankelijk van de gewenste resolutie.

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Introduction

The improvement of material properties involves a time-consuming cycle of manipulation of the underlying microstructure, e.g., chemistry, composition and processing, and testing of the modified material. While some "rule of thumb" guidelines can be used to enhance the properties in the direction that is intended, these rules cannot achieve the level of targeted goals which are dictated by a design bureau or market requirements. Understanding the effect of different parameters at the microscopic level on the (effective) response of the material requires a detailed description of the geometry and parameters. Together these two can grow into a huge set of data. The computational power that can obtain a solution on such a detailed domain in an acceptable amount of time is scarce by even today's computational resources. Multiscale methods, among other methods, can be used to reduce the computational cost by decomposing a single, detailed simulation of the domain into multiple, concurrent or hierarchical sets of simulations.

1.1 Multiscal methods: Overview

Multiscale methods can be classified either as hierarchical or concurrent [39], although this classification is not mutually exclusive since concurrent methods can be embedded in a hierarchical approach when bridging disparate length scales and, conversely, hierarchical methods can be used to provide constitutive information in a concurrent calculation, as explained below. Hierarchical methods use a lower-scale model to determine an effective material behavior that is used in a large-scale problem. In this approach, the lower-scale problem is weakly coupled to the large-scale problem and in general can be solved independently of the large-scale problem. The coupling is achieved through suitable initial, boundary and/or average conditions for the representative volume element (RVE) associated to each macroscopic point. An attractive feature of the hierarchical approach is its modularity: numerical codes or models for different length scales can be developed independently from each other and connected through a relatively simple interface, which also simplifies parallelization. The lower-scale problem in hierarchical methods can be solved analytically or semi-analytically (see, e.g., [11]). In situations where no analytical techniques can be used, the hierarchical approach is implemented in a fully numerical fashion at the level of an RVE (i.e., its purpose is to numerically provide macroscopic constitutive information during the simulation). In concurrent methods, the approach is to simultaneously solve the small and large-scale models, typically within the same domain representing the large-scale domain, which results in a strong coupling between scales. The intention is to use the small-scale model sparsely and the method requires a suitable coupling between the regions where each model is used through a so-called handshake region, where information is passed back and forth from the distinct models. An illustrative example of a concurrent approach is the simulation of nanoindentation, where an atomistic model is used in regions close to the tip of the indenter, whereas a discrete dislocation approach, which is computationally less costly, can be used in regions away from the nanoindenter (see, e.g., [16]). However, the advantage of a computationally efficient coarse model is often limited to situations where there is a priori knowledge of the applicability of each model. Although the concurrent approach does not enjoy the modularity advantage of hierarchical methods, it is usually deemed necessary when there is a strong coupling between two scales (e.g., development of discrete cracks or strain localizations), which prevents the use of a hierarchical approach. A common problem of fully numerical algorithms (either hierarchical or concurrent) is that they are computationally very demanding. Adaptive procedures that combine concurrent and hierarchical approaches are useful for mentioned computationally expensive multiscale problems as they provide a balance between computational cost and accuracy. Within the context of finite element simulations, adaptive techniques have traditionally been used for the socalled hp-adaptivity, where the mesh size parameter h and/or the polynomial order p of the shape functions are modified depending on a desired error tolerance ([1, 28]). In the same manner, model refinement can improve the accuracy and it fits naturally within a concurrent multiscale method ([46, 47]). The basic strategy is to assume the existence of a so-called fine-scale model that provides the most accurate response of a material. Usually the fine-scale model is never solved (as in fact it might not be known). Rather, simpler models are used and, in conjunction with the solution of a so-called surrogate problem (adjoint problem), an error estimate can be obtained for each model. A less rigorous but computationally more efficient approach is to use (a posteriori) error indicators, which are useful whenever the formulation of the adjoint problem is not known, as is the case for complex constitutive models. Depending on a quantity of interest to be controlled

(the goal, usually a parameter relevant for the large-scale solution), a choice can be made regarding the use of a specific coarse scale model in a given region of the domain. The computationally less expensive coarse model is used whenever it provides a reasonable response compared to the fine-scale model (model coarsening) and, conversely, lower scale models are selectively applied in regions and/or time intervals where they are deemed necessary (model refinement). The key ingredient in this strategy is the identification of a suitable quantity of interest that indicates whether model refinement is required or model coarsening is possible. An objective of this thesis is to develop methods with various degrees of complexity and accuracy such that an adaptive model refinement methodology can employ them to determine the complex material behavior as in the case of multiphase materials.

1.2 Multiscale Modeling of Multiphase Materials

The modeling of multiphase materials for engineering applications, such as forming and crash simulations, require models that on the one hand are sufficiently accurate to represent the influence of microstructural information on the constitutive response of a material and , on the other hand, are sufficiently simple to achieve a solution within a reasonable computational time. Furthermore, the evolution of material at the microscale is (often) a thermomechanical process rather than a purely thermal or mechanical process. Thus, for any multiscale method to capture the effective response of the underlying material one has to employ a set of thermomechanical constitutive laws. A prominent example of this class of materials is the transformation-induced plasticity (TRIP) steels. A distinctive characteristic of a TRIP steel is the presence of grains of metastable austenite inside the ferritic matrix. The ferritic phase can deform plastically while the austenitic phase can transform into the harder, brittle martensitic phase upon application of thermomechanical loading.

As the focus of this thesis is on the computational aspects of TRIP steels rather than the material modeling, in order to familiarize the reader with the underlying material, the following subsection describes shortly the metallurgical properties of TRIP steels.

1.2.1 Multiphase TRIP-steels; Composition and chemistry

A typical microstructure of TRIP-steel consists of ferrite as the most dominant phase, accompanied by bainite, retrained austenine and occasionaly a small fraction of thermal martensite, at room temperature. Intercritical ferrite forms up to 75% (volumetric) of the microstructure. Ferrite has a body-centered cubic (BCC) lattice and it is the softest phase in the mixture. Nano-indentation tests by Furnémont [21] indicate the hardness of ferrite in a typical multiphase steel to be about 5 GPa. The size of ferritic grains in a typical TRIP-steel varies between 5 to 10 μm , according to [21, 32].

As opposed to ferrite, bainite does not possess a single-phase structure, with the microstructure consisting of an assembly of layers of iron carbide (cementite) and bainitic ferrite. The formation of bainite is achieved by an isothermal process which holds bainite at a temperature between 600 and 700 K. Bainite is a harder phase than the ferritic phase duo to its smaller grain size and the existence of carbide precipitations. The size of bainite grains ranges typically between 1 to 6 μm . Additionally, a higher dislocation density for initial bainite is reported in [32]. The composition of chemicals in TRIP steels is such that the formation of carbides is restricted, resulting in a bainite that is almost carbon-free, but still possesses a fine plate-like structure [32, 21, 31].

As opposed to other stable phases in TRIP steel, retained austenite is a metastable phase. Austenite possesses a face-centered cubic (FCC) structure and it is stable at a high temperature. Several factors contribute to metastability of austenite at room temperature, such as local carbon enrichment and the constraining effect from the neighboring grains. The transformation of metastable austenite into martensite is achieved through a combination of mechanical and thermal loading, thus generating the TRIP-effect. A rapid cooling (or quenching) of austenite may result into a small fraction of martensite (called thermal martensite). Martensite has a body-centered tetragonal structure (BCT). The brittleness of martensite can be attributed to supersaturated interstitial carbons, which results in strain fields that restrict the movement of dislocations in the lattice.

1.2.2 Thermomechanical modeling and simulation in TRIP steels

In oder to describe the crystal plasticity and transformation at the level of a single grain, kinematics of the two phenomena are expressed by means of an averaging scheme coupling the lower microscale to the upper microscale. Both processes can be written as a weighted average of individual systems that account for their relevant processes [75]. Together with proper evolution laws, constitutive relations can be obtained by integrating the resulting equations from the so-called Coleman-Noll procedure [15]. Because of the thermomechanical nature of these processes, it is desirable to incorporate the thermoelastic coupling effect into the set of kinematical laws [72]. Upon the introduction of such generalization, the thermomechanical consistency of the model cannot be satisfied by using the same decomposition and integration schemes as before. Neglecting the consistency could lead to models that violate the second law of thermoelastic coupling effects.

The retained (metastable) austenite in TRIP steels can be transformed into martensite through application of thermal and mechanical loadings. This process is also accompanied by a relative (positive) change of volume. The plastic deformation in the austenitic and ferritic phases is also a dissipative process. Therefore, a fully coupledthermomechanical simulation of TRIP-steels is justified by considering the fact that both of these processes (phase transformation and plasticity) can interact with each other via mechanical and thermal loadings. As such, neglecting the coupling effects of thermal and mechanical fields for any non-isothermal process, e.g., an adiabatic situation or a high rate test, can lead to unreliable results. It is therefore desirable to study these phenomena in a fully coupled thermomechanical numerical scheme.

1.3 Objectives and outlines

The objective of the current manuscript is twofold: 1- To better understand the multiphysics and interaction of thermal and mechanical fields in multiphase steels, both at the level of the modeling and numerical simulations, and 2- To bring together the tools and techniques that enable an efficient multiscale simulation of materials with complex microstructures. In doing that, we first turn our attention to the thermomechanics of TRIP steels and identify the current pitfall and shortcomings. The proposed model is then used to simulate and investigate the effect of the mechanical and thermal fields on each other. Next, the underlying material is used to build numerical tools and homogenization techniques that can make a link between the mechanical properties of the material at the microscale and its effective response at the macroscale. In the subsequent sections, purely mechanical simulations are considered. The focus of the thesis will be to understand the effect of texture on the overall response of these microstructures through the direct numerical simulation (DNS) as well as the development of an algebraic, cost-efficient method for obtaining the effective properties of the microstructure. The two described sections are outlined as follows:

1. Thermo-mechanical interaction in TRIP steels: The thermomechanical modeling and simulation of low-alloyed TRIP steels is analyzed, by taking into account the coupling between the thermal and mechanical fields (chapter 2). The two-way coupling is considered both at the level of the micromechanical (mesoscale) model as well as a set of numerical simulations. In order to construct the constitutive relations, the model proposed by Turteltaub and Suiker [75] and expanded by Tjahjanto et. al. [72] is adopted and the kinematics of the model is extended by considering the thermal deformation gradient as a function of the reversible entropy. Unlike the classical situations, the resulting equations obtained from the Coleman-Noll procedure cannot be decoupled from each other. This coupling leads to challenges in the integration of the constitutive relations. The derivation is proceeded by considering the internal energy potential instead of the Helmholtz free energy potential, as is the case for the decoupled situations. The thermomechanical driving forces are identified and the effect of the thermal deformation gradient in the terms is highlighted. For the numerical simulations, the linear momentum and the energy equations are solved simultaneously (coupled system) in a fully-implicit numerical scheme. The coupling effects are illustrated for both single crystals of austenite and aggregates of austenitic and ferritic grains. The interaction of the thermal and the mechanical fields are highlighted through these numerical examples and the differences with the purely mechanical simulations

are pointed out.

2. Homogenization of microstructures: The influence of the spatial distribution of the secondary phase, i.e., the austenitic phase, embedded in a ferritic matrix is analyzed in chapter 3. The main tool for this is the numerical homogenization of representative volume elements (RVEs) with distinct microstructural morphologies. For that, several volume elements (VE) with increasing number of grains are considered. In each VE, a random distribution of crystal orientation is assigned to both phases. The VEs are simulated subjected to periodic, non-redundant, boundary conditions. The macroscopic responses in VEs are analyzed and the minimum number of grains to form an RVE is identified. A material with the second phase clustered in a band-like region is compared with a benchmark distribution, which consist of microstructures with a randomly-dispersed secondary phase inside the matrix. Key parameters that affect the macroscopic response are compared between the banded and the disperse samples with the same volume fraction. An efficient, algebraic, method for the calculation of the macroscopic response of typical microstructure, that compromises of Voronoi cells of arbitrary shape, is presented in chapter 4. A key assumption of constant strain per grain is introduced in order to simplify and reduce the number of unknowns in the solution space. It is shown that at the interface of two neighboring grains the compatibility equation has to be considered alongside the linear momentum equation. An iterative minimization scheme based on the *constrained gradient descent* is adopted for numerical solution of the discretized field equations (the linear momentum and the compatibility). To demonstrate the dependency of the solution method on the initial estimate at each step, different methods for constructing the initial estimate are discussed and their effects on the macroscopic response are discussed through a set of numerical examples. Finally, the capability of the method in capturing a broad range of responses in the underlying material is demonstrated and the influencing parameters on the effective response of the domain are calibrated in order to approximate the macroscopic response of the DNS.

1.4 Nomenclature

The scheme of notation described here is used consistently throughout this manuscript. Scalar quantities are written as light-face italic letters. Unless mentioned explicitly, vectors are denoted as boldface lower case (e.g., $\mathbf{a}, \boldsymbol{\xi}$). Second order tensors are written as boldface capital letters (e.g., $\mathbf{A}, \boldsymbol{\Sigma}$), where as the fourth order tensors are denoted as black board capital letters (e.g., \mathbf{C}, \mathbf{A}). Boldface sans-serif letters are used to denote matrices and vectors in the linear algebra context, e.g., $\mathbf{L}\mathbf{x} = \mathbf{f}$, for the linear transformation \mathbf{L} acting on vector \mathbf{x} . Cartesian components of vectors and tensors are expressed in an orthonormal coordinate system, i.e., the covariant and contra-variant components are the same. For the index notation, and unless indicated otherwise, implicit summation on re-

peated indices is assumed. A single contraction between two second order tensors or a tensor and vector is assumed as \mathbf{FF}^{T} or \mathbf{Fx} , respectively. A double contraction is implied between a fourth order tensor and a second order tensor, e.g., \mathbb{CE} and the full contraction between two tensors of the same rank is denoted by a centered dot. The tensor product (dyadic product) between two tensors is denoted by $\mathbf{m} \otimes \mathbf{n}$, i.e., $m_i n_j$. The transpose of a tensor and the differential operator are denoted by a superscript, roman font, T and d, respectively. Unless idicated otherwise, subscripts A, M and F indicate the quantities corresponding to material properties of austenite, martensite and ferrite, respectively.

CHAPTER 1. INTRODUCTION

2

Coupled thermomechanical modeling and simulation of TRIP steels

¹Low-alloyed multiphase steels assisted by transformation-induced plasticity, commonly known as TRIP steels, have been identified as ideal candidates for applications requiring high strength-to-mass ratios, particularly in the automotive industry where fuel efficiency and safety are primary concerns. A distinctive characteristic of a TRIP steel is the presence of grains of metastable austenite in its microstructure, with volume fractions usually between 5 to 20%, embedded in a ferrite-based matrix [61, 32, 34]. Due to the addition of small quantities of alloying elements such as Al or Si, the austenite is retained in the material during processing as it is cooled down to room temperature. The presence of retained austenite is critical for the transformation-induced plasticity effect. Indeed, upon subsequent application of mechanical and/or thermal loads during forming or operation, the austenite may transform into a harder phase, martensite, providing the material with enhanced work-hardening characteristics compared to more conventional high-strength steels.

In order to understand the details of the transformation-induced plasticity effect, various models have been proposed in the literature ranging from micromechanically-based formulations to purely phenomenological constitutive relations at a macroscopic level [6, 30, 41, 59, 38, 42, 37, 56, 54]. These models have been mostly applied to study the *isothermal* response of a multiphase steel, typically at room temperature. Tensile tests

¹This chapter is based upon S. Yadegari, S. Turteltaub, A.S.J. Suiker, Mech Mat, 53, 1-14, 2012

conducted at various externally-controlled temperatures have shown that the martensitic transformation rate strongly depends on temperature (see, e.g., [5, 36]), which indicates that a comprehensive investigation of this class of steels should include their thermal behavior. The thermal sensitivity of TRIP steels has been studied under different thermal loading paths in [72], where it was shown that the onset of inelastic response decreases with temperature. Nonetheless, that study also showed that upon continued deformation, the strength of a TRIP steel becomes the largest at the lowest temperature considered in the analyses. The simulations presented in [72] were carried out under the assumption that the temperature was externally-controlled and uniform within the sample, hence the energy equation was trivially satisfied. However, during actual operational conditions, the temperature is usually not controlled, hence the thermal behavior of the material depends on the internal heat generated by inelastic processes (transformation and plasticity). In particular, the phase transformation is accompanied by the release of a considerable amount of energy per unit volume (latent heat) which affects the local temperature as shown in non-isothermal tensile tests presented in [51]. Under those circumstances, the thermomechanical behavior of a material sample needs to be obtained as the solution of a coupled problem involving the balance of both linear momentum and energy. The coupling occurs in both directions since the thermal response is affected by the internal heat stemming from mechanical processes and, conversely, the mechanical response depends on the thermal behavior.

The present contribution focusses on the formulation and the numerical analysis of a fully-coupled thermomechanical model for multiphase steels. The model, presented in Section 2.1, is based on the work originally proposed in [75, 73], which was expanded in [70] to account for crystalline plasticity in the austenitic phase and the surrounding matrix and further extended in [72] to incorporate thermoelastic coupling effects. From a theoretical point of view, one important refinement in the present formulation relates to the decomposition of the entropy density, where the entropic counterpart of the thermal strain is *derived* from thermodynamic requirements. Although the resulting formulation is similar to that presented in [72], the new entropy decomposition formally provides thermodynamic *consistency*. This model has been implemented in a fully-implicit numerical framework in order to solve simultaneously the equations of linear momentum and energy. To illustrate the predictions of the model, Section 2.2.1 includes simulations of a single crystal of austenite undergoing plastic deformation and/or phase transformation. These simulations are carried out at different initial temperatures and compared to the predictions of isothermal simulations. Subsequently, in Section 2.2.2, the basic behavior of a grain of austenite embedded in a ferritic matrix is simulated to study the influence of the surrounding matrix on the thermomechanical behavior of austenite.

2.1 Thermomechanical model for multiphase steels

In this section, a constitutive model is developed to describe the thermo-elasto-plastic response of single-crystal FCC austenite that may transform into one or more martensitic BCT phases (referred to as *transformation systems*). The model is based on the work presented in [75, 73, 70, 72] and incorporates new features to satisfy consistency from a thermodynamical point of view. To this end, the deformation gradient and the entropy are decomposed analogously to each other with special attention given to the terms that account for the coupling between the entropy and the deformation.

2.1.1 Kinematics

To describe the deformation of a single-crystal grain of austenite that may partially or totally transform into martensite, the total deformation gradient \mathbf{F} is multiplicatively decomposed as

$$\mathbf{F} = \mathbf{F}_{e} \mathbf{F}_{th} \mathbf{F}_{p} \mathbf{F}_{tr}, \qquad (2.1)$$

where \mathbf{F}_{e} , \mathbf{F}_{th} , \mathbf{F}_{p} and \mathbf{F}_{tr} are the elastic, thermal, plastic and transformation contributions to the total deformation gradient, respectively. This decomposition defines several (local) intermediate configurations \mathcal{B}_{i} (i = 1, 2, 3) between the reference configuration \mathcal{B}_{0} (chosen to coincide with a stress-free state of the underlying material) and the current configuration \mathcal{B} as shown schematically below



The transformation deformation gradient includes lower length-scale kinematical information of the product martensitic phase(s) through crystallographic information derived from the theory of martensitic transformations [75]. A material point x in the reference configuration \mathcal{B}_0 is interpreted as representing a small neighborhood containing a mixture of austenite and one or more martensitic transformation systems. The mixture is quantified using the volume fractions $\xi^{(\alpha)}$ of the martensitic transformation system α (measured per unit referential volume). The total possible number of transformation systems for an FCC to BCT transformations is M = 24. Each transformation system characterized by a pair of vectors, $\mathbf{b}^{(\alpha)}$ and $\mathbf{d}^{(\alpha)}$ that represent, respectively, the shape strain vector and the normal to the habit plane (interface between a martensitic transformation system α and austenite). The (unconstrained) transformation deformation gradient associated with an individual martensitic transformation system α is $\mathbf{F}^{(\alpha)} = \mathbf{b}^{(\alpha)} \otimes \mathbf{d}^{(\alpha)}$ and the corresponding change in volume due to the transformation is, for any system α , given by

$$J_{\rm tr}^{(\alpha)} = \det \mathbf{F}^{(\alpha)} = 1 + \delta_{\rm T} \text{ with [75]}$$
$$\delta_{\rm T} := \mathbf{b}^{(\alpha)} \cdot \mathbf{d}^{(\alpha)} . \tag{2.2}$$

The time rate of change of the effective transformation gradient of a mixture, $\dot{\mathbf{F}}_{tr}$, is given by the volume average (in the reference configuration) of the rates of the transformation deformation gradients of all active martensitic transformation systems, which can be expressed as (see [70, 75, 73])

$$\dot{\mathbf{F}}_{\rm tr} = \sum_{\alpha=1}^{M} \dot{\xi}^{(\alpha)} \mathbf{b}^{(\alpha)} \otimes \mathbf{d}^{(\alpha)}, \qquad (2.3)$$

The evolution of the plastic deformation is described by the effective plastic velocity gradient L_p that is related to the effective plastic deformation gradient F_p through

$$\mathbf{L}_{\mathrm{p}} = \dot{\mathbf{F}}_{\mathrm{p}} \mathbf{F}_{\mathrm{p}}^{-1}.$$
 (2.4)

The effective plastic velocity gradient is expressed as a volume average, measured in the second intermediate configuration \mathcal{B}_2 , of the plastic velocity gradients of the austenitic phase, $\mathbf{L}_{p,A}$, and the martensitic phases, $\mathbf{L}_{p}^{(\alpha)}$, see [70]. In the present model it is assumed that the high-carbon martensite does not deform plastically (i.e., $\mathbf{L}_{p}^{(\alpha)} = \mathbf{0}$), in accordance to experimental observations, see [33]. Consequently, the effective plastic velocity gradient can be related to the plastic gradient of the austenitic phase in the second intermediate configuration as [70]

$$\mathbf{L}_{\mathrm{p}} = \tilde{\xi}_{\mathrm{A}} \mathbf{L}_{\mathrm{p},\mathrm{A}} = \frac{\xi_{\mathrm{A}}}{J_{\mathrm{tr}} J_{\mathrm{p}}} \mathbf{L}_{\mathrm{p},\mathrm{A}} = \frac{\xi_{\mathrm{A}}}{J_{\mathrm{tr}}} \mathbf{L}_{\mathrm{p},\mathrm{A}}, \tag{2.5}$$

where ξ_A and $\tilde{\xi}_A$ represent the austenitic volume fraction in the reference (\mathcal{B}_0) and second intermediate (\mathcal{B}_2) configurations, respectively, J_{tr} represents the determinant of the effective transformation deformation gradient, and J_p is the determinant of the effective plastic deformation gradient. The austenitic volume fraction in the reference configuration is given by $\xi_A = 1 - \sum_{\alpha=1}^{M} \xi^{(\alpha)}$. Observe that the last relation in (2.5) is obtained assuming that the plastic deformation is isochoric, i.e., $J_p = 1$. Consistent with a crystal plasticity description of slip along the slip systems $i = 1, \ldots, N = 24$ of FCC austenite, the effective plastic velocity gradient is expressed as [70]

$$\mathbf{L}_{\mathrm{p}} = \sum_{i=1}^{N} \dot{\gamma}^{(i)} \mathbf{m}_{\mathrm{A}}^{(i)} \otimes \mathbf{n}_{\mathrm{A}}^{(i)}, \qquad (2.6)$$

where $\mathbf{m}_{A}^{(i)}$ and $\mathbf{n}_{A}^{(i)}$ are the unit vectors parallel to the slip direction and normal to the slip plane for the austenitic slip system *i*, respectively, and $\dot{\gamma}^{(i)}$ represents the effective

plastic slip rate on slip system *i*, given by [70]

$$\dot{\gamma}^{(i)} = \frac{\xi_{\rm A}}{J_{\rm tr}} \dot{\gamma}_{\rm A}^{(i)},$$
(2.7)

with $\dot{\gamma}_{\rm A}^{(i)}$ the rate of slip along the austenitic slip system *i* (measured within the austenitic region).

The effective thermal deformation gradient \mathbf{F}_{th} is expressed as the volume average of the thermal deformation gradients (in the second intermediate configuration) of the austenitic phase, $\mathbf{F}_{th,A}$, and martensitic phases, $\mathbf{F}_{th}^{(\alpha)}$, i.e.,

$$\mathbf{F}_{\rm th} = \frac{1}{J_{\rm tr}} \left(\xi_{\rm A} \mathbf{F}_{\rm th,A} + (1 + \delta_{\rm T}) \sum_{\alpha=1}^{M} \xi^{(\alpha)} \mathbf{F}_{\rm th}^{(\alpha)} \right) , \qquad (2.8)$$

where, as before, the plastic deformation has been taken as isochoric. The dependency of the thermal deformation gradient on thermal variables will be discussed below after introducing a decomposition for the entropy.

2.1.2 Entropy

In an entropy-based thermodynamical framework, the entropy plays for the thermal fields an analogous role as the deformation gradient does for the mechanical fields [9]. In order to develop a thermodynamically-consistent formulation, the following decomposition for the total entropy density per unit mass η is used:

$$\eta = \eta_{\rm e} + \eta_{\rm m} + \eta_{\rm p} + \eta_{\rm tr}, \qquad (2.9)$$

where η_e is referred to as the thermal part of the reversible entropy density (analogous to the elastic deformation gradient), η_m is the reversible entropy density that accounts for the coupling between the mechanical and thermal fields (analogous to the thermal deformation gradient) and η_p and η_{tr} are the entropy densities related to plastic and transformation processes, respectively (analogous to the plastic and transformation deformation gradients).

The rate of change of the transformational entropy density η_{tr} is expressed as (see [75, 70])

$$\dot{\eta}_{\rm tr} = \sum_{\alpha=1}^{M} \dot{\xi}^{(\alpha)} \frac{\lambda_{\rm T}^{(\alpha)}}{\theta_{\rm T}},\tag{2.10}$$

where $\lambda_{\rm T}^{(\alpha)}$ is the latent heat at the transformation temperature $\theta_{\rm T}$, which is the heat (per unit mass) required to transform austenite into a specific martensitic transformation

system α during an isothermal process at $\theta = \theta_{\rm T}$. Similarly, the rate of change of the plastic entropy density $\eta_{\rm p}$ is formally written as (see [70])

$$\dot{\eta}_{\rm p} = \xi_{\rm A} \sum_{i=1}^{N} \dot{\gamma}_{\rm A}^{(i)} \phi_{\rm A}^{(i)} = J_{\rm tr} \sum_{i=1}^{N} \dot{\gamma}^{(i)} \phi_{\rm A}^{(i)}, \qquad (2.11)$$

where $\phi_A^{(i)}$ measures the change in entropy per unit slip along the slip system *i*. The form of the term η_m will be discussed in more detail in the context of thermodynamical consistency.

2.1.3 State and internal variables

State and internal variables need to be chosen to characterize the internal energy density of the material. From the decomposition of the deformation gradient and the entropy, convenient state variables are the elastic deformation gradient $\mathbf{F}_{\rm e}$ and the thermal part of the reversible entropy $\eta_{\rm e}$. In addition, the volume fractions of the martensitic transformation systems $\boldsymbol{\xi} = (\xi^{(1)}, \xi^{(2)}, \dots, \xi^{(M)})$ and the amounts of plastic slip $\boldsymbol{\gamma} = (\gamma^{(1)}, \gamma^{(2)}, \dots, \gamma^{(N)})$ are used as variables that characterize internal structural changes in the material due to phase transformations and plastic deformations. Whenever required for partial differentiation, functions that depend on some or all the variables $\mathbf{F}_{\rm e}, \eta_{\rm e}, \boldsymbol{\xi}$ and $\boldsymbol{\gamma}$ will be denoted in the sequel with a superimposed tilde.

For subsequent use, assumptions are made regarding the dependency of the coupling terms \mathbf{F}_{th} and η_m that appear in the decompositions (2.1) and (2.9) of the deformation gradient and the entropy, respectively. The classical model for the thermal deformation gradient assumes that \mathbf{F}_{th} depends on the temperature θ . However, since the temperature is not chosen as a primary variable, it is instead assumed that the thermal deformation gradient depends on the (purely thermal) reversible entropy η_e . Furthermore, in view of (2.8), it may be observed that the thermal deformation gradient also depends on $\boldsymbol{\xi}$; consequently it is assumed that

$$\mathbf{F}_{\rm th} = \tilde{\mathbf{F}}_{\rm th} \left(\eta_{\rm e}, \boldsymbol{\xi} \right). \tag{2.12}$$

At a later stage, a classical model of the thermal deformation gradient as a function of the temperature will be introduced with a suitable change of variables.

As will be shown in subsequent sections, the reversible entropy associated with the thermomechanical coupling η_m cannot be independently specified from the thermal deformation gradient (2.12); however it is possible to formally express η_m as follows:

$$\eta_{\rm m} = \tilde{\eta}_{\rm m} \left(\mathbf{F}_{\rm e}, \eta_{\rm e}, \boldsymbol{\xi} \right) \ . \tag{2.13}$$

Observe that the decomposition of the deformation gradient and the entropy is done in terms of two types of variables, namely (i) quantities related to reversible processes
$(\mathbf{F}_{e}, \mathbf{F}_{th}, \eta_{e}, \eta_{m})$ and (ii) quantities representing irreversible processes $(\mathbf{F}_{p}, \mathbf{F}_{tr}, \eta_{p}, \eta_{tr})$. The existence of relations of the types (2.12) and (2.13) is consistent with the notion of reversibility.

2.1.4 Thermodynamical relations

Useful thermodynamical relations can be established as a result of the procedure established by Coleman and Noll [15]. To this end, consider the dissipation rate \mathscr{D} (per unit volume) at a material point given by

$$\mathscr{D} := -\rho_0 \dot{\epsilon} + \mathbf{P} \cdot \mathbf{F} + \rho_0 \theta \dot{\eta} - \nabla \theta \cdot \mathbf{\Phi}, \qquad (2.14)$$

where ρ_0 is the referential mass density, $\dot{\epsilon}$ is the rate of change of the internal energy density ϵ (per unit mass), **P** is the first Piola-Kirchhoff stress, $\dot{\mathbf{F}}$ is the rate of change of the deformation gradient, θ is the temperature, $\dot{\eta}$ is the rate of change of the entropy, $\nabla \theta$ is the (referential) temperature gradient and Φ is the entropy flux, all written for a material point in the reference configuration.

Using the kinematic relations (2.3), (2.6), (2.4) and (2.12) and applying the chain rule, the internal mechanical power $\mathbf{P} \cdot \dot{\mathbf{F}}$ can be expressed as

$$\mathbf{P} \cdot \dot{\mathbf{F}} = \mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \mathbf{F}_{\mathrm{th}}^{\mathrm{T}} \cdot \dot{\mathbf{F}}_{\mathrm{e}} + \mathbf{F}_{\mathrm{e}}^{\mathrm{T}} \mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \cdot \frac{\partial \ddot{\mathbf{F}}_{\mathrm{th}}}{\partial \eta_{\mathrm{e}}} \dot{\eta_{\mathrm{e}}} + \sum_{\alpha=1}^{M} \left(\tau_{\mathrm{tr}}^{(\alpha)} + \mathbf{F}_{\mathrm{e}}^{\mathrm{T}} \mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \cdot \frac{\partial \tilde{\mathbf{F}}_{\mathrm{th}}}{\partial \xi^{(\alpha)}} \right) \dot{\xi}^{(\alpha)} + \sum_{i=1}^{N} \tau_{\mathrm{p}}^{(i)} \dot{\gamma}^{(i)},$$
(2.15)

with $\tau_{tr}^{(\alpha)}$ and $\tau_{p}^{(i)}$ denoting the resolved stresses on the transformation system α and on the plastic slip system *i*, respectively. The resolved stress for transformation has the form

$$\tau_{\rm tr}^{(\alpha)} = \mathbf{F}_{\rm p}^{\rm T} \mathbf{F}_{\rm th}^{\rm T} \mathbf{F}_{\rm e}^{\rm T} \mathbf{P} \cdot \left(\mathbf{b}^{(\alpha)} \otimes \mathbf{d}^{(\alpha)} \right).$$
(2.16)

and the resolved stress for plastic slip is given by

$$\tau_{\mathbf{p}}^{(i)} = \mathbf{F}_{\mathbf{th}}^{\mathrm{T}} \mathbf{F}_{\mathbf{e}}^{\mathrm{T}} \mathbf{P} \mathbf{F}_{\mathbf{tr}}^{\mathrm{T}} \mathbf{F}_{\mathbf{p}}^{\mathrm{T}} \cdot \left(\mathbf{m}_{\mathrm{A}}^{(i)} \otimes \mathbf{n}_{\mathrm{A}}^{(i)} \right), \qquad (2.17)$$

The internal thermal power $\rho_0 \theta \dot{\eta}$ in (2.14) can be expanded in a similar way using (2.9), (2.10), (2.11) and the dependency condition for η_m in (2.13), i.e.,

$$\rho_{0}\theta\dot{\eta} = \rho_{0}\theta\frac{\partial\tilde{\eta}_{m}}{\partial\mathbf{F}_{e}}\cdot\dot{\mathbf{F}}_{e} + \rho_{0}\theta\left(1 + \frac{\partial\tilde{\eta}_{m}}{\partial\eta_{e}}\right)\dot{\eta}_{e} + \sum_{\alpha=1}^{M}\left(\zeta_{tr}^{(\alpha)} + \rho_{0}\theta\frac{\partial\tilde{\eta}_{m}}{\partial\xi^{(\alpha)}}\right)\dot{\xi}^{(\alpha)} + \sum_{i=1}^{N}\zeta_{p}^{(i)}\dot{\gamma}^{(i)},$$

$$(2.18)$$

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where $\zeta_{tr}^{(\alpha)}$ and $\zeta_{p}^{(i)}$ are the thermal analogues of the resolved stresses $\tau_{tr}^{(\alpha)}$ and $\tau_{p}^{(i)}$, respectively, given by

$$\zeta_{\rm tr}^{(\alpha)} = \rho_0 \theta \frac{\lambda_{\rm T}^{(\alpha)}}{\theta_{\rm T}}, \quad \zeta_{\rm p}^{(i)} = \rho_0 J_{\rm tr} \theta \phi_{\rm A}^{(i)}. \tag{2.19}$$

The rate of change of the internal energy can be expressed in terms of rates of state and internal variables and, more generally, might also depend on fluxes. The model that will be used here to take into account the stored energy associated with plastic deformations is relatively simple. With this in mind, for the purposes of the present model, it is sufficient to assume that the internal energy does not arbitrarily depend on all components of γ but only through a specific combination of them. To this end, a strain-like variable β is defined (in rate form) as a weighted sum of the rates of plastic slips $\dot{\gamma}^{(i)}$ [70], i.e.,

$$\dot{\beta} = \sum_{i=1}^{N} w^{(i)} \dot{\gamma}^{(i)}, \qquad (2.20)$$

where the form of the weighting functions $w^{(i)}$ will be derived at the end of Section 2.1.6 in terms of a hardening model. The scalar quantity β plays the role of an equivalent plastic (micro) strain and is henceforth treated as an internal variable (see [70] for details). Correspondingly, it is assumed that the internal energy ϵ is given by a function $\tilde{\epsilon}$ that depends on the state and internal variables \mathbf{F}_{e} , η_{e} , $\boldsymbol{\xi}$ and β and, a priori, may also depend on the fluxes $\dot{\boldsymbol{\xi}}$, $\dot{\beta}$, and $\boldsymbol{\Phi}$, i.e.,

$$\epsilon = \tilde{\epsilon} \left(\mathbf{F}_{\mathrm{e}}, \eta_{\mathrm{e}}, \boldsymbol{\xi}, \beta; \dot{\boldsymbol{\xi}}, \dot{\boldsymbol{\beta}}, \boldsymbol{\Phi} \right).$$
(2.21)

Combining (2.15), (2.18), (2.20) and (2.21) with (2.14) results in the following expression

for the dissipation:

$$\begin{aligned} \mathscr{D} &= \left(\mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \mathbf{F}_{\mathrm{th}}^{\mathrm{T}} + \rho_{0} \theta \frac{\partial \tilde{\eta}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{e}}} - \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \mathbf{F}_{\mathrm{e}}} \right) \cdot \dot{\mathbf{F}}_{\mathrm{e}} \\ &+ \rho_{0} \left(\theta + \theta \frac{\partial \tilde{\eta}_{\mathrm{m}}}{\partial \eta_{\mathrm{e}}} + \frac{1}{\rho_{0}} \mathbf{F}_{\mathrm{e}}^{\mathrm{T}} \mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \cdot \frac{\partial \tilde{\mathbf{F}}_{\mathrm{th}}}{\partial \eta_{\mathrm{e}}} - \frac{\partial \tilde{\epsilon}}{\partial \eta_{\mathrm{e}}} \right) \dot{\eta}_{\mathrm{e}} \\ &+ \sum_{\alpha=1}^{M} \left(\tau_{\mathrm{tr}}^{(\alpha)} + \zeta_{\mathrm{tr}}^{(\alpha)} + \mathbf{F}_{\mathrm{e}}^{\mathrm{T}} \mathbf{P} \mathbf{F}_{\mathrm{tr}}^{\mathrm{T}} \mathbf{F}_{\mathrm{p}}^{\mathrm{T}} \cdot \frac{\partial \tilde{\mathbf{F}}_{\mathrm{th}}}{\partial \xi^{(\alpha)}} \right. \end{aligned} \tag{2.22} \\ &+ \rho_{0} \theta \frac{\partial \tilde{\eta}_{\mathrm{m}}}{\partial \xi^{(\alpha)}} - \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \xi^{(\alpha)}} \right) \dot{\xi}^{(\alpha)} - \sum_{\alpha=1}^{M} \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \dot{\xi}^{(\alpha)}} \ddot{\xi}^{(\alpha)} \\ &+ \sum_{i=1}^{N} \left(\tau_{\mathrm{p}}^{(i)} + \zeta_{\mathrm{p}}^{(i)} - \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \beta} w^{(i)} \right) \dot{\gamma}^{(i)} \\ &- \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \dot{\beta}} \ddot{\beta} - \nabla \theta \cdot \mathbf{\Phi} - \rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \mathbf{\Phi}} \cdot \dot{\mathbf{\Phi}}. \end{aligned}$$

The second law of thermodynamics states that for every thermomechanical process, the local entropy rate must be non-negative, $\Gamma \geq 0$, which for this case, it is equivalent to $\mathscr{D} = \Gamma \theta \geq 0$, since the temperature is always positive. Furthermore, the terms in (2.22) that are multiplied by the rates $\dot{\mathbf{F}}_{e}$, $\dot{\eta}_{e}$, $\ddot{\beta}$, $\ddot{\boldsymbol{\xi}}$ and $\dot{\boldsymbol{\Phi}}$ must vanish, since otherwise a process can be specified for which the dissipation is negative (see [15]). Correspondingly, it can be concluded that

$$\rho_{0} \frac{\partial \tilde{\epsilon}}{\partial \mathbf{F}_{e}} = \mathbf{P} \mathbf{F}_{tr}^{T} \mathbf{F}_{p}^{T} \mathbf{F}_{th}^{T} + \rho_{0} \theta \frac{\partial \tilde{\eta}_{m}}{\partial \mathbf{F}_{e}},$$

$$\frac{\partial \tilde{\epsilon}}{\partial \eta_{e}} = \theta + \theta \frac{\partial \tilde{\eta}_{m}}{\partial \eta_{e}} + \frac{1}{\rho_{0}} \mathbf{F}_{e}^{T} \mathbf{P} \mathbf{F}_{tr}^{T} \mathbf{F}_{p}^{T} \cdot \frac{\partial \tilde{\mathbf{F}}_{th}}{\partial \eta_{e}},$$

$$\frac{\partial \tilde{\epsilon}}{\partial \dot{\beta}} = 0, \quad \frac{\partial \tilde{\epsilon}}{\partial \dot{\boldsymbol{\xi}}} = \mathbf{0}, \quad \frac{\partial \tilde{\epsilon}}{\partial \boldsymbol{\Phi}} = \mathbf{0}.$$
(2.23)

As a result of the last three relations in (2.23), the internal energy cannot depend on the fluxes, which reduces (2.21) to

$$\epsilon = \tilde{\epsilon} \left(\mathbf{F}_{\mathrm{e}}, \eta_{\mathrm{e}}, \boldsymbol{\xi}, \beta \right). \tag{2.24}$$

Enforcing (2.23) in (2.22), the dissipation can be written as $\mathscr{D} = \mathscr{D}_{tr} + \mathscr{D}_{p} + \mathscr{D}_{q}$, where \mathscr{D}_{tr} , \mathscr{D}_{p} and \mathscr{D}_{q} are the dissipations due to phase transformation, plastic deformation and heat conduction, respectively, defined as

$$\mathscr{D}_{\rm tr} := \sum_{\alpha=1}^{M} f^{(\alpha)} \dot{\xi}^{(\alpha)}, \quad \mathscr{D}_{\rm p} := \sum_{i=1}^{N} g^{(i)} \dot{\gamma}^{(i)}, \quad \mathscr{D}_{\rm q} := -\nabla \theta \cdot \Phi, \tag{2.25}$$

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with $f^{(\alpha)}$ and $g^{(i)}$ the driving forces for transformation and plasticity, respectively, given by

$$f^{(\alpha)} := \tau_{\rm tr}^{(\alpha)} + \zeta_{\rm tr}^{(\alpha)} + \mathbf{F}_{\rm e}^{\rm T} \mathbf{P} \mathbf{F}_{\rm tr}^{\rm T} \mathbf{F}_{\rm p}^{\rm T} \cdot \frac{\partial \mathbf{F}_{\rm th}}{\partial \xi^{(\alpha)}} + \rho_0 \theta \frac{\partial \tilde{\eta}_{\rm m}}{\partial \xi^{(\alpha)}} - \rho_0 \frac{\partial \tilde{\epsilon}}{\partial \xi^{(\alpha)}}, \qquad (2.26)$$
$$g^{(i)} := \tau_{\rm p}^{(i)} + \zeta_{\rm p}^{(i)} - \rho_0 \frac{\partial \tilde{\epsilon}}{\partial \beta} w^{(i)}.$$

For the kinetic relations of the present model, it will be assumed that a strong form of the dissipation inequality applies, namely that the dissipation associated with individual processes is non-negative, i.e., it will be required that

$$\mathscr{D}_{\mathrm{tr}} \ge 0, \quad \mathscr{D}_{\mathrm{p}} \ge 0, \quad \mathscr{D}_{\mathrm{q}} \ge 0.$$
 (2.27)

Observe that the Coleman-Noll procedure yields two types of results, namely (i) relations for the partial derivatives of the (stored) internal energy (see $(2.23)_{1,2}$) and (ii) expressions for the transformational and plastic driving forces (see (2.26)). After introducing specific constitutive models between the dependent variables \mathbf{P} , θ , \mathbf{F}_{th} and η_m and the state variables \mathbf{F}_e and η_e , the first set of thermodynamical relations from the Coleman-Noll procedure can be integrated to obtain an expression for the internal energy. Once the expression for $\tilde{\epsilon}$ has been established, the second set of thermodynamical relations (2.26) can be applied to further develop specific forms for the driving forces. Finally, kinetic relations that relate the evolution of the internal variables to the driving forces can be proposed such that the dissipation inequality is satisfied for all possible processes. These steps are carried out in the subsequent sections.

2.1.5 Models for the internal energy, thermal deformation gradient and reversible entropy

To obtain an expression for the internal energy density ϵ , it is convenient to work with a different set of state variables. In particular, since the constitutive relation between the stress and the (elastic) deformation must be frame indifferent, the stress tensor cannot depend on (elastic) rotations. This can be guaranteed using a strain measure where the rotation has been factored out, such as the elastic Green-Lagrange strain defined as

$$\mathbf{E}_{e} = \tilde{\mathbf{E}}_{e}(\mathbf{F}_{e}) = \frac{1}{2} \left(\mathbf{F}_{e}^{\mathrm{T}} \mathbf{F}_{e} - \mathbf{I} \right) .$$
(2.28)

Furthermore, the classical models for the thermal deformation gradient and the thermal energy are expressed in terms of the temperature θ and not the (purely thermal) reversible entropy η_e . It is assumed that there is a one-to-one correspondence between θ and η_e of

the form $\theta = \tilde{\theta}(\eta_{e}, \boldsymbol{\xi})$, which can be inverted as $\eta_{e} = \hat{\eta}_{e}(\theta, \boldsymbol{\xi})$. Accordingly, a new set of state and internal variables, namely $(\mathbf{E}_{e}, \theta, \boldsymbol{\xi}, \beta)$, is used in the foregoing analysis. Henceforth, a superimposed "hat" on a function indicates that it depends on some or all of the variables $\mathbf{E}_{e}, \theta, \boldsymbol{\xi}$ and β . It is worth pointing out that in order to use the temperature as a state variable, the most natural formulation is in terms of the Helmholtz energy ψ , which, assuming a one-to-one correspondence between conjugate variables, can be obtained from a Legendre transformation, namely $\hat{\psi}(\mathbf{E}_{e}, \theta, \boldsymbol{\xi}, \beta) = \tilde{\epsilon}(\mathbf{E}_{e}, \hat{\eta}_{e}(\theta, \boldsymbol{\xi}), \boldsymbol{\xi}, \beta) - \theta \hat{\eta}_{e}(\theta, \boldsymbol{\xi})$. However, in anticipation of a numerical implementation that is based on the internal energy, it is more convenient to perform a direct change of variables instead of a Legendre transform. This choice requires the use of the chain rule, but otherwise provides an equivalent formulation as the Legendre transform.

Based on the aforementioned assumptions, the change of variables can be achieved employing the following relations for a (scalar, vector or tensor-valued) function **f**:

$$\frac{\partial \tilde{\mathbf{f}}}{\partial \mathbf{F}_{e}} = \mathbf{F}_{e} \frac{\partial \hat{\mathbf{f}}}{\partial \mathbf{E}_{e}}, \quad \mathbf{P} = J_{tr} J_{th} \mathbf{F}_{e} \mathbf{S} \mathbf{F}_{th}^{-T} \mathbf{F}_{p}^{-T} \mathbf{F}_{tr}^{-T},$$

$$\frac{\partial \tilde{\mathbf{f}}}{\partial \eta_{e}} = \frac{\partial \tilde{\theta}}{\partial \eta_{e}} \frac{\partial \hat{\mathbf{f}}}{\partial \theta}, \quad \frac{\partial \hat{\eta}_{e}}{\partial \theta} = \left(\frac{\partial \tilde{\theta}}{\partial \eta_{e}}\right)^{-1},$$

$$\frac{\partial \tilde{\mathbf{f}}}{\partial \xi^{(\alpha)}} = \frac{\partial \hat{\mathbf{f}}}{\partial \xi^{(\alpha)}} + \frac{\partial \tilde{\theta}}{\partial \xi^{(\alpha)}} \frac{\partial \hat{\mathbf{f}}}{\partial \theta}, \quad \frac{\partial \tilde{\mathbf{f}}}{\partial \beta} = \frac{\partial \hat{\mathbf{f}}}{\partial \beta},$$
(2.29)

where **S** corresponds to the second Piola-Kirchhoff stress tensor in the third intermediate configuration \mathcal{B}_3 . Employing the relations (2.29), equations (2.23)_{1,2} can be written as

$$\rho_{0} \frac{\partial \hat{\epsilon}}{\partial \mathbf{E}_{e}} = J_{tr} J_{th} \mathbf{S} + \rho_{0} \theta \frac{\partial \hat{\eta}_{m}}{\partial \mathbf{E}_{e}},$$

$$\rho_{0} \frac{\partial \hat{\epsilon}}{\partial \theta} = \rho_{0} \theta \frac{\partial}{\partial \theta} \left(\hat{\eta}_{e} + \hat{\eta}_{m} \right) + J_{tr} J_{th} \mathbf{F}_{e}^{T} \mathbf{F}_{e} \mathbf{S} \cdot \frac{\partial \hat{\mathbf{F}}_{th}}{\partial \theta} \mathbf{F}_{th}^{-1}.$$
(2.30)

It is assumed that the stress tensor S and its conjugate strain tensor E_e are related through the constitutive relation

$$\mathbf{S} = \hat{\mathbf{S}} \left(\mathbf{E}_{\mathrm{e}}, \boldsymbol{\xi} \right) = \mathbb{C} \left(\boldsymbol{\xi} \right) \mathbf{E}_{\mathrm{e}}, \tag{2.31}$$

where $\mathbb{C} = \mathbb{C}(\xi)$ is an effective fourth order elasticity tensor for the mixture of austenite and martensite that, in the present model, is estimated as a volume average in the third intermediate configuration, i.e.,

$$\mathbb{C}\left(\boldsymbol{\xi}\right) = \frac{1}{J_{\mathrm{tr}}J_{\mathrm{th}}} \left(J_{\mathrm{th},\mathrm{A}}\xi_{\mathrm{A}}\mathbb{C}_{\mathrm{A}} + (1+\delta_{\mathrm{T}})\sum_{\alpha=1}^{M} J_{\mathrm{th}}^{(\alpha)}\xi^{(\alpha)}\mathbb{C}^{(\alpha)} \right), \qquad (2.32)$$

where \mathbb{C}_{A} and $\mathbb{C}^{(\alpha)}$ are the stiffness tensors of austenite and twinned martensite, respectively, and $J_{th} = \det \mathbf{F}_{th}$, $J_{th,A} = \det \mathbf{F}_{th,A}$ and $J_{th}^{(\alpha)} = \det \mathbf{F}_{th}^{(\alpha)}$. Specific forms for

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 \mathbb{C}_A and $\mathbb{C}^{(\alpha)}$ are given in [75]. It is noted that the effective stiffness \mathbb{C} formally depends on the temperature since the thermal deformation gradients $\mathbf{F}_{th,A}$ and $\mathbf{F}_{th}^{(\alpha)}$ depend on θ . However, this dependency is not intrinsically physical because it is only related to the approximation scheme used, namely the volume averaging. In the sequel, it will be assumed that the dependency of \mathbb{C} on θ is *weak* in the sense that

$$\frac{\partial}{\partial \theta} \left(J_{\rm tr} J_{\rm th} \mathbb{C} \right) \approx 0 \,. \tag{2.33}$$

Correspondingly, the formal dependency of \mathbb{C} on θ is not indicated in (2.32).

Integrating $(2.30)_1$ with respect to \mathbf{E}_e yields

$$\hat{\epsilon} \left(\mathbf{E}_{\mathrm{e}}, \theta, \boldsymbol{\xi}, \beta \right) = \hat{\epsilon}_{\mathrm{m}} \left(\mathbf{E}_{\mathrm{e}}, \boldsymbol{\xi} \right) + \theta \hat{\eta}_{\mathrm{m}} \left(\mathbf{E}_{\mathrm{e}}, \theta, \boldsymbol{\xi} \right) + \hat{\epsilon}_{1} \left(\theta, \boldsymbol{\xi}, \beta \right),$$
(2.34)

where $\hat{\epsilon}_1$ is a function that does not depend on \mathbf{E}_e and $\hat{\epsilon}_m$ is the strain energy given by

$$\hat{\epsilon}_{\rm m} \left(\mathbf{E}_{\rm e}, \boldsymbol{\xi} \right) = \frac{J_{\rm tr} J_{\rm th}}{2\rho_0} \mathbb{C}(\boldsymbol{\xi}) \mathbf{E}_{\rm e} \cdot \mathbf{E}_{\rm e}.$$
(2.35)

Taking the partial derivative of (2.34) with respect to the temperature (accounting for the assumption (2.33)), equating the resulting expression with $(2.30)_2$ and rearranging the terms leads to

$$\hat{\eta}_{\rm m} = \frac{1}{\rho_0} J_{\rm tr} J_{\rm th} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm e} \mathbf{S} \cdot \frac{\partial \hat{\mathbf{F}}_{\rm th}}{\partial \theta} \mathbf{F}_{\rm th}^{-1} + \left(\theta \frac{\partial \hat{\eta}_{\rm e}}{\partial \theta} - \frac{\partial \hat{\epsilon}_1}{\partial \theta}\right).$$
(2.36)

As discussed in Section 2.1.2, the term $\hat{\eta}_m$ accounts for the entropy associated with an elastic deformation. Consequently, $\hat{\eta}_m$ should vanish in the absence of an elastic deformation, i.e.,

$$\hat{\eta}_{\rm m} \left(\mathbf{E}_{\rm e} = \mathbf{0}, \theta, \boldsymbol{\xi} \right) = 0. \tag{2.37}$$

Observe that the relation shown in (2.37) should hold for arbitrary values of the temperature θ and the volume fractions $\boldsymbol{\xi}$. By setting $\mathbf{E}_{\rm e} = \mathbf{0}$ (and hence $\mathbf{S} = \mathbf{0}$) in (2.36), and in view of (2.37), it follows that

$$\theta \frac{\partial \hat{\eta}_{\rm e}}{\partial \theta} - \frac{\partial \hat{\epsilon}_1}{\partial \theta} = 0. \tag{2.38}$$

Consistent with the foregoing assumptions, the above relation is valid for arbitrary values of θ and ξ and does not depend on the elastic deformation. The term ϵ_1 can be obtained upon integration of (2.38), which requires a constitutive relation between θ and η_e . The following constitutive relation is then proposed [75]:

$$\eta_{\rm e} = \hat{\eta}_{\rm e}(\theta, \boldsymbol{\xi}) = h(\boldsymbol{\xi}) \ln\left(\frac{\theta}{\theta_{\rm T}}\right) + \eta_{\rm T}, \qquad (2.39)$$

where $h = h(\boldsymbol{\xi})$ stands for the effective specific heat (per unit mass), $\theta_{\rm T}$ is the transformation temperature at zero elastic deformation and $\eta_{\rm T}$ denotes the value of $\eta_{\rm e}$ at the transformation temperature. The above model corresponds to assuming that the specific heat remains constant during a purely thermal process. The effective specific heat h is estimated as a volume average of the specific heat of the austenitic phase, h_A , and the specific heats of the martensitic transformation systems, $h^{(\alpha)}$ (see [75]), i.e.,

$$h(\boldsymbol{\xi}) = \xi_{\rm A} h_{\rm A} + \sum_{\alpha=1}^{M} \xi^{(\alpha)} h^{(\alpha)} .$$
 (2.40)

Using (2.39) in (2.38) and integrating with respect to θ results in

$$\hat{\epsilon}_1(\theta, \boldsymbol{\xi}, \beta) = \hat{\epsilon}_{\rm th}(\theta, \boldsymbol{\xi}) + \hat{\epsilon}_2(\boldsymbol{\xi}, \beta), \qquad (2.41)$$

where $\hat{\epsilon}_2$ is a function that does not depend on the temperature and $\hat{\epsilon}_{th}$ is the thermal internal energy, which corresponds to a classical model, i.e.,

$$\hat{\epsilon}_{\rm th}(\theta, \boldsymbol{\xi}) = h(\boldsymbol{\xi})\theta . \tag{2.42}$$

The function $\hat{\epsilon}_2$ is used to introduce two other forms of (lower-scale) energy that play a role at the mesoscale, namely a defect energy $\hat{\epsilon}_d$ that represents the elastic distortion of the lattice due to the presence of dislocations and a surface energy $\hat{\epsilon}_s$ stored in the austenite-twinned martensite interfaces. Correspondingly, the function $\hat{\epsilon}_2$ is expressed as

$$\hat{\epsilon}_{2}(\boldsymbol{\xi},\beta) = \hat{\epsilon}_{d}(\boldsymbol{\xi},\beta) + \hat{\epsilon}_{s}(\boldsymbol{\xi}) + \hat{\epsilon}^{*}(\boldsymbol{\xi}).$$
(2.43)

Adopting the models presented in previous works [73, 75, 70], the defect energy and the surface energy are formulated as

$$\hat{\epsilon}_{\rm d}\left(\boldsymbol{\xi},\beta\right) = \frac{1}{2\rho_0} J_{\rm tr} J_{\rm th} \omega_{\rm A} \mu(\boldsymbol{\xi}) \beta^2,$$

$$\hat{\epsilon}_{\rm s}\left(\boldsymbol{\xi}\right) = \frac{\chi}{l_0 \rho_0} \sum_{\alpha=1}^M \xi^{(\alpha)} \left(1 - \xi^{(\alpha)}\right),$$
(2.44)

where ω_A is a scaling factor for the strain energy of an assembly of dislocations, β is the strain-like internal variable related to plastic slip through (2.20), χ is an interface energy per unit referential area and l_0 is a length-scale parameter representing the volumeto-surface ratio of a circular platelet of martensite within a spherical grain of austenite (see [75] and [74] for details). The term $\mu = \mu(\boldsymbol{\xi})$ is an equivalent (isotropic) shear modulus (obtained through averaging the modulus μ_A of austenite and $\mu^{(\alpha)}$ of martensite, see [70]), i.e.,

$$\mu\left(\boldsymbol{\xi}\right) = \frac{1}{J_{\mathrm{tr}}J_{\mathrm{th}}} \left(J_{\mathrm{th},\mathrm{A}}\xi_{\mathrm{A}}\mu_{\mathrm{A}} + \left(1 + \delta_{\mathrm{T}}\right)\sum_{\alpha=1}^{M} J_{\mathrm{th}}^{(\alpha)}\xi^{(\alpha)}\mu^{(\alpha)} \right)$$

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Similar to the approach adopted for the stiffness \mathbb{C} , it is assumed that the dependency of μ on θ is weak in the sense that $\partial (J_{tr}J_{th}\mu)/\partial\theta \approx 0$.

The last term in the decomposition (2.43), $\hat{\epsilon}^*$, is used to satisfy an additional requirement on the energy at the transformation temperature θ_T , namely that the transformation driving force (for all systems) should vanish when the transformation process takes place at the transformation temperature, at zero elastic strain (hence at zero stress), at zero plastic deformation (hence at zero plastic microstrain) and in the absence of a surface energy. The previous requirement can be formally expressed as

$$f^{(\alpha)}\Big|_{\mathbf{E}_{e}=\mathbf{0},\ \theta=\theta_{\mathrm{T}},\ \beta=0,\ \chi=0} = 0.$$
 (2.45)

Upon using (2.16), (2.19)₁, (2.29)₂, (2.31), (2.34), (2.35), (2.36), (2.40), (2.42), (2.43) and (2.44) in (2.26)₁ (with $\mathbf{E}_{e} = \mathbf{0}, \theta = \theta_{T}, \beta = 0, \chi = 0$), the condition (2.45) results in

$$\lambda_{\rm T}^{(\alpha)} - \left(h^{(\alpha)} - h_{\rm A}\right)\theta_{\rm T} - \frac{\partial \hat{\epsilon}^*}{\partial \xi^{(\alpha)}} = 0, \qquad (2.46)$$

Integration of (2.46) gives the following expression for $\hat{\epsilon}^*$:

$$\hat{\epsilon}^{*}\left(\boldsymbol{\xi}\right) = \sum_{\alpha=1}^{M} \lambda_{\mathrm{T}}^{(\alpha)} \boldsymbol{\xi}^{(\alpha)} - h\left(\boldsymbol{\xi}\right) \boldsymbol{\theta}_{\mathrm{T}}.$$
(2.47)

It is convenient to combine the term $\hat{\epsilon}^*$ with the thermal internal energy $\hat{\epsilon}_{th}$ given in (2.42) into a thermal energy $\hat{\epsilon}_{th}^*$ that also accounts for the latent heat, i.e.,

$$\hat{\epsilon}_{\rm th}^*(\theta, \boldsymbol{\xi}) = h(\boldsymbol{\xi})(\theta - \theta_{\rm T}) + \sum_{\alpha=1}^M \lambda_{\rm T}^{(\alpha)} \boldsymbol{\xi}^{(\alpha)} .$$
(2.48)

Before closing this section, a classical model for the thermal deformation gradient is considered. In particular, the thermal deformation gradient is assumed to depend linearly on the temperature, i.e., $\mathbf{F}_{th,A} = \mathbf{I} + \mathbf{A}_A(\theta - \theta_0)$ and $\mathbf{F}_{th}^{(\alpha)} = \mathbf{I} + \mathbf{A}^{(\alpha)}(\theta - \theta_0)$, with θ_0 being a reference temperature and \mathbf{A}_A and $\mathbf{A}^{(\alpha)}$ the tensors of thermal expansion of the austenitic and martensitic phases, respectively. In view of the relations above, expression (2.8) becomes

$$\mathbf{F}_{\rm th} = \mathbf{F}_{\rm th} \left(\theta, \boldsymbol{\xi} \right) = \mathbf{I} + \mathbf{A}(\boldsymbol{\xi}) \left(\theta - \theta_0 \right) \tag{2.49}$$

with \mathbf{A} the effective tensor of thermal expansion given by

$$\mathbf{A}(\boldsymbol{\xi}) = \frac{1}{J_{\rm tr}} \left(\xi_{\rm A} \mathbf{A}_{\rm A} + (1 + \delta_T) \sum_{\alpha=1}^{M} \xi^{(\alpha)} \mathbf{A}^{(\alpha)} \right) \,. \tag{2.50}$$

The specific form of the reversible entropy $\hat{\eta}_{m}$ associated with the thermomechanical coupling can be obtained by substitution of (2.32), (2.35) and (2.49) in (2.36) (accounting

for (2.38)), i.e.,

$$\hat{\eta}_{\rm m} \left(\mathbf{E}_{\rm e}, \theta, \boldsymbol{\xi} \right) = \frac{1}{\rho_0} J_{\rm tr} J_{\rm th} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm e} \mathbf{S} \mathbf{F}_{\rm th}^{-{\rm T}} \cdot \mathbf{A} .$$
(2.51)

In view of (2.28), (2.31) and (2.49), the term $\hat{\eta}_{\rm m}$ is interpreted as a function of $\mathbf{E}_{\rm e}, \theta$ and $\boldsymbol{\xi}$. The explicit form of the internal energy, i.e.,

$$\hat{\epsilon} = \hat{\epsilon}_{\rm m} + \theta \hat{\eta}_{\rm m} + \hat{\epsilon}_{\rm th}^* + \hat{\epsilon}_{\rm s} + \hat{\epsilon}_{\rm d} , \qquad (2.52)$$

can be obtained from (2.35), (2.44), (2.48) and (2.51).

2.1.6 Driving forces and kinetic relations

To complete the thermomechanical formulation, the driving forces for transformation and plasticity and the kinetic relations for the evolution of the internal variables of the model are presented in this section. Explicit forms for the driving forces corresponding to the internal energy developed in the previous section can be computed using (2.26) together with the change of variables (2.29) and the expressions for the distinct terms of the internal energy given in (2.52). After some algebra, where the simplifying assumption $\partial (J_{\rm tr})^{-1}/\partial \xi^{(\alpha)} \approx 0$ is used, it is possible to decompose the driving forces based on their relevant mechanism as follows:

$$\begin{aligned} f_{\rm tr}^{(\alpha)} &= f_{\rm m}^{(\alpha)} + f_{\rm m,th}^{(\alpha)} + f_{\rm th}^{(\alpha)} + f_{\rm d}^{(\alpha)} + f_{\rm s}^{(\alpha)}, \\ g_{\rm A}^{(i)} &= g_{\rm m}^{(i)} + g_{\rm th}^{(i)} + g_{\rm d}^{(i)}, \end{aligned} (2.53)$$

where $f_{\rm m}^{(\alpha)}$, $f_{\rm m,th}^{(\alpha)}$, $f_{\rm th}^{(\alpha)}$, $f_{\rm d}^{(\alpha)}$ and $f_{\rm s}^{(\alpha)}$ stand for the purely mechanical contribution, the coupled thermomechanical contribution, the purely thermal contribution, the defect energy contribution and the surface energy contribution, respectively, as given by

$$f_{\rm m}^{(\alpha)} = J_{\rm tr} J_{\rm th} \mathbf{F}_{\rm p}^{\rm T} \mathbf{F}_{\rm th}^{\rm T} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm e}^{-\rm T} \mathbf{F}_{\rm p}^{-\rm T} \mathbf{F}_{\rm tr}^{-\rm T} \cdot \left(\mathbf{b}^{(\alpha)} \otimes \mathbf{d}^{(\alpha)} \right) + \frac{1}{2} \left(J_{\rm th,A} \mathbb{C}_{\rm A} - (1 + \delta_{\rm T}) J_{\rm th}^{(\alpha)} \mathbb{C}^{(\alpha)} \right) \mathbf{E}_{\rm e} \cdot \mathbf{E}_{\rm e}, \\f_{\rm m,th}^{(\alpha)} = J_{\rm th} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm e} \mathbf{S} \mathbf{F}_{\rm th}^{-\rm T} \cdot \left((1 + \delta_{\rm T}) \mathbf{A}^{(\alpha)} - \mathbf{A}_{\rm A} \right) (\theta - \theta_{0}), \\f_{\rm th}^{(\alpha)} = \rho_{0} \frac{\lambda_{\rm T}^{(\alpha)}}{\theta_{\rm T}} \left(\theta - \theta_{\rm T} \right) \\+ \rho_{0} \left(h_{\rm A} - h^{(\alpha)} \right) \left(\theta - \theta_{\rm T} - \theta \ln \left(\frac{\theta}{\theta_{\rm T}} \right) \right), \\f_{\rm d}^{(\alpha)} = \frac{\omega_{\rm A}}{2} \left(J_{\rm th,A} \mu_{\rm A} - (1 + \delta_{\rm T}) J_{\rm th}^{(\alpha)} \mu^{(\alpha)} \right) \beta^{2}, \\f_{\rm s}^{(\alpha)} = \frac{\chi}{l_{0}} \left(2\xi^{(\alpha)} - 1 \right). \end{cases}$$
(2.54)

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Similarly, the contributions of the mechanical energy, the thermal energy and the defect energy to the driving force for plasticity are, respectively,

$$g_{\rm m}^{(i)} = J_{\rm th} \mathbf{F}_{\rm th}^{\rm T} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm e}^{\rm T} \mathbf{F}_{\rm th}^{\rm -T} \cdot \left(\mathbf{m}_{\rm A}^{(i)} \otimes \mathbf{n}_{\rm A}^{(i)} \right),$$

$$g_{\rm th}^{(i)} = \rho_0 \theta \phi_{\rm A}^{(i)},$$

$$g_{\rm d}^{(i)} = -\omega_{\rm A} \mu \beta w^{(i)}.$$
(2.55)

Typically, the most relevant contributions to the transformation driving force are $f_{\rm m}^{(\alpha)}$ and $f_{\rm th}^{(\alpha)}$ given by $(2.54)_{1,3}$. More specifically, the main contribution is the first term in each of these expressions (i.e., the stress resolved on a transformation system in $(2.54)_1$ and its thermal analogue in $(2.54)_3$). Other terms in the transformation driving force that account for changes in energy due to changes in material properties may have a significant influence if, for example, there is a large difference in stiffness, thermal expansion and/or specific heat between the parent phase (austenite) and the product phase (martensite). Similarly, the most important contribution for the plastic driving force is $g_{\rm m}^{(i)}$ (i.e., the stress resolved on a slip system). The thermal analogue to the resolved stress (i.e., $g_{\rm th}^{(i)}$ in $(2.55)_2$) appears to have a minor contribution. Finally, the term $g_{\rm d}^{(i)}$, which is meant to account for the increase in stored energy due to elastic distortion around dislocation cores, is always negative and thus acts against plastic slip. However, $g_{\rm d}^{(i)}$ has typically a minor contribution compared to the resolved stress.

Following the approach of Onsager for irreversible thermodynamics [9], constitutive relations for the evolution of the internal variables $\boldsymbol{\xi}$ and γ need to be specified in the form of kinetic relations. These relations must comply with the dissipation inequality that in the present framework is assumed to take the form given in (2.27). For the phase transformation process, the following kinetic relation for the rate of growth of the volume fraction of system α is adopted [73, 75]

$$\dot{\xi}^{(\alpha)} = \begin{cases} \dot{\xi}_0 \tanh\left(\frac{f^{(\alpha)} - f^{(\alpha)}_{cr}}{\nu f^{(\alpha)}_{cr}}\right) & \text{if } f^{(\alpha)} \ge f^{(\alpha)}_{cr}, \\ 0 & \text{otherwise,} \end{cases}$$
(2.56)

where $\dot{\xi}_0 > 0$ is the maximum value of the transformation rate, ν is a dimensionless, viscosity-like parameter and $f_{\rm cr}^{(\alpha)}$ is a critical value that acts as an energy barrier for the transformation process.

Similarly, the following kinetic relation is used for the evolution of plastic slip on system i in the austenite [70]

$$\dot{\gamma}_{\mathbf{A}}^{(i)} = \begin{cases} \dot{\gamma}_{0}^{\mathbf{A}} \left(\left(\frac{g_{\mathbf{A}}^{(i)}}{s_{\mathbf{A}}^{(i)}} \right)^{\left(\frac{1}{n_{\mathbf{A}}}\right)} - 1 \right) & \text{if } g_{\mathbf{A}}^{(i)} \ge s_{\mathbf{A}}^{(i)}, \\ 0 & \text{otherwise,} \end{cases}$$
(2.57)

where $\dot{\gamma}_0^A$ is a reference slip rate, n_A is the rate-sensitivity exponent and $s_A^{(i)}$ is the resistance against slip on system *i*. The resistance against slip is taken to evolve according to the following hardening relation:

$$\dot{s}_{\rm A} = \sum_{j=1}^{N} H_{\rm A}^{(i,j)} \dot{\gamma}_{\rm A}^{(j)},$$
 (2.58)

where the hardening moduli of the austenite $H_{\rm A}^{(i,j)}$ are given as

$$H_{\rm A}^{(i,j)} = \left((1 - q_{\rm A}) \delta_{ij} + q_{\rm A} \right) k_{\rm A}^{(j)} .$$
(2.59)

In (2.59), q_A is the latent hardening ratio, which accounts for the difference between cross and self-hardening, $k_A^{(j)}$ is the single slip hardening modulus of slip system j and δ_{ij} is Kronecker's delta. The evolution of the single slip hardening modulus is given by [70]

$$k_{\rm A}^{(i)} = k_0^{\rm A} \left(1 - \frac{s_{\rm A}^{(j)}}{s_{\infty}^{\rm A}} \right)^{u_{\rm A}}, \tag{2.60}$$

where k_0^A is a reference hardening modulus, s_{∞}^A is the hardening saturation value, and u_A is the hardening exponent.

In order to determine the form of the weighting functions $w^{(i)}$ introduced in (2.20), a kinetic relation for the evolution of the effective plastic microstrain β is presented. Analogous to the expression used for the effective plastic velocity gradient in (2.5), the rate of change of the effective plastic microstrain β is related to the rate of change of the plastic microstrain β_A within the austenitic phase as

$$\dot{\beta} = \tilde{\xi}_{\rm A} \dot{\beta}_{\rm A} = \frac{\xi_{\rm A}}{J_{\rm tr}} \dot{\beta}_{\rm A}.$$
(2.61)

The rate of change of β_A is assumed to depend linearly on the rate of change of the slip resistance in austenite as

$$c_{\rm A}\mu_{\rm A}\dot{\beta}_{\rm A} = \frac{1}{N}\sum_{i=1}^{N}\dot{s}_{\rm A}^{(i)},$$
 (2.62)

where μ_A is the equivalent isotropic shear modulus of the austenite and c_A is a scaling factor that accounts for dislocation interaction [70]. Combining (2.7), (2.58), (2.61) and (2.62) results in

$$\dot{\beta} = \frac{1}{c_{\rm A}\mu_{\rm A}N} \sum_{i=1}^{N} \sum_{j=1}^{N} H_{\rm A}^{(i,j)} \dot{\gamma}^{(j)} .$$
(2.63)

Comparing (2.63) and (2.20) allows to identify the weighting functions $w^{(i)}$ as

$$w^{(i)} = \frac{1}{c_{\rm A}\mu_{\rm A}N} \sum_{j=1}^{N} H_{\rm A}^{(j,i)}.$$
(2.64)

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The last kinetic relation necessary to complete the model is the heat conduction relation for which a classical model is used (Fourier's law), i.e., taking the entropy flux as $\Phi = q/\theta$, with q the heat flux, then

$$\mathbf{q} = -\mathbf{K}\nabla\theta\,,\tag{2.65}$$

where **K** is the heat conductivity tensor. The kinetic relations (2.56), (2.57) and (2.65) satisfy the dissipation inequality (2.27) with appropriate restrictions (e.g., the tensor **K** must be positive semi-definite). For simplicity, isotropic models are adopted for thermal expansion and thermal conduction, i.e., $\mathbf{A}_{A} = \alpha_{A}\mathbf{I}$, $\mathbf{A}^{(\alpha)} = \alpha^{(\alpha)}\mathbf{I}$, $\mathbf{K}_{A} = k_{A}\mathbf{I}$ and $\mathbf{K}^{(\alpha)} = k^{(\alpha)}\mathbf{I}$, with α_{A} , $\alpha^{(\alpha)}$, k_{A} and $k^{(\alpha)}$ the corresponding coefficients of thermal expansion and heat conduction for the austenite and martensite.

In the sequel, simulations will be presented for single crystals of austenite and for grains of austenite embedded in an aggregate of ferritic grains. The model used for ferrite may be formally derived from the model for austenite by suppressing all features related to phase transformation. However, since ferrite has a BCC structure while austenite is FCC, there are some differences in the formulation. Apart from using different slip systems (and numerical values for the model parameters), the model for BCC ferrite includes a non-Schmid term in the resistance to plastic slip. Details are omitted here and can be found in [71]. These models are used to simulate the response of austenitic and ferritic grains subjected to quasi-static thermomechanical loading.

2.2 Numerical Simulations

To illustrate the features of the proposed model under thermomechanical loading, two sets of simulations are presented in this section. The first set consists of a single crystal of austenite under homogeneous tension. The second set is a tensile test for a multiphase TRIP steel microstructure composed of a single-crystalline grain of austenite surrounded by a ferritic matrix. The simulations are performed using the finite element package ABAQUS and the constitutive models are implemented using the UMAT and UMATHT subroutines for a fully-coupled thermomechanical analysis. Details about the numerical time integration of the phase transformation model can be found in [62]. The initial-boundary value problem consists of solving simultaneously the balance of linear momentum (for a quasi-static process in the absence of body forces) and the balance of energy (in the absence of non-contact heat exchange), i.e.,

$$\operatorname{div} \mathbf{P} = \mathbf{0}, \quad \rho_0 \dot{\epsilon} = \mathbf{P} \cdot \dot{\mathbf{F}} - \operatorname{div} \mathbf{q} , \qquad (2.66)$$

together with appropriate initial and boundary conditions for the thermal and mechanical fields.

The material parameters for the austenite, martensite and ferrite used in the simulations are shown in Table 2.1 with the sub- or superscripts A, M or F indicating the corresponding phase. These parameters are equal to those presented in [72] (see also



Figure 2.1: Austenitic single crystal sample loaded in two distinct crystalline orientations.

references therein for additional information on the calibration of those parameters). Detailed crystallographic data for the transformation systems can be found in [75]. Plastic deformation in the FCC austenite is accounted for by considering slip along the systems of the $\langle 110 \rangle_A \{111\}_A$ family. For the BCC ferrite, plastic deformation is modeled based on the $\langle 111 \rangle_F \{110\}_F$ family and data for the non-Schmid contribution to slip resistance can be found in [71]. In addition, representative values for the specific heat and thermal conductivities of typical low-allowed carbon steels are taken from [65]. Observe that, for simplicity, the conductivity and the specific heat of all phases are taken equal to that of a multiphase steel and they do not depend on temperature, which is a reasonable assumption for the range of temperatures considered in the present analysis.

2.2.1 Austenitic single crystal under uniaxial tension

A simulation is performed on a cubical sample of a single crystal of austenite subjected to an axial nominal strain up to $\varepsilon_{11} = 0.2$ using a strain rate of $10^{-4}s^{-1}$, where the nominal strain is $\varepsilon = \mathbf{V} - \mathbf{I}$, with \mathbf{V} the left stretch tensor in the polar decomposition of the deformation gradient \mathbf{F} . To achieve this mechanical loading condition, three mutually perpendicular faces of the cube are constrained along their normals while pulling the top plane of the specimen in x_1 -direction with the prescribed loading rate (see Fig. 4.1). The two remaining faces are set to be traction-free. A zero heat-flux boundary condition is applied in the thermomechanical simulation, hence there is no heat exchanged with the surrounding environment. To study the effect of the internal heat generated from inelastic mechanisms (transformation and plasticity) on the mechanical response, each thermomechanical simulation is repeated under isothermal conditions for comparison purposes. In the isothermal simulations only the linear momentum equation is solved with a temperature equal to the initial temperature of its thermomechanical counterpart. To assess the effect of the initial temperature, each type of simulation, i.e., isothermal and thermomechanical, is performed for two different values of the initial temperature, namely

Parameter(s)	Value(s)	Equation(s)
Mechanical Elastic moduli	$\begin{split} \kappa_1^{\rm A} &= 286.8, \kappa_2^{\rm A} = 166.4, \kappa_3^{\rm A} = 145.0 \ ({\rm GPa}) \\ \kappa_1^{\rm M} &= 372.4, \kappa_2^{\rm M} = 345.0, \kappa_3^{\rm M} = 191.0 \ ({\rm GPa}) \\ \kappa_4^{\rm M} &= 508.4, \kappa_5^{\rm M} = 201.9, \kappa_6^{\rm M} = 229.5 \ ({\rm GPa}) \\ \kappa_1^{\rm F} &= 233.5, \kappa_2^{\rm F} = 135.5, \kappa_3^{\rm F} = 118.0 \ ({\rm GPa}) \end{split}$	(2.32)
Transformation kinetic parameters	$\dot{\xi}_0 = 0.003 (\mathrm{s}^{-1}), \nu = 0.17,$ $f_{\mathrm{cr}}^{(\alpha)} = 227 (\mathrm{MPa})$	(2.56)
Surface energy parameters	$\chi = 0.2 \left({\rm J} \cdot {\rm m}^{-2} \right), l_0 = 0.05 \left(\mu {\rm m} \right)$	$(2.44)_2, (2.54)_5$
Plastic kinetic parameters	$\begin{split} \dot{\gamma}_0^{\rm A} &= 0.001 \left({\rm s}^{-1} \right), n_{\rm A} = 0.02 \\ \dot{\gamma}_0^{\rm F} &= 0.001 \left({\rm s}^{-1} \right), n_{\rm F} = 0.02 \end{split}$	(2.57)
Defect energy parameters	$\begin{split} \beta_{\rm A,0} &= 0.0056, c_{\rm A} = 0.5, \omega_{\rm A} = 10 \\ \beta_{\rm F,0} &= 0.0056, c_{\rm F} = 0.5, \omega_{\rm F} = 7 \\ \mu_{\rm A} &= 67.5, \mu^{(\alpha)} = 98.4, \mu_{\rm F} = 55.0 \; (\rm GPa) \end{split}$	(2.44) ₁ ,(2.62), (2.63),(2.64)
Hardening parameters	$s_{A,0} = 189, s_{\infty}^{A} = 579 \text{ (MPa)}$ $k_{0}^{A} = 3 \text{ (GPa)}, u_{A} = 2.8, q_{A} = 1$ $s_{F,0} = 154, s_{\infty}^{F} = 412 \text{ (MPa)}$ $k_{0}^{F} = 1.9 \text{ (GPa)}, u_{F} = 2.8, q_{F} = 1$	(2.60),(2.59)
Thermal		
Thermal driving force parameters	$\begin{split} \lambda_{\rm T}^{(\alpha)} &= -50.5 \ \left({\rm kJ} \cdot {\rm kg}^{-1} \right), \\ \phi_{\rm A}^{(i)} &= 5.13 \ \left({\rm J} \cdot {\rm kg}^{-1} \cdot {\rm K}^{-1} \right) \\ \phi_{\rm F}^{(i)} &= 4.27 \ \left({\rm J} \cdot {\rm kg}^{-1} \cdot {\rm K}^{-1} \right), \ \theta_{\rm T} = 633 ({\rm K}) \end{split}$	$(2.48),(2.54)_3,$ $(2.55)_2$
Specific heat	$h_{\mathrm{A}} = h^{(\alpha)} = h_{\mathrm{F}} = 450 \ \left(\mathbf{J} \cdot \mathbf{kg}^{-1} \cdot \mathbf{K}^{-1} \right)$	(2.40)
Thermal expansion coefficient	$\begin{split} \alpha_{\rm A} &= \alpha^{(\alpha)} = 2.1 \times 10^{-5} \ \left({\rm K}^{-1} \right), \\ \alpha_{\rm F} &= 1.7 \times 10^{-5} \ \left({\rm K}^{-1} \right) \end{split}$	(2.49),(2.50)
Heat conductivity	$k_{\rm A} = k^{(\alpha)} = k_{\rm F} = 60 \ \left({\rm W} \cdot {\rm m}^{-1} \cdot {\rm K}^{-1} \right)$	(2.65)

Table 2.1: Model parameters for austenite, martensite and ferrite. The elasto-plastic models used for ferrite and austenite are formally similar; see section 2.1.6.

 $\theta_0 = 300 \text{ K}$ and $\theta_0 = 350 \text{ K}$. Due to the anisotropic mechanical properties of the austenite and the martensite, the aforementioned simulations are performed for two crystalline orientations such that the loading direction x_1 corresponds to the crystallographic directions $[100]_A$ and $[111]_A$, measured with respect to the austenitic crystal lattice as shown in Fig. 4.1. The sample is initially fully austenitic, stress-free and the reference temperature θ_0 for the thermal strains is set to coincide with the initial temperature, hence the initial thermal deformation gradient is identity.

Tension along the $[100]_A$ direction

The results for the sample loaded along the $[100]_A$ direction are shown in Fig. 4.2. The figure indicates the evolution of (a) the axial component T_{11} of the Cauchy stress tensor **T**, (b) the temperature θ , (c) the total martensitic volume fraction $\xi_{\rm M} = \sum_{\alpha=1}^{N} \xi^{(\alpha)}$ and (d) the plastic microstrain β , as a function of the axial logarithmic strain e_{11} , where the logarithmic strain is $e = \ln V$. The total volume fraction ξ_M monitors the nucleation and subsequent growth of the martensitic phase whereas plastic slip can be correlated to the plastic microstrain β . From Fig. 4.2a, it can be observed that the evolution of the axial stress T_{11} is significantly different for the thermomechanical case (labeled as "th.mech.") and the isothermal case (labeled as "iso.th."). In the isothermal case, there is a clear stress plateau as the austenite gradually transform into martensite, i.e., as $\xi_{\rm M}$ increases from 0 to 1 (see Fig. 4.2c). The stress response curve exhibits a plateau in accordance with the constitutive model that does not contemplate hardening as a direct result of the phase transformation mechanism (i.e., nucleation of new martensite is not hindered by the previous appearance of that phase). The stress plateau for the isothermal deformation at $\theta_0 = 300 \,\mathrm{K}$ starts at a lower strain than for the isothermal deformation at $\theta_0 = 350 \,\mathrm{K}$ since, in the latter case, the austenite deforms plastically prior to the nucleation of martensite (compare the evolution of $\xi_{\rm M}$ and β in Figures 4.2c and 4.2d, respectively). Moreover, from Fig. 4.2d, it can be seen that for the isothermal deformation at $\theta_0 = 300 \,\mathrm{K}$ there is no plastic slip and for the isothermal deformation at $\theta_0 = 350 \,\mathrm{K}$ plastic slip is suppressed as soon as the material starts to transform (see Fig. 4.2c and Fig. 4.2d). The end of the stress plateau for both temperatures corresponds to the point where the austenite has fully transformed into martensite, which behaves elastically.

In contrast to the isothermal case, the stress in the austenite in the thermomechanical case under zero heat flux boundary conditions shows a gradual increase with continuous deformation. Both inelastic mechanisms (plasticity and transformation) are active throughout the process as shown in Figures 4.2c and 4.2d, i.e., in this case the transformation mechanism does not suppress the plastic deformation. The difference in the stress response between the isothermal and thermomechanical cases can be explained as follows: The heat generated from the inelastic processes increases the temperature of the material as shown in Fig. 4.2b. According to $(2.54)_3$, an increase in temperature results in a decrease in the thermal contribution to the transformation driving force $f_{th}^{(\alpha)}$ (ob-

serve that, in view of the values shown in Table 2.1, $f_{\rm th}^{(\alpha)}$ is a monotonically decreasing function of the temperature). This feature reflects the fact that austenite is more stable at higher temperatures. The main contributions of the total transformation driving force $f^{(\alpha)}$ are the thermal part, $f_{\rm th}^{(\alpha)}$, and the mechanical part, $f_{\rm m}^{(\alpha)}$. Consequently, in order to further activate the phase transformation mechanism, as the thermal part $f_{\rm th}^{(\alpha)}$ decreases with temperature, a *larger* stress is required for the mechanical part $f_{\rm m}^{(\alpha)}$ to increase up to the point where the total driving force $f^{(\alpha)}$ reaches the critical value $f_{\rm cr}^{(\alpha)}$. Hence, an increase in temperature produces an apparent stress "hardening" observed in the stress response curves that is not directly associated with plastic hardening (see, e.g., the stress response in Fig. 4.2a for the thermomechanical case with $\theta_0 = 300$ K where initially there is no plastic deformation as can be observed from Fig. 4.2d).

For the thermomechanical case, the evolution of the temperature θ is depicted in Fig. 4.2b. Since the specimen is subjected to zero normal heat flux at external boundaries, the change in temperature occurs due to the internal heat generated from the inelastic processes. In view of the fact that there is an explicit expression for the internal energy, the temperature field can be obtained as the solution of (2.66) without the need to assume that a constant portion of the inelastic mechanical power is converted into heat (i.e., a fraction of the last two terms on the right hand side of (2.15)). Instead, the expression given in (2.52) is used to solve $(2.66)_2$ iteratively, in the present case with a Newton-Raphson algorithm. As can be seen in Fig. 4.2b, the temperature in the simulation with the lower initial temperature ($\theta_0 = 300 \,\mathrm{K}$) increases at a *higher rate* and eventually becomes *larger* than the temperature in the simulation with the larger initial temperature ($\theta_0 = 350$ K). This result, which at first sight might be counterintuitive, can be traced back to the underlying deformation mechanisms. Indeed, as indicated in Fig. 4.2c, more austenite transforms into martensite in the simulation with $\theta_0 = 300 \text{ K}$ than in the simulation with $\theta_0 = 350 \text{ K}$. Conversely, from Fig. 4.2d, more plastic deformation is observed in the simulation with $\theta_0 = 350 \,\mathrm{K}$ than in the simulation with $\theta_0 = 300 \,\mathrm{K}$. Thus, it may be concluded that more heat is generated due to the phase transformation than due to plastic deformation, which correlates with the evolutions of the temperatures shown in Fig. 4.2b. This feature also serves to explain why the initial "thermal" stress hardening discussed above and shown in Fig. 4.2a is higher for the simulation with $\theta_0 = 300 \,\mathrm{K}$ than in the simulation with $\theta_0 = 350 \,\mathrm{K}.$

Tension along the $[111]_{\rm A}$ direction

The results for the sample loaded in the $[111]_A$ direction, for two initial temperatures $\theta_0 = 300 \text{ K}$ and $\theta_0 = 350 \text{ K}$ and the corresponding isothermal cases, are shown in Fig. 2.3 in terms of the evolution of the axial Cauchy stress T_{11} , the temperature θ , the total martensitic volume fraction ξ_M and the plastic microstrain β . In this case, except for the isothermal simulation at $\theta = 300 \text{ K}$, all responses are nearly identical in terms of the stress, transformation and plastic behavior (see Fig. 2.3a,c and d, respectively). In the



Figure 2.2: Response of a single crystal of austenite loaded in the $[100]_A$ direction for two initial temperatures $(\theta_0 = 300 \text{ K} \text{ and } \theta_0 = 350 \text{ K})$ for the isothermal and thermomechanical (zero heat flux) cases: Evolution as a function of the axial logarithmic strain e_{11} of (a) the Cauchy axial stress T_{11} , (b) temperature θ , (c) martensitic volume fraction ξ_M and (d) plastic microstrain β .



Figure 2.3: Response of a single crystal of austenite loaded in the $[111]_A$ direction for two initial temperatures $(\theta_0 = 300 \text{ K} \text{ and } \theta_0 = 350 \text{ K})$ for the isothermal and thermomechanical (zero heat flux) cases: Evolution as a function of the axial logarithmic strain e_{11} of (a) the Cauchy axial stress T_{11} , (b) temperature θ , (c) martensitic volume fraction ξ_M and (d) plastic microstrain β .

isothermal simulation at $\theta = 300$ K both inelastic mechanisms (plasticity and transformation) are active until the austenite fully transforms into martensite, effectively suppressing plasticity since the martensite deforms elastically. In contrast, the other three simulations (isothermal at $\theta = 350$ K and thermomechanical with initial temperatures $\theta_0 = 300$ K and $\theta_0 = 350$ K), are dominated by plastic deformation with little or no phase transformation and, from this point of view, the corresponding responses differ significantly from those of the sample loaded along the $[100]_A$ direction shown in Fig. 4.2. The plastic driving force, as given in (2.55), has only a weak dependence on the temperature for the given set of material parameters indicated in Table 2.1. Consequently, the stress response for the thermomechanical case does not significantly diverge from the isothermal case in a process dominated by plasticity.

The differences between the responses of the specimens loaded in the $[100]_A$ and [111]_A directions can be traced back to the mechanical part of the transformation driving force shown in $(2.54)_1$, in particular the first term that involves an inner product with the transformation strain $\mathbf{b}^{(\alpha)} \otimes \mathbf{d}^{(\alpha)}$. Indeed, based on the crystallographic data for the transformation systems (see [75]), the axial stress required to nucleate martensite is significantly *larger* when a specimen is loaded in the $[111]_A$ direction compared to a specimen loaded in the $[100]_A$ direction. Similarly, in view of the expression of the mechanical plastic driving force $g_{\rm m}^{(i)}$ given by (2.55)₁ (i.e., the Schmid stress), the axial stress required to trigger plastic slip is also larger for a specimen loaded in the [111]_A direction compared to a specimen loaded in the [100]_A direction. Nevertheless, the stress required to activate plasticity is less than the stress required to nucleate a transformation system for a specimen loaded in the $[111]_{A}$ -direction, thus plastic slip becomes the preferred inelastic mechanism. In addition, as the temperature increases, the thermal part of the transformation driving force decreases (see $(2.54)_3$ and note that $\lambda_T < 0$) while the thermal part of the plastic driving forces increases (see $(2.55)_2$), which reinforces the preference of plasticity as an inelastic mechanism at larger temperatures.

The results of the simulations for a single crystal of austenite shown in this section are in good qualitative agreement with high-energy X-ray diffraction measurements recently presented in [8] where it was observed that the transformation rate increases with decreasing temperature and that the transformation occurs preferentially when the grain is loaded in the [100]_A-direction.

2.2.2 Austenitic grain embedded in a ferritic matrix

To study the thermomechanical interaction between the constituent phases of a typical low-alloyed multiphase TRIP steel, a cubic sample consisting of a single grain of retained austenite embedded in a matrix of six ferritic grains is considered in this section, as shown in Fig. 2.4. The cubic sample has a side length of 3μ m and the polyhedral austenitic grain has a characteristic size of 2μ m and occupies approximately 13% of the total volume (i.e., the initial volume fraction of austenite is $\xi_{A,0} = 0.13$). The samples are discretized with a



Figure 2.4: Grain of retained austenite surrounded by a ferrite-based matrix. The sample is loaded along the x_1 -direction and two distinct crystal orientations are considered (see inset).

total number of 864 linear hexahedral elements. The loading of the sample is similar to the uniaxial deformation tests in the previous section with an average extensional strain rate of 10^{-4} s⁻¹ along the x_1 -direction that is achieved by imposing a normal displacement on the top face, zero normal displacements imposed on the bottom and two lateral faces and traction-free conditions prescribed on the remaining directions and external faces. For the thermomechanical simulations, a uniform initial temperature of $\theta_0 = 300 \,\mathrm{K}$ is applied and zero heat flux is prescribed on the external surfaces of the specimen. Heat can flow and be exchanged between the distinct phases according to Fourier's law of heat conduction. The sample is initially stress-free with zero thermal strain prior to the loading, i.e., the reference temperature for the thermal strains in all phases is set equal to the initial temperature θ_0 . To explore the influence of the crystal orientations on the sample's response, two crystal orientations are analyzed, namely (i) all ferritic grains and the austenitic grain are oriented such that the loading direction x_1 coincides respectively with the $[100]_{\rm F}$ and $[100]_{\rm A}$ directions and (ii) all ferritic grains and the austenitic grain are oriented such that the loading direction x_1 coincides respectively with the $[111]_F$ and $[111]_A$ directions. In Fig. 2.4 these two orientations are denoted as $[100]_{A,F}$ and $[111]_{A,F}$. The motivation for this choice of orientations is that they represent "soft" and "hard" responses, thus they characterize lower and upper limits for the possible combinations of the crystallographic orientations of the two phases.

The isothermal and thermomechanical response are shown in Fig. 2.5 in terms of (a) the average axial Cauchy stress \overline{T}_{11} , (b) the average temperature $\overline{\theta}$, (c) the normalized austenitic volume fraction $\overline{\xi}_{A} = \xi_{A}/\xi_{A,0}$ and (d) the phase-averaged plastic microstrain $\overline{\beta}$ for each phase (i.e., β averaged over the austenitic grain as shown on the left, and β averaged over the ferritic grains as sown on the right). The stress, strain and the temperature



Figure 2.5: Response of an aggregate of austenitic and ferritic grains for an isothermal simulation at θ = 300 K and a thermomechanical (zero heat flux) simulation with initial temperature θ_0 = 300 K: Evolution as a function of the average axial logarithmic strain e_{11} of (a) the average Cauchy axial stress T_{11} , (b) the average temperature θ , (c) the normalized austenitic volume fraction $\bar{\xi}_A$ and (d) the phase-averaged plastic microstrain β .

are averaged over the whole cubic sample whereas the microstrains are averaged over the corresponding phases (ferrite and austenite).

As anticipated, the stress response for the $[111]_{A,F}$ -loaded sample is considerably higher than for the $[100]_{A,F}$ -loaded sample, both for the isothermal and thermomechanical cases (see Fig. 2.5a). However, the differences between the isothermal and thermomechanical cases for the same orientation are relatively small. This is due to the facts that (i) the samples contain mostly ferrite, whose stress response dominates the overall behavior and (ii) in the present model the isothermal and thermomechanical responses for the ferritic phase are similar since the plastic driving force only depends weakly on temperature and the resistance to plastic slip is taken to be temperature-independent.

The increase in temperature in the thermomechanical simulations of the aggregate of ferrite and austenite is on average *smaller* than for the single crystal of austenite (compare Fig. 2.5b with Fig. 4.2b and Fig. 2.3b for $\theta_0 = 300$ K). As for the stress response, the significant amount of ferrite in the sample (87%) dominates the overall thermal behavior. The internal heat generation in the ferrite is only due to plastic deformation and it is less significant than the heat generated due to phase transformation in the austenite. Consequently, the average heat generated per unit volume in the aggregate of ferrite and austenite is less than in the austenitic single crystal. Moreover, contour plots of the temperature (not presented here) indicate that the loading is sufficiently slow for the heat generated in the austenite from the transformation to be conducted towards the ferritic matrix, as a result of which the temperature field is nearly spatially uniform. Hence, as the heat generated in the austenite due to transformation is conducted towards the ferritic matrix, the austenitic grain remains cooler in an aggregate compared to the single crystal case. Since the temperature in the austenite in an aggregate does not increase as much as for the single crystal, it is easier to trigger a phase transformation in the former case than in the latter. This phenomenon also serves to explain why the (normalized) transformation rates $d\xi_M/d\bar{e}_{11}$ in the thermomechanical simulations of aggregates loaded in the $[100]_{A,F}$ and $[111]_{A,F}$ -directions are higher than the transformation rates $d\xi_{\rm M}/de_{11}$ in the thermomechanical simulations of a single crystal for the corresponding loading directions $[100]_A$ and $[111]_A$ (compare Fig. 2.5c with the thermomechanical curves for $\theta_0 = 300$ K in Fig. 4.2c and Fig. 2.3c keeping in mind that $\bar{\xi}_M = 1 - \bar{\xi}_A$ hence $d\bar{\xi}_M/d\bar{e}_{11} = -d\bar{\xi}_A/d\bar{e}_{11}$). Nevertheless, as in the single crystal case, the transformation rates in the *thermomechanical* simulations of austenite-ferrite aggregates remain lower than the transformation rates for the corresponding *isothermal* simulations in the same aggregates due to the increase in temperature in the former case (see Fig. 2.5c).

2.3 Conclusion

A thermomechanical model applicable to individual single-crystal grains of austenite undergoing plastic deformation and phase transformation has been developed with special emphasis on a thermodynamically-consistent formulation for the thermomechanical coupling. Consistency is achieved through a decomposition of the entropy density that includes an entropic counterpart of the thermal deformation gradient. The model was used to analyze fully-coupled thermomechanical deformations of a single crystal of austenite as well as an aggregate of austenitic and ferritic grains. The simulations indicate that for a single crystal of austenite, the increase in temperature associated with the latent heat of transformation reduces the transformation rate and significantly *delays* the transformation-induced plasticity effect. Consequently, the effective hardening response under axial deformation of a thermally-insulated sample is initially higher but eventually lower compared to a sample deformed under isothermal conditions. However, the delay in the transformation-induced plasticity effect due to the latent heat is relatively small when the ferritic matrix is taken into account. The ferritic matrix absorbs the latent heat generated in the austenite and, since ferrite accounts for a large volume in a multiphase steel, it effectively acts as a thermal sink, thus mitigating the temperature increase. In that case, the effective stress responses for the isothermal and thermomechanical cases are similar. However, it is relevant to indicate that the conclusions from the present study are applicable to quasi-static processes where there is sufficient time for the heat generated in the austenite to flow to the surrounding ferritic matrix. For materials with a more significant volume fraction of austenite (e.g., austenitic alloys) as well as for impact problems involving high strain rates, it can be anticipated that thermal effects may be more significant than for low-alloyed multiphase steels under quasi-static loading.

CHAPTER 2. COUPLED THERMOMECHANICAL MODELING AND SIMULATION OF TRIP STEELS

RVE simulation of different TRIP steel microstructures

¹A thorough understanding of the link between the microstructural-level characteristics of a material and its macroscale response is critical for the development of new multiphase materials with enhanced effective mechanical properties. Typical microstructures of high-strength low-alloyed multiphase steel assisted by transformation-induced plasticity (TRIP steels) are composed of grains of retained austenite embedded in a ferritic matrix. Upon mechanical deformation, the austenite transforms into martensite, which is a harder phase, thus increasing the effective hardening of the material compared with a steel without retained austenite. The microstructure of a multiphase steel can be modified through its processing route [4, 77]. For a TRIP steel, microstructural characteristics such as the initial volume fraction of austenite, the carbon concentration in the retained austenite and crystallographic texture, have a strong influence on the stability of the retained austenite, and, consequently, on the overall mechanical response [69]. Grain size also greatly affects the macroscopic properties, an issue that has been analyzed with continuum and discrete models [74, 54]. In the present study, attention is focused on determining the influence of the *spatial distribution* of the austenite on the macroscopic mechanical response.

In general, the macroscopic properties of a multiphase steel not only depend on the initial volume fraction of the austenite, but also on how the austenite is distributed within

¹This chapter is based upon S. Yadegari, S. Turteltaub, A.S.J. Suiker, P.J.J. Kok, *Comp Mat Sci*, **84**, 339-349, 2014

the ferritic matrix. Two distinct, technologically-relevant distributions are analyzed and compared, namely (i) a benchmark microstructure with isolated, randomly-distributed austenitic grains embedded in the ferritic matrix and (ii) a microstructure where the austenitic grains are clustered in a plate-like region (band). The benchmark distribution is typically encountered in cold-rolled TRIP steels that are subsequently subjected to a twostep annealing (intercritical annealing followed by isothermal heat treatment). Retained austenite is typically found in grains wedged between ferritic grains. On the other hand, austenitic grains clustered in a band-like region may appear during hot-rolling (i.e. hightemperature mechanical deformation during processing), whenever the banded morphology is not completely removed during further heat treatment (see [53]). The relevance of banded morphologies in ferrous alloys has been discussed in [23, 13, 66]. Using a discrete dislocation-transformation model, the effect of a banded microstructure was analyzed in [55], where it was found that a microstructure composed of randomly-distributed grains of austenite is optimal in terms of strength since it delays the onset of plastic localization compared with banded microstructures. The present analysis is based on a continuum approach which, compared with the aforementioned discrete model, allows to extend the analysis to a three-dimensional setting and for a larger range of deformations (i.e. not only for the onset of plastic deformation), thus providing a more comprehensive insight on the effect of spatial distribution.

In order to establish a direct link between the spatial distribution of austenite and the macroscopic properties of a multiphase steel, simulations are conducted in banded and dispersed microstructures while keeping all other relevant microstructural features the same (i.e. initial volume fraction of austenite, average crystallographic orientation, carbon content, etc.). The constitutive models used for ferrite and austenite are summarized in Section 3.1. A multilevel Voronoi algorithm is used in Section 3.2 to generate microstructural computational samples of aggregates of grains. These samples are used in a convergence analysis to establish the required size of a representative volume element used to determine macroscopic properties. The effect of a banded microstructure is analyzed in Section 3.3 based on a comparison with benchmark simulations. Conclusive remarks are provided in Section 3.4.

3.1 Micromechanical modeling of multiphase TRIP steels

The microstructures considered in the present analysis consist of an aggregate of ferritic grains (primary phase) and metastable retained austenitic grains (secondary phase). Upon loading, the austenitic grains may partially or totally transform into a martensitic phase. The goal of the present work is to determine the collective response of the aggregate of grains for which separate constitutive models are used for each phase. The main characteristics of the models are summarized in this section and the interested reader is referred to relevant publications for further details.

3.1.1 Elasto-plastic-transformation model for austenitic grains

The elastoplastic response of the austenitic phase and its possible transformation into the martensitic phase is simulated using the model originally proposed by Turteltaub and Suiker [75, 73, 62] and subsequently extended by Tjahjanto et al. [70] and Yadegari et al. [82]. The model assumes that, upon loading, a region inside each grain (i.e. at the sub-grain length scale) may undergo a plastic deformation through slip and/or a sudden change in crystalline structure, i.e., martensitic phase transformation. The transformation of austenite, which possesses a face-centered cubic (FCC) structure, into twinned martensite, composed of pairs of body-centered tetragonal (BCT) martensitic variants, is described according to the theory of martensitic transformations [3]. The distinct pairs of (twinned) variants of martensite, referred to as transformation systems, are characterized by two vectors, namely the habit plane normal and the shape strain vector. The transformation model is coupled to a crystal plasticity model to simulate the sub-grain interaction between transformation and plastic deformation [70]. Plastic deformation at the sub-grain level is described by slip occurring on active slip systems. Following the approach used in crystal plasticity, individual slip systems are characterized by a pair of vectors that represent the slip plane normal and the slip direction.

The sub-grain length scale behavior of a collection of slip systems and transformation systems is translated to the mesoscale (grain-level) by considering the weighted average of active systems that account for the corresponding inelastic mechanisms. This averaging is performed within sub-regions in the grains, which allows to simulate non-homogeneous plastic deformations and/or transformations inside individual grains. The averaged response for the martensitic transformation is obtained upon time-integration of the rate of change of the volume fractions of the individual transformation systems. This set of rates is denoted as $\dot{\boldsymbol{\xi}} = (\dot{\xi}^{(1)}, \ldots, \dot{\xi}^{(N)})$, where $\dot{\xi}^{(\alpha)}$ represents the rate of change of the volume fraction of the α -th martensitic system within a sub-region inside a grain and N is the total number of available transformation systems. For plasticity, the averaged responsed is determined from the rate of slip in each system, i.e., from $\dot{\gamma} = (\dot{\gamma}^{(1)}, \ldots, \dot{\gamma}^{(M)})$, where $\dot{\gamma}^{(i)}$ denotes the rate of slip in the *i*-th system and M is the total number of slip systems in the underlying material. Although the martensite is assumed to deform only elastically, the model takes into account the amount of plastic slip that occurred in the austenite prior to transformation.

The rates of change for transformation and plastic slip upon loading are modeled using a formulation that is thermodynamically-consistent with respect to the dissipation inequality. The isothermal model used in the present simulations is derived from a thermomechanical formulation using a constant homogeneous temperature such that the thermal deformation gradient is equal to identity [82]. Following the formalism proposed by Onsager [9] and guided by the so-called Coleman-Noll procedure [15], the terms in the dissipation inequality are expressed as a sum of products of affinities (i.e. driving forces) and fluxes (i.e. rates of change for volume fractions and plastic slip) for each inelastic mechanism. The model includes constitutive evolution relations between fluxes and affinities, i.e., kinetic relations. In particular, the transformation of the austenitic phase into the martensite is described by a tangent hyperbolic function that relates the rate of transformation of each individual transformation system to the driving force of the corresponding system. Similarly, the plastic deformation in the austenite is governed by a power law that relates the plastic slip rate of each individual slip system to the corresponding plastic driving force. The evolution of plastic slip resistance is accounted for by a hardening power law. The kinetic relations are complemented by initiation criteria that indicate the onset of the inelastic deformation. Detailed expressions for the driving forces and the kinetic relations can be found in [70] and [82].

At the mesoscale (grain-level), the kinematical description of the austenitic phase is based on a large deformation framework where the deformation gradient at a given material point is multiplicatively decomposed as follows:

$$\mathbf{F} = \mathbf{F}_{\mathrm{e}} \mathbf{F}_{\mathrm{p}} \mathbf{F}_{\mathrm{tr}},\tag{3.1}$$

where \mathbf{F}_{tr} is the transformation deformation gradient, \mathbf{F}_{p} is the plastic deformation gradient and \mathbf{F}_{e} is the elastic portion of the deformation gradient, respectively. The mesoscale Cauchy stress tensor \mathbf{T} is determined from the elastic deformation gradient and an effective stiffness for a mixture of austenite and martensite (see [75] for details). The mesoscopic Helmholtz energy, which contains contributions related to the "bulk" elastic strain energy, a surface energy and a lattice defect energy, is described by a state function that depends on the elastic strain \mathbf{E}_{e} defined as $\mathbf{E}_{e} = (1/2)(\mathbf{F}_{e}^{T}\mathbf{F}_{e} - \mathbf{I})$ and on internal state variables, namely the volume fractions of the transformation systems $\boldsymbol{\xi}$ and a so-called microstrain β that is meant to reflect the elastic distortion in the crystalline lattice due to the presence of dislocations (see [70] and [82] for details).

To monitor the evolution of the martensitic transformation at the mesoscale, results are reported using the total martensitic volume fraction, defined as $\xi_M = \sum_{\alpha} \xi^{(\alpha)}$, with $\xi_M = 1$ being reached for a fully-transformed sub-region inside an austenitic grain. For monitoring the overall plastic deformation in the austenite, the accumulated amount of plastic slip is correlated to the microstrain β_A in the austenitic phase.

3.1.2 Elastoplastic model for ferritic grains

The elastoplastic deformation of the ferritic grains is simulated using a crystal plasticity model suitable for a body-centered cubic (BCC) phase. The model is similar to the one used for the austenitic phase, except that it incorporates an additional term in the resistance to slip to account for non-symmetric behavior in the twinning and anti-twinning directions (see [71] for details). At the mesoscale (grain-level), the kinematical description of the ferritic phase is decomposed as follows:

$$\mathbf{F} = \mathbf{F}_{\mathrm{e}} \mathbf{F}_{\mathrm{p}},\tag{3.2}$$

where the plastic deformation gradient \mathbf{F}_{p} is computed based on the contributions of the active slip systems. It is worth pointing out that the models used for the austenitic and ferritic phases are anisotropic and explicitly incorporate the orientation of the underlying crystalline lattice.

3.2 Representative volume element

To establish a representative link between the mesoscale response, characterized by the individual behavior of grains, and the macroscale response, governed by the collective behavior of a large number of grains, one has to analyze a material volume element containing a sufficiently large number of grains N_G such that the average response of the aggregate does not vary as the number of grains is further increased (i.e., the macroscale response converges within a desired tolerance). A representative volume element (RVE), comprising at least N_G grains, characterizes the macroscopic bulk response of the material. Note that the establishment of an RVE depends on the choice of the quantities used to monitor convergence. Since the current study aims at establishing the macroscopic mechanical response, the major components of the stress are chosen as a primary set of interest for the establishment of an RVE. In a multiscale framework, the upper scale does not contain an explicit constitutive relation; instead, the response relies on the information from the lower scale that is necessary to provide a macroscopic state of equilibrium under quasi-static loading, i.e., the average stress computed from lower scale information. In order to establish an RVE based on convergence of other quantities, such as crystallographic texture or internal variables, typically a different number of grains is required than for the mechanical response.

3.2.1 Microstructural volume elements

In order to identify the minimum number of grains required for an RVE, the responses of seven microstructural samples are analyzed. The samples consist of aggregates of ferritic and austenitic grains with a total number of grains increasing from 8 to 800 as indicated in Table 3.1. The volume fraction of the secondary phase (austenite) in each sample is approximately 12%, which is a typical value for multiphase TRIP steels (see, e.g., [61, 32]). The geometrical construction of the microstructures is achieved with a newly-developed, three-dimensional algorithm that is based on the generation of Voronoi-shaped polyhedrons. Standard Voronoi cells are convex, a property which is not consistent with the mesoscale morphology of grains. In order to perform simulations with more realistic, non-convex grains, the following two-level algorithm is proposed: At the first level, a standard periodic Voronoi tessellation is generated, i.e., seed points are randomly-chosen within a cubic region and the seed point field is fully-replicated in all adjacent cubic regions, thus forming a 3x3x3 stacking (i.e., the central cubic region is translated in 26 directions). Subsequently, Voronoi cells are generated from the complete seed point field

Sample #	Austenitic grains	Ferritic grains	Volume fraction
1	1	7	12.0
2	8	56	12.1
3	12	88	12.2
4	24	176	11.9
5	56	394	12.0
6	72	525	12.0
7	100	700	11.9

Table 3.1: Composition and volume fraction of different microstructural samples used in the RVE convergence study.



Figure 3.1: Two-dimensional illustration of a microstructure obtained from a multilevel Voronoi tessellation. The first level (fine tessellation) contains 200 cells and the second level (coarse tessellation) has 30 cells. White lines and small circles show, respectively, the cells and Voronoi seed points of the first level tessellation. The thin black lines show the cells of the second level tessellation. The bold black lines show the resulting complex-shaped grain structure. The grain size is largely determined by the coarse tessellation while the fine tessellation controls the grain morphology, particularly the grain boundaries.

in the 27 cubic domains. Only the Voronoi cells of the central cubic region are used to create a periodic structure; the cells that are cut by the cube's faces are modified to fit exactly in the cubic domain. These first-level Voronoi cells are referred to as the *fine* tessellation. At the second level, a *coarser* tessellation is created, also with randomly-chosen seed point field, but with a smaller seed point density compared with the density of the first tessellation. Cells from the coarse tessellation are used as master regions for the construction of complex-shaped grains. To this end, all cells of the finer tessellation, whose seed points are in the interior of the same master cell, are merged to form a single grain. This procedure is illustrated in Figure 3.1 for the two-dimensional case. By modifying the point field densities at both levels (fine and coarse), it is possible to generate a broad range of different shapes and sizes of grains.

For a multiphase material, the next step is to assign a phase to each newly-shaped grain. In the present study, two phases are distributed within the microstructure, namely ferrite and austenite, with a given volume fraction. For the samples indicated in Table 3.1, the spatial distribution of the secondary phase (austenite) inside the matrix (ferrite) is done

randomly. An iterative procedure is employed to satisfy the given volume fraction of each phase. However, since a sample contains a finite number of grains with volumes obtained from a random process, the targeted volume fraction cannot in general be matched exactly (see Table 3.1).

3.2.2 Crystallographic orientation

In the current study, the orientation distribution of an aggregate of grains is assumed to be *isotropic* for both the austenitic and ferritic phases. The orientation of the crystalline lattice of an individual grain with respect to a global vector basis is described in terms of Euler angles using the 313 convention, i.e., each grain orientation is represented by three angles that characterize rotations around three coordinate axes. In order to cover the whole orientation space without using the symmetry properties of the underlying crystalline structure, the three Euler angles range, respectively, from 0 to 2π , 0 to π and 0 to 2π . For a sufficiently large number of grains, a uniform (isotropic) orientation distribution can be achieved by choosing the three Euler angles as, respectively, $2\pi a$, $\cos^{-1} (2b - 1)$, and $2\pi c$, where a, b and c are random variables ranging between 0 and 1. Note that the expression used for the second Euler angle guarantees an unbiased orientation distribution by decoupling the composite Euler rotations. For each of the samples indicated in Table 3.1, four distinct random orientation distributions are chosen to study the influence of the grain orientation. Typical distributions, displayed as [100]-pole figures, are shown in Figure 3.2 for the first, fourth and seventh samples listed in Table 3.1.

3.2.3 Numerical simulations

All volume elements are subjected to an *average* simple shear deformation $\bar{\mathbf{F}} = \mathbf{I} + \bar{\gamma} \mathbf{e}_1 \otimes$ \mathbf{e}_3 where $\bar{\gamma}$ is the amount of shear, \mathbf{e}_i , i = 1, 2, 3 is an orthonormal basis aligned with the cubic samples and \otimes denotes the tensor product. The samples are quasi-statically loaded from $\bar{\gamma} = 0$ to $\bar{\gamma} = 0.2$ with an applied rate of deformation equal to $10^{-4} \ s^{-1}$. Periodic boundary conditions are prescribed on the external surfaces of the cubic sample, which ensure that the average deformation gradient corresponds to the prescribed value F during loading, i.e., $\langle \mathbf{F} \rangle = \mathbf{F}$, where $\langle \cdot \rangle$ denotes the volume average. Details of the numerical implementation of a non-redundant set of periodic boundary conditions are given in A.1. It is worth recalling that simulations with periodic boundary conditions generally provide a softer response (and usually a more physically-meaningful prediction) compared with simulations based on pointwise affine boundary conditions. All simulations are performed on a mesh with $30 \times 30 \times 30$ elements. Linear hexahedral elements with reduced integration are used in the simulations and geometrically-nonlinear strain measures are used in the solution of the linear momentum equation. The update of the internal variables is performed by means of an implicit iterative-scheme. Details of this implementation can be found in [62]. A complete list of material parameters used for the constitutive models can be found in [82].



Figure 3.2: Typical [100]-pole figures for the first sample (a, b), fourth sample (c,d) and seventh sample (f, g) listed in Table 3.1. The left column corresponds to austenite and the right one to ferrite.

The results of a typical set of simulations for four distinct randomly-chosen crystal orientation distributions (indicated as O1, O2, O3 and O4) that are used in the same volume element (in this case sample 4 from Table 3.1), are shown in Figure 3.3 as a function of the average amount of shear $\bar{\gamma}$. Figures 3.3(a,b) indicate the average Cauchy stress components T_{31} and T_{11} , respectively, where the average is carried out over all grains (ferrite and austenite). Figure 3.3(c) shows the average microstrain in the ferrite (averaged over ferritic grains only) and Figure 3.3(d) shows the average total volume fraction of martensite $\xi_{\rm M}$ (averaged over austenitic grains only). For sample 4, the influence of the crystal orientation distribution on the plastic response of the *ferritic* matrix, as monitored using the average microstrain $\beta_{\rm F}$, is relatively small as shown in Figure 3.3(c). However, the crystal orientation has a relatively important effect on the response of the *austenitic* grains (secondary phase) as may be inferred from Figure 3.3(d), which shows the evolution of the average normalized martensitic volume fraction $\xi_{\rm M}$. Since sample 4 contains 176 grains of ferrite but only 24 grains of austenite, it is expected that the scatter of the responses of the secondary phase would be larger than for the primary phase. Due to the distinct evolutions of the martensitic phase transformation in the secondary phase for



Figure 3.3: Typical results of simulations for sample 4 (with a total of 200 grains) for four distinct crystal orientations, labeled O_i , with i = 1, ..., 4).

different crystal orientation distributions, the average Cauchy stress component \overline{T}_{11} also evolves quantitatively differently as may be observed in Figure 3.3(b). Similar results, not shown here, are observed for the average stress components T_{22} and T_{33} . Nevertheless, the influence of the crystal orientation is less noticeable for the main average Cauchy shear stress component T_{31} , as can be seen in Figure 3.3(a). This trend can be ascribed to the fact that a phase transformation induces a (local) volumetric expansion, which needs to be compensated for by a volumetric contraction elsewhere in the domain (i.e., in the untransformed austenite and/or the ferritic matrix) since the imposed average simple shear deformation is isochoric. Since the normal components are affected by the (average) bulk properties, this dilatation behavior has a stronger effect on the average normal stress components \bar{T}_{ii} , i = 1, 2, 3, than on the average shear stress component \bar{T}_{31} . The dilatation response of the secondary phase is thus responsible for both negative values for the average normal components as well as a larger scatter in the responses compared with the average shear component. In particular, observe that the normal (compressive) stress T_{11} for orientation O1 is the largest (in absolute value) for all orientations analyzed, which correlates with the highest amount of transformation $\bar{\xi}_{M}$, obtained for the same orientation. The influence of the crystal orientation on the response of the computational samples is further analyzed in the next section.



Figure 3.4: Stress state of volume elements at $\bar{\gamma} = 0.2$: (a)-(d) average Cauchy stress components \bar{T}_{31} , \bar{T}_{11} , \bar{T}_{22} and \bar{T}_{33} , respectively.

3.2.4 Convergence analysis

In order to establish a lower bound for the number of grains required for an RVE, the final states of the simulations (i.e., at $\bar{\gamma} = 0.2$) for the seven volume elements indicated in Table 3.1 are plotted in Figure 3.4 in terms of the average Cauchy stress components and in Figure 3.5 in terms of the average plastic deformation in the ferritic and austenitic grains and the average volume fraction of martensite. In Figures 3.4 and 3.5, the results are shown as a function of the total number of grains in the samples (which are also labeled with the corresponding sample numbers as indicated in Table 3.1). For each sample, the four data points (shown as crosses) correspond to the results of four distinct random crystal orientations. To better visualize these results, an interpolated area bounded by the upper and lower simulation values is shaded in gray and the interpolated mean value (mean value of the four orientation distributions) is shown by a dashed line.

From Figure 3.4(a), it can be observed that the main shear stress component T_{31} converges, within an acceptable tolerance, for samples comprising about 200 grains or more. The plastic deformation in the ferritic matrix also converges for a similar number of grains, as can be seen in Figure 3.5(a) in terms of the microstrain $\bar{\beta}_{\rm F}$. However, convergence of the normal stress components \bar{T}_{ii} , i = 1, 2, 3, is relatively low as shown in Figure 3.4. The low rate of convergence on the normal stress components can be traced



Figure 3.5: Inelastic state variables of volume elements at $\bar{\gamma} = 0.2$: (a) average ferritic microstrain $\bar{\beta}_{\rm F}$, (b) average austenitic microstrain $\bar{\beta}_{\rm A}$ and (c) average normalized martensitic volume fraction $\bar{\xi}_{\rm M}$.

back to the low rate of convergence of the response of the secondary phase, austenite, as discussed in Section 3.2.3. Indeed, as can be inferred from Figures 3.5(b,c), the inelastic response of the secondary phase, measured in terms of the amount of plastic deformation in the austenite and its transformation into martensite, shows a scatter due to the limited number of austenitic grains in the samples (see Table 3.1). Nevertheless, as may be observed in Figures 3.4 and 3.5, three out of the four simulations for the largest sample (sample 7, with 100 grains of austenite), already show a reasonable convergence as these results are clustered around the mean value.

The convergence analysis indicates that the macroscopic shear stress in a multiphase steel under simple shear may be determined with a relatively small number of total grains (e.g., 200), but the macroscopic normal components require a larger number of grains of the secondary phase. Reasonable results may be expected with about 100 grains of the secondary phase. These guidelines are used in the next section to study the effect of the spatial distribution of the secondary phase on the overall response of a multiphase steel.

3.3 Effect of a banded microstructure on the response of a multiphase steel

In this section, the influence of the spatial distribution of the secondary phase (austenite) on the macroscopic properties of a multiphase steel is analyzed. In particular, the mechanical behavior of a material where the austenitic grains are clustered in a plate-like region (band) is compared with the response of a benchmark microstructure where the austenitic grains are randomly scattered within the ferritic matrix. These two microstructures are henceforth referred to as the *banded* and the *dispersed* microstructures, respectively.

3.3.1 Volume elements with banded microstructure

The analysis is carried out for three pairs of banded and dispersed microstructures with austenitic volume fractions of 10%, 20% and 30% as shown in Table 3.2. The microstructural samples are generated using the same multi-level periodic Voronoi tessellation as described in Section 3.2. The banded microstructures were created by defining a banded region and, within that region, assigning grains to the austenitic phase iteratively until the targeted volume fraction of austenite (for the whole sample) approximately matched the targeted value. As indicated in Table 3.2, all microstructures contain more than 200 grains in total, which was identified in Section 3.2.4 as a threshold for an RVE based on the macroscopic shear stress. The microstructures contain between 47 and 144 grains of the secondary phase (austenite), which should provide reasonable to accurate predictions for the normal stresses and the internal variables. Due to the multilevel Voronoi generation, there are less grains of austenite in the banded microstructures than in the corresponding dispersed microstructures, hence nominally the austenitic grains in the banded microstructures are larger than those of the dispersed microstructures (with an average grain size that scales with the cubic root of the volume). The difference in average austenitic grain size of the banded and dispersed microstructures range from 13% to 22%, which is relatively small. Moreover, since the purpose of the present analysis is to study the effect of the spatial distribution of the austenite rather than grain size effects, a length scale parameter in the model that is related to the grain size (see [74]) has been kept the same for all simulations.


Table 3.2: Volume elements with distinct initial volume fractions of austenite. Austenitic grains are displayed in dark gray while the ferritic grains are shown in light gray. The microstructures with randomly-dispersed austenitic grains are shown in the top row while the banded microstructures are indicated in the bottom row. The number of austenitic and ferritic grains is indicated below each sample.



Transverse shear In-plane shear Figure 3.6: Simple shear naming convention with respect to the band's plane: (a) transverse shearing case and (b) in-plane shearing case. The dark gray band represents the region where the austenitic grains are clustered.

3.3.2 Numerical simulations with banded microstructures

As in Section 3.2, all microstructures are subjected to a macroscopic simple shear from $\bar{\gamma} = 0$ to $\bar{\gamma} = 0.2$. The loading rate and periodic boundary conditions are the same as those indicated in Section 3.2.3. Randomly-chosen crystal orientations, as explained in Section 3.2.2, are used in the simulations. Although some fluctuations in the response may still occur for distinct randomly-chosen crystal orientations, it is expected from the convergence study in Section 3.2.4 that these would not qualitatively affect the simulations based on the number of grains used in the samples shown in Table 3.2.

As opposed to a dispersed microstructure, which is essentially macroscopically isotropic, a banded microstructure may be sheared in distinct ways depending on the orientation of the shearing direction and the shearing plane with respect to the band-like region where the secondary phase is clustered. This motivates separate simulations and comparisons of the samples for different shear loading cases. Two extreme shear loading cases are shown in Figure 3.6, where the plate-like austenitic region is represented as an idealized band in the middle of a cubic-sample. The two loading cases are referred to as *transverse* and *in-plane* shearing, respectively. Other possible shearing directions have been omitted for brevity because their responses are bounded by the results of the in-plane and transverse shear loading cases.

The average Cauchy shear stress component \overline{T}_{31} , the average normalized martensitic volume fraction $\overline{\xi}_{M}$ and the average ferritic microstrain $\overline{\beta}_{F}$ are shown as functions of the average amount of shear $\overline{\gamma}$ in Figure 3.7 for the transverse shear loading case and in Figure 3.8 for the in-plane shear loading case. The results for the banded microstructures are indicated by black curves and for the benchmark dispersed microstructures in gray. Dotted, dashed and solid line patterns are used to identify the results for microstructures with, respectively, 10%, 20% and 30% volume fraction of austenite.



Figure 3.7: Evolution under transverse shear loading of (a) the average main Cauchy shear stress, (b) the average martensitic volume fraction and (c) the average ferritic microstrain as functions of the macroscopic amount of shear. Graph (d) contains the relative difference between the response at $\bar{\gamma} = 0.2$ of the banded and dispersed microstructures.

3.3.3 Influence of the initial austenitic volume fraction

From Figure 3.7(a), which corresponds to the transverse shear loading case, it can be observed that for the microstructures with dispersed grains of austenite (gray lines), the shear strength increases with increasing initial volume fraction of austenite. However, for the banded microstructures (black lines), the trend is not monotonic as the response of the sample with 10% austenite has a slightly higher strength than the sample with 20% austenite. The influence on the shear strength of a higher initial volume fraction of austenite in the banded microstructure only becomes noticeable for the sample with 30% austenite. In contrast, for the banded microstructure loaded under in-plane shearing, the dependence of the shear strength on the austenitic volume fraction shows a similar trend as for the dispersed microstructures, see Figure 3.8(a). In that case, the shear strength always increases with increasing initial volume fraction of austenite.

Although strictly speaking there is no monotonic dependence of the martensitic transformation rate on the initial volume fraction of austenite, from Figures 3.7(b) and 3.8(b), one may conclude that the general trend is that the martensitic transformation rate under simple shear *decreases* with increasing austenitic volume fraction. This trend applies to both the transverse and in-plane shear loading cases. However, it is noted that this trend refers to the amount of martensite formed in the austenitic grains and not to the total amount of martensite in the sample, which depends on the initial volume fraction



Figure 3.8: Evolution under in-plane shear loading of (a) the average main Cauchy shear stress, (b) the average martensitic volume fraction and (c) the average ferritic microstrain as functions of the macroscopic amount of shear. Graph (d) contains the relative difference between the response at $\bar{\gamma} = 0.2$ of the banded and dispersed microstructures.

of austenite. Indeed, despite that the transformation rate is smaller with increasing initial volume fraction of austenite, the *total* amount of martensite formed during deformation *increases* with increasing initial volume of austenite, which explains the increase in shear strength since martensite is the hardest phase.

The plastic deformation in the ferrite appears to be rather insensitive to the initial volume fraction of austenite except for the banded microstructure under transverse shear loading, where the plastic deformation in the ferrite slightly increases with increasing initial volume fraction of austenite, see Figure 3.7(c).

3.3.4 Influence of the spatial distribution of austenite

To compare the responses of the banded and dispersed microstructures for samples with equal amount of austenite, the relative differences between the shear stress, martensitic volume fraction and microstrains of the banded and dispersed microstructures at the end of the simulations are indicated in Figures 3.7(d) and 3.8(d) for the transverse and inplane shear loading cases, respectively. The relative difference for the main shear stress is defined as

$$\Delta \bar{T}_{31} = \frac{\bar{T}_{31}^{\text{banded}} - \bar{T}_{31}^{\text{dispersed}}}{\bar{T}_{31}^{\text{dispersed}}} \bigg|_{\bar{\gamma}=0.2}$$

and similar formulas are used for the internal variables.

One can observe from Figure 3.7(d) that the banded microstructures have a lower shear strength than the dispersed ones under transverse shear for all austenitic volume fractions analyzed (i.e., the values of $\Delta \bar{T}_{31}$ are negative). Moreover, the absolute value of the relative difference in strength, i.e., $|\Delta \bar{T}_{31}|$, increases with increasing initial volume fraction of austenite. This trend may be correlated to the response of the secondary phase (austenite) and its effect on the primary phase (ferrite). Indeed, as shown in Figure 3.7(d), the amount of transformation as well as the plastic deformation in the austenite are significantly lower in the banded microstructures than in the dispersed ones (up to 50%difference). Observe that, within the austenitic phase, a decrease in transformation is not compensated for by an increase in plastic deformation. Rather, both inelastic mechanisms within the austenite show the same decreasing trend (i.e., less plastic deformation and less transformation for the banded microstructure compared with the dispersed microstructure). Consequently, this indicates that the austenite tends to deform less when it is clustered around a band-like region compared with microstructures with randomly distributed isolated grains of austenite inside the ferritic matrix. Correspondingly, in order to achieve the same imposed average shear deformation, the ferritic matrix tends to deform more in the banded microstructures compared with the dispersed ones. This behavior can be confirmed from the values of $\Delta\beta_{\rm F}$, which measures the differences between the microstrains in the ferritic matrix of the banded and dispersed microstructures, as shown in Figure 3.7(d). Indeed, the amount of plastic deformation in the ferritic matrix is higher for banded microstructures than for dispersed ones, which in relative terms diminishes the contribution to the overall strength of the (harder) secondary phase in banded microstructures. This prediction of the simulations is consistent with experimental observations reported by [53], albeit for tensile tests. In the experimental results, a significant portion of the deformation was carried by the ferritic matrix while the austenite in the banded regions experienced a smaller deformation and, consequently, a relatively small transformation rate. In the cited experimental work, the authors attributed the reduction in the transformation rate to unfavorable crystal orientations with respect to the external loading; however, the present simulations suggest that a reduced transformation rate in the austenite may be ascribed to a relatively high deformation of the ferritic matrix.

For the in-plane shear loading case, the shear strength of the banded microstructures is somewhat similar to the strength of the corresponding dispersed microstructures, as can be observed in Figures 3.8(a) and 3.8(d). In contrast to the transverse shear loading case, under in-plane shear loading there is *more* transformation and plastic deformation in the austenite for the banded microstructures than for the dispersed ones (see Figures 3.8(b,d)). Correspondingly, there is *less* plastic deformation in the ferrite for banded microstructures than for dispersed ones (see Figures 3.8(c,d)). Nevertheless, the distinct behavior of the banded and dispersed microstructures under in-plane shear is not sufficient to achieve significantly different shear strengths.

In order to gain a better insight in the different responses of banded microstructures



Transverse shearIn-plane shearFigure 3.9: Deformed shape at $\bar{\gamma} = 0.2$ of banded microstructure for (a) transverse shear and (b) in-plane shearfor samples with 30% initial volume fraction of austenite.

under transverse and in-plane shearing, the deformed shapes of the samples are shown in Figure 3.9 (see also sketch in Figure 3.6). The samples shown in the figure correspond to 30% initial volume fraction of austenite. As illustrated in Figure 3.9(a), the austenitic region deforms less than the ferritic matrix under transverse shear. In this case the (softer) ferritic matrix carries most of the deformation. In contrast, the deformation under in-plane shear is more homogeneous, hence the shear deformation is more evenly distributed between the ferrite and austenite. Correspondingly, the austenitic region carries a relatively smaller amount of the load under transverse shear than under in-plane shear. Indeed, the average shear stress in the austenite, $\bar{T}_{31}^{\rm A}$, at the end of the simulation is 400 MPa for the transverse shear loading case. The corresponding average shear stresses in the ferrite, $\bar{T}_{31}^{\rm F}$, are 367 MPa for the transverse shear loading case. Since for both loading cases the average stresses in the ferrite are similar, the shear stress \bar{T}_{31} averaged over the whole domain is lower under transverse loading (377 MPa) than under in-plane loading (413 MPa).

3.4 Conclusions

A convergence analysis is carried out to establish the size of representative volume elements for multiscale simulations using non-convex grain shapes that are generated from a multilevel Voronoi tessellation. From the numerical simulations of microstructures with banded and dispersed austenitic grains, it is found that:

• The shear strength of a TRIP steel increases with increasing volume fraction of austenite for microstructures with randomly-dispersed grains of austenite. For mi-

crostructures with clustered austenitic grains in band-like regions, the shear strength does not necessarily increase with increasing volume fraction of austenite.

- In a multiphase steel with a banded microstructure loaded under transverse shear, the plastic deformation localizes in the (softer) ferritic matrix, which diminishes the contribution of the secondary austenitic phase.
- The shear strength of a TRIP steel with clustered grains of austenite in a band-like region may be lower than the shear strength of a steel with similar composition but with the austenitic grains being dispersed.

From the aforementioned findings, one may conclude that clustering of the austenite in band-like regions in general has a negative effect on the hardening contribution of the secondary phase.

Generalized grain cluster method for multiscale response of multiphase materials

¹The constitutive behavior of metals and alloys is strongly influenced by their microstructural characteristics, such as the size, fraction, orientation and composition of the individual metallic phases. The need for understanding the evolution of microstructural characteristics with deformation has stimulated the development of advanced micromechanical models that accurately describe the underlying physical phenomena, e.g., recrystallization [12, 43], martensitic phase transitions [73, 48, 50], phase separation and coarsening by diffusion [17], twinning and detwinning [26, 79], dislocation interactions [22, 19], and cracking and damage growth [14, 63, 7, 20]. In order to apply state-of-the-art micromechanical models for the analysis of large-scale engineering problems, efficient and generic multiscale methods need to be developed for keeping the computational times within manageable bounds.

Starting with the landmark contributions of Voigt [78] and Reuss [49], substantial research effort has been devoted to efficiently transferring information from small length scales to the macroscopic scale, leading to a wide spectrum of analytical and numerical formulations for the effective mechanical behavior of composites [52, 67, 25, 27, 29, 80, 44, 10, 64, 81, 85]. Although for a broad range of materials these methods have

¹This chapter is based upon S. Yadegari, S. Turteltaub, A.S.J. Suiker, Comp Mech, 56, 193-219, 2015

provided an impetus to the homogenization of basic constitutive properties (elasticity, (rate-dependent) plasticity, power law creep), their extension towards the description of advanced microstructures composed of a diversity of phases with relatively complex constitutive behavior often is far from straightforward, and poses considerable mathematical challenges. Furthermore, the description of sophisticated micromechanical phenomena may introduce complementary conditions on the static and/or kinematic hypotheses adopted in classical homogenization approaches, such as the well-known Taylor assumption that demands the deformation in each microstructural phase to be equal to the applied macroscopic deformation. For example, for polycrystalline materials this kinematic assumption appears to be too restrictive for adequately simulating grain size effects [19] and deformation texture [76]; hence, during the last decade this has triggered the development of homogenization schemes in which deformation heterogeneity among grains is explicitly accommodated for by *relaxing* the Taylor assumption [40, 19, 76, 18, 68]. This relaxation can be formulated in various ways and at different degrees, and essentially comes down to requiring that the macroscopic deformation is no longer imposed on each grain individually, but rather on specific *clusters of grains*, by equating it to the weighted average of the grain deformations within a cluster. Accordingly, the distribution of strain remains homogeneous within each grain, but not within a cluster of grains.

To date, the grain cluster-type formulations presented in the literature typically consider relatively small clusters of 2 to 8 hexahedral (rectangular) grains, with the deformation incompatibilities at the grain boundaries being described by a set of additional kinematic variables, i.e., the a-priori unknown relaxations [19, 76, 18, 68]. These local relaxations are computed by minimizing the total work of the system, whereby the stationarity condition with respect to the relaxations results in the corresponding equations for traction continuity at the grain boundaries. For providing the relaxations with a physical background, the deformation mismatch at grain boundaries, commonly expressed by the Nye tensor [45, 24], often is constitutively connected to the development of dislocation networks, see [19, 68].

Despite their efficiency in terms of computational time, the current grain cluster-type formulations are not very suitable for being extended to clusters composed of a vast number of grains with realistic (convex and non-convex) shapes, since the incorporation of numerous relaxations at grain boundaries of arbitrary orientation makes the mathematical implementation relatively cumbersome. For this reason, in the present chapter a *generalized grain cluster method* (GGCM) is proposed in which these limitations are removed. In specific, the general character of this formulation can be defined by means of three distinctive aspects, namely: (i) the method is able to model grains in a computationally tractable way, thereby explicitly accounting for interactions between individual grains, (iii) the method is formulated within a geometrically nonlinear framework and is independent of the actual micromechanical model(s) applied within the grains. The latter aspect allows for the analysis of an aggregate of dissimilar (multiphase) grains with different,

user-defined constitutive properties.

The basic starting point of the method is to assume that each grain in a polycrystalline aggregate deforms homogeneously, whereby the deformation gradient is allowed to vary from grain to grain. However, as opposed to other grain cluster-type models, both traction discontinuities and deformation incompatibilities along grain boundaries are minimized simultaneously in the cluster, by means of iteratively adjusting the deformation gradients in the individual grains. This key ingredient is based upon the construction of a representative objective functional, which brings in the advantage that the method can be straightforwardly applied to a large number of grains of arbitrary shape. The use of separate weighting factors in the objective functional on the conditions for traction continuity and deformation compatibility makes it possible to cover the range of effective nonlinear responses lying between the Taylor bound (uniform deformation in the grains) and the Sachs bound (uniform stress in the grains). Although the method does allow for describing the incompatibilities at grain boundaries in terms of any particular localized deformation mechanism, such as geometrically necessary dislocations or intergranular cracks, for reasons of simplicity and generality these incompatibilities here are straightforwardly adopted as a consequence of the kinematic assumptions made in the formulation.

This chapter is organized as follows. The generalized grain cluster method is formulated in Section 4.1 and its numerical implementation is treated in Section 4.2. The calibration of the weighting factors and a detailed analysis of the efficiency and accuracy of the method is demonstrated in Section 4.3 through a series of simulations on grain clusters of various sizes. The simulations were performed for a multiphase material composed of ferritic grains undergoing plastic deformation and austenitic grains undergoing a combination of plastic deformation and phase transformation. The advanced microstructural geometries considered in the analyses were generated by means of a multilevel Voronoi algorithm developed recently in Section 3.2.1, and represent a steel experiencing transformation-induced plasticity, i.e., a TRIP steel. The plasticity and transformation phenomena activated under shear loading were simulated by means of crystallographically-based models presented in previous works by the authors [73, 75, 71, 70, 82]. One important objective for the development of the GGCM is to have a flexible scheme that can be used in a so-called multiscale adaptive algorithm. Within that algorithm, microscale simulations may be conducted using either the GGCM or a fullyresolved finite-element simulation at the level of individual grains, depending on the required resolution. In view of this, the performance of the GGCM is compared to (finite element-based) direct numerical simulations for the same microstructure (Chapter 3, Section 3.2.3). This illustrates that the generalized grain cluster method is able to efficiently account for the evolution of the stress and history variables, such as plastic slip and transformation volume fractions. Some concluding remarks are provided in Section 4.4 on the coupling of the GGCM with commercial FEM software, and the bifurcation sensitivity of microstructural responses.



Figure 4.1: Periodic aggregate of grains Ω .

4.1 Formulation of generalized grain cluster method

4.1.1 Basic assumptions

Consider an aggregate of $N_{\rm gr}$ grains, with each grain $N = 1, \ldots, N_{\rm gr}$ occupying a region Ω_N , as shown schematically in Fig. 4.1. The region filled by the cluster of grains is denoted as Ω , i.e.,

$$\Omega = \bigcup_{N=1}^{N_{\rm gr}} \Omega_N \,. \tag{4.1}$$

This aggregate of grains is assumed to be periodic in space. Each grain N is taken as a polyhedron, although not necessarily convex. The boundary of each polyhedral grain N is composed of M_N faces, denoted by $\Gamma_{N,\gamma}$ and identified using the global grain index N and a local face index $\gamma = 1, \ldots, M_N$. For notational purposes, it is convenient to introduce a global interface index I given by $I = \hat{I}(N, \gamma)$. The common interface Γ_I between adjacent grains N and N' (corresponding to the local indices γ and γ' , respectively), is uniquely identified as $I = \hat{I}(N, \gamma) = \hat{I}(N', \gamma')$, as illustrated in Fig. 4.1. Furthermore, observe that parts of grains on the "external" boundary of Ω appear as disconnected, but are in fact treated as a single grain due to periodicity. In that case, the index N refers to the whole grain and the index I to the whole interface, see Fig. 4.1. Correspondingly, the total number of interfaces in the cluster is

$$N_{\rm int} = \frac{1}{2} \sum_{N=1}^{N_{\rm gr}} M_N .$$
 (4.2)

The description of a deformation $\hat{\mathbf{y}}$ from a reference configuration is written as

$$\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x}, t) \quad \text{with} \quad \mathbf{x} \in \Omega \quad \text{and} \quad \mathbf{y} \in \Omega_t ,$$
 (4.3)

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where Ω and Ω_t denote the regions occupied by the grain cluster in the reference and the current configurations (at time t), respectively, x is a (material) point in the reference configuration and y denotes the current location of x at time t. The deformation gradient **F** is defined as

$$\mathbf{F} := \nabla \hat{\mathbf{y}} , \qquad (4.4)$$

where $\nabla = \partial / \partial \mathbf{x}$ designates the gradient with respect to \mathbf{x} .

Previous grain cluster-type formulations rely on variables that describe the deformation of *interfaces*, see [19, 76, 18, 68]. While this approach is adequate for the description of cubic-like grains, it becomes cumbersome and requires enforcement of redundant constraints for grains with an arbitrary polyhedral shape. In order to reduce the number of variables while preserving the simplicity of the grain cluster method, it is more efficient to work directly with the *deformation gradient* of the grain as the primary variable. This modification allows for an extension of the range of applications to a large number of grains of arbitrarily complex shapes; hence, the method is termed the *generalized grain cluster method* (GGCM). In view of developing the weak formulation of the GGCM, the deformation field \hat{y} and a generic test function \hat{w} are assumed to be *linear* inside each grain, i.e.,

$$\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x}, t) = \mathbf{F}_N(t)\mathbf{x} + \mathbf{c}_N(t),$$

$$\mathbf{w} = \hat{\mathbf{w}}(\mathbf{x}, t) = \mathbf{G}_N(t)\mathbf{x} + \mathbf{d}_N(t),$$

(4.5)

for x in Ω_N . At a given time t, the tensor \mathbf{F}_N and the vector \mathbf{c}_N thus are considered as *uniform* in grain N, with \mathbf{F}_N the deformation gradient; note that for an admissible deformation it is required that det $(\mathbf{F}_N) > 0$. The deformation gradient and the displacement are allowed to vary discontinuously from grain to grain. From this perspective, the proposed method shares similarities with non-conforming Galerkin finite element methods, where displacements are allowed to be discontinuous at element boundaries, see, e.g., [2]. The tensor \mathbf{G}_N and the vector \mathbf{d}_N characterizing the test functions in (4.5)₂ are assumed to be constant in the interior of each grain. Further, at the common interface I between two adjacent grains N and N', these quantities are taken as a simple average, i.e.,

$$\mathbf{G}_{I} := \frac{1}{2} \left(\mathbf{G}_{N} + \mathbf{G}_{N'} \right),$$

$$\mathbf{d}_{I} := \frac{1}{2} \left(\mathbf{d}_{N} + \mathbf{d}_{N'} \right),$$

(4.6)

with $I = \hat{I}(N, \gamma) = \hat{I}(N', \gamma')$ representing a global interface index, see the inset in Fig. 4.1. As will be shown below, the relevance of using (4.6) is to (approximately) recover continuity of traction and kinematic compatibility across grain boundaries.

4.1.2 Weak formulation and discretization of the balance of linear momentum

Neglecting body forces, for a quasi-static process the balance of linear momentum in terms of the first Piola-Kirchhoff stress tensor \mathbf{P} is expressed as

$$\operatorname{div}\mathbf{P} = \mathbf{0},\tag{4.7}$$

with $div = div_x$ denoting the divergence in the reference configuration. Multiplying (4.7) with a suitable test function w gives

$$\operatorname{div} \mathbf{P} \cdot \mathbf{w} = \operatorname{div} \left(\mathbf{P}^{\mathrm{T}} \mathbf{w} \right) - \mathbf{P} \cdot \nabla \mathbf{w} = 0 , \qquad (4.8)$$

where $(\cdot)^T$ designates the transpose of a tensor.

In the classical formulation of a boundary value problem the macroscopic boundary conditions are applied on the external boundary of the domain Ω . However, due to the periodicity of the present microstructure, all interfaces of the domain Ω are treated as internal boundaries, for which the boundary data is not explicitly defined. For this reason, the macroscopic deformation is imposed pointwise on the *interior* of the grain cluster instead, by means of the following multiscale kinematic constraint:

$$\int_{\Omega} \left(\mathbf{F} - \bar{\mathbf{F}} \right) \mathrm{d}v = \mathbf{0},\tag{4.9}$$

where \mathbf{F} is the deformation gradient in a microscopic material point and $\bar{\mathbf{F}}$ reflects the deformation gradient at the macroscopic level. Observe that the multiscale kinematic constraint (4.9) cannot be transformed to pointwise periodic boundary conditions, since the displacement field is not continuous across grains. Taking a variation in (4.9) with respect to the deformation gradient, it follows that a (virtual) deformation gradient $\delta \mathbf{F} = \nabla \mathbf{w}$ should satisfy that its average over the domain Ω is zero. Consequently, a suitable test function \mathbf{w} is assumed to fulfill the condition

$$\int_{\Omega} \nabla \mathbf{w} \mathrm{d}v = \mathbf{0} \,. \tag{4.10}$$

Integrating (4.8) over the reference domain Ω , followed by using the decomposition (4.1) and incorporating the constraint (4.10), gives

$$\sum_{N=1}^{N_{\rm gr}} \left[\int_{\Omega_N} \left(\operatorname{div} \left(\mathbf{P}^{\mathrm{T}} \mathbf{w} \right) - \mathbf{P} \cdot \nabla \mathbf{w} \right) \mathrm{d}v + \mathbf{\Sigma} \cdot \int_{\Omega_N} \nabla \mathbf{w} \mathrm{d}v \right] = 0, \qquad (4.11)$$

where Σ is a Lagrange multiplier tensor. Since the assumed displacement field u presented in (4.5) may be discontinuous across grain boundaries, the divergence term in (4.11) may not be defined at the internal interfaces. However, it is still possible to use the divergence theorem for each grain separately, which leads to

$$\sum_{N=1}^{N_{\rm gr}} \left[\sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \left(\mathbf{Pn} \right) \cdot \mathbf{w} da - \int_{\Omega_N} \mathbf{P} \cdot \nabla \mathbf{w} dv + \mathbf{\Sigma} \cdot \int_{\Omega_N} \nabla \mathbf{w} dv \right] = 0, \quad (4.12)$$

where $\mathbf{n} = \mathbf{n}(N, \gamma)$ refers to the outward normal unit vector of face $\Gamma_{N,\gamma}$. Rewriting (4.12) using the assumed fields (4.5) yields the following expression for the weak form

$$\sum_{N=1}^{N_{\rm gr}} \left[\sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \left(\mathbf{P}_N \mathbf{n} \right) \cdot \left(\mathbf{G}_I \mathbf{x} + \mathbf{d}_I \right) \mathrm{d}a - \int_{\Omega_N} \left(\mathbf{P}_N - \mathbf{\Sigma} \right) \cdot \mathbf{G}_N \mathrm{d}v \right] = 0 , \quad (4.13)$$

where \mathbf{P}_N refers to the first Piola-Kirchhoff stress in grain N and \mathbf{G}_I and \mathbf{d}_I are given by (4.6) with $I = \hat{I}(N, \gamma)$. Consistent with the assumption of a homogeneous grain subjected to a uniform deformation gradient \mathbf{F}_N , the stress \mathbf{P}_N is taken as *uniform* within an individual grain N.

To elaborate further on expression (4.13), observe that the first term refers to a summation over all grains N and all interfaces γ (local index), hence it involves surface integrals on both sides of each interface $I = \hat{I}(N, \gamma) = \hat{I}(N', \gamma')$. For a specific grain N that shares an interface I with a neighboring grain N', the contribution from both grains to the first term in (4.13) is, using relation (4.6),

$$\begin{split} &\int_{\Gamma_{N,\gamma'}} \left(\mathbf{P}_{N} \mathbf{n}(N,\gamma) \right) \cdot \left(\mathbf{G}_{\hat{I}(N,\gamma)} \mathbf{x} + \mathbf{d}_{\hat{I}(N,\gamma)} \right) da \\ &+ \int_{\Gamma_{N',\gamma'}} \left(\mathbf{P}_{N'} \mathbf{n}'(N',\gamma') \right) \cdot \left(\mathbf{G}_{\hat{I}(N',\gamma')} \mathbf{x} + \mathbf{d}_{\hat{I}(N',\gamma')} \right) da \\ &= \int_{\Gamma_{N,\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N} \mathbf{n}(N,\gamma) \right) \cdot \left(\left(\mathbf{G}_{N} + \mathbf{G}_{N'} \right) \mathbf{x} + \left(\mathbf{d}_{N} + \mathbf{d}_{N'} \right) \right) da \\ &+ \int_{\Gamma_{N',\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N'} \mathbf{n}'(N',\gamma') \right) \cdot \left(\left(\mathbf{G}_{N'} + \mathbf{G}_{N} \right) \mathbf{x} + \left(\mathbf{d}_{N'} + \mathbf{d}_{N} \right) \right) da \\ &= \int_{\Gamma_{N,\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N} \mathbf{n}(N,\gamma) + \mathbf{P}_{N'} \mathbf{n}'(N',\gamma') \right) \cdot \left(\mathbf{G}_{N} \mathbf{x} + \mathbf{d}_{N} \right) da \\ &+ \int_{\Gamma_{N',\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N'} \mathbf{n}'(N',\gamma') + \mathbf{P}_{N} \mathbf{n}(N,\gamma) \right) \cdot \left(\mathbf{G}_{N'} \mathbf{x} + \mathbf{d}_{N'} \right) da \\ &= \int_{\Gamma_{N,\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N} - \mathbf{P}_{N'} \right) \mathbf{n}(N,\gamma) \cdot \left(\mathbf{G}_{N} \mathbf{x} + \mathbf{d}_{N'} \right) da \\ &+ \int_{\Gamma_{N',\gamma'}} \frac{1}{2} \left(\mathbf{P}_{N'} - \mathbf{P}_{N} \right) \mathbf{n}'(N',\gamma') \cdot \left(\mathbf{G}_{N'} \mathbf{x} + \mathbf{d}_{N'} \right) da , \end{split}$$

...



Figure 4.2: Common interface of grains N and N'.

where the last expression follows from the fact that the outward normal unit vector of face $\Gamma_{N',\gamma'}$ satisfies $\mathbf{n}' = \mathbf{n}'(N',\gamma') = -\mathbf{n}(N,\gamma)$, as shown in Fig. 4.2. Consequently, the first term in (4.13) may be expressed as follows:

$$\sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} (\mathbf{P}_N \mathbf{n}) \cdot (\mathbf{G}_I \mathbf{x} + \mathbf{d}_I) \, \mathrm{d}a$$

$$= \sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \frac{1}{2} (\mathbf{P}_N - \mathbf{P}_{N'}) \, \mathbf{n} \cdot (\mathbf{G}_N \mathbf{x} + \mathbf{d}_N) \, \mathrm{d}a , \qquad (4.15)$$

where, to simplify the notation, the arguments of **n** have been suppressed. A further simplification in (4.15) may be achieved by using the fact that the traction vector $\mathbf{P}_N \mathbf{n}$ in each interface *I* is constant, hence

$$\sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \frac{1}{2} \left(\mathbf{P}_N - \mathbf{P}_{N'} \right) \mathbf{n} \cdot \left(\mathbf{G}_N \mathbf{x} + \mathbf{d}_N \right) \mathrm{d}a$$

=
$$\sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \frac{1}{2} A_{N,\gamma} \left(\mathbf{P}_N - \mathbf{P}_{N'} \right) \mathbf{n} \cdot \left(\mathbf{G}_N \mathbf{r}_{N,\gamma} + \mathbf{d}_N \right), \qquad (4.16)$$

where $\mathbf{r}_{N,\gamma}$ represents the position vector of the centroid of interface $I = \hat{I}(N,\gamma)$ and $A_{N,\gamma}$ is the corresponding area. From the assumptions (4.5) and in view of (4.16), it follows that (4.13) may be written as

$$\sum_{N=1}^{N_{\rm gr}} \left[\sum_{\gamma=1}^{M_N} \frac{1}{2} A_{N,\gamma} \left(\mathbf{P}_N - \mathbf{P}_{N'} \right) \mathbf{n} \cdot \left(\mathbf{G}_N \mathbf{r}_{N,\gamma} + \mathbf{d}_N \right) - V_N \left(\mathbf{P}_N - \boldsymbol{\Sigma} \right) \cdot \mathbf{G}_N \right] = 0 ,$$
(4.17)

with V_N reflecting the volume of the N-th grain.

In the weak formulation (4.17), which needs to be satisfied for all test tensors \mathbf{G}_N and test vectors \mathbf{d}_N , the unknowns are the deformation gradient tensors \mathbf{F}_N with $N = 1, \ldots, N_{\text{gr}}$ and the Lagrange multiplier Σ ; observe that the vectors \mathbf{c}_N have no contribution in this formulation. Note that the first Piola-Kirchhoff stress \mathbf{P}_N in grain N depends on the deformation gradient \mathbf{F}_N through the constitutive law of grain N, whereas the first Piola-Kirchhoff stress $\mathbf{P}_{N'}$ in an adjacent grain N' depends in a similar fashion on the deformation gradient $\mathbf{F}_{N'}$. Here, it is implicitly assumed that, with the actual constitutive relation, the stress (or stress rate) depends objectively on the deformation through an appropriate formulation.

Since the test tensors \mathbf{G}_N can be specified independently of the test vectors \mathbf{d}_N , the (virtual) deformation $\mathbf{G}_N \mathbf{r}_{N,\gamma} + \mathbf{d}_N$ of the *centroid* of an interface γ may be defined independently of the (virtual) deformation gradient \mathbf{G}_N of the grain. Consequently, the formulation (4.17), together with the constraint (4.9), leads to the following system of equations for each grain and each interface:

$$A_{N,\gamma} \left(\mathbf{P}_N - \mathbf{P}_{N'} \right) \mathbf{n} = \mathbf{0}$$

$$V_N \left(\mathbf{P}_N - \mathbf{\Sigma} \right) = \mathbf{0}$$
for all $N = 1, \dots, N_{\text{gr}}, \gamma = 1, \dots, M_N$
subjected to:
$$\frac{N_{\text{gr}}}{N_{\text{gr}}}$$
(4.18)

$$\sum_{N=1}^{N_{ ext{gr}}} V_N \left(\mathbf{F}_N - ar{\mathbf{F}}
ight) = \mathbf{0} \; .$$

In principle this is an over-determined system of equations since, in view of (4.2) and (4.18), there are $N_{int} + N_{gr} + 1$ distinct tensor-valued equations and only $N_{gr} + 1$ tensor-valued unknowns, i.e., the deformations gradients in each grain and the global Lagrange multiplier. Observe that one solution of this system of equations corresponds to a uniform state of stress, with the Lagrange multiplier Σ representing the actual macroscopic stress value.

As mentioned before, equation $(4.18)_3$ enforces compatibility between the volumeaveraged microscopic deformation gradients \mathbf{F}_N in the grains and the macroscopic deformation gradient $\mathbf{\bar{F}}$ of the whole cluster of grains. However, in analogy with a displacement-controlled process in which $\mathbf{\bar{F}}$ is prescribed, it also acts as the "external loading" for which the system of equations $(4.18)_{1,2}$ must be satisfied. In particular, note that in the absence of the loading term $(4.18)_3$, equations $(4.18)_{1,2}$ are trivially satisfied with a stress-free state $\Sigma = \mathbf{0}$. Accordingly, a state of equal stress in the grains, which reflects the well-known Sachs bound, requires the solution for the deformation gradients \mathbf{F}_N that satisfies $(4.18)_3$. Obviously, this solution neglects kinematic compatibility across grain boundaries, which indeed would induce a non-uniform state of stress in the grain cluster. The incorporation of the kinematic compatibility equation in the formulation is treated in the section below.

4.1.3 Weak formulation and discretization of the kinematic compatibility equation

As mentioned in Section 4.1.1, the basic kinematic assumption adopted in the generalized grain cluster method is that the displacement field is linear within each grain, but generally may be discontinuous across grain boundaries. This discontinuity can be related to a physical mechanism, such as crack formation or dislocation activity [19, 68], but for simplicity and generality is considered here as a direct result of the above kinematic assumptions. Accordingly, the purpose is to find piecewise linear displacement fields that *minimize* the kinematic incompatibilities at grain boundaries. To this end, the equation of kinematic compatibility, which guarantees continuity of a displacement field, is *explicitly* incorporated in the formulation as a field equation.

Referring to a cartesian basis, the components of a vector **n** and a tensor **F** are, respectively, given by n_i and F_{ij} , with i, j = 1, 2, 3. Accordingly, the curl of the tensor field $\mathbf{F} = \mathbf{F}(\mathbf{x})$ and the cross product between **n** and **F** can be expressed as

$$(\nabla \times \mathbf{F})_{ij} = \varepsilon_{imn} F_{jn,m} ,$$

($\mathbf{n} \times \mathbf{F}$)_{ij} = $\varepsilon_{imn} n_m F_{jn} .$ (4.19)

Here, implicit summation on repeated indices is assumed, $(\cdot)_{\cdot,m}$ refers to partial differentiation with respect to x_m , $\varepsilon_{ijk} = (1/2)(i-j)(j-k)(k-i)$ represents the alternator (or permutation) tensor, and $\nabla \times (\cdot)$ designates the curl of a tensor (in the reference configuration). When interpreting **F** as the microscopic deformation gradient, the kinematic compatibility equation can be written as

$$\nabla \times \mathbf{F} = \mathbf{0} \,. \tag{4.20}$$

Multiplying (4.20) by a suitable tensor-valued test function **G** and using the identity (B.5) (see appendix) yields

$$(\nabla \times \mathbf{F}) \cdot \mathbf{G} = \operatorname{tr} \left(\nabla \times (\mathbf{GF}) \right) + \left(\nabla \times \mathbf{G}^{\mathrm{T}} \right) \cdot \mathbf{F}^{\mathrm{T}} = 0, \qquad (4.21)$$

where tr indicates the trace of a tensor. Integrating (4.21) over the domain Ω and using the decomposition (4.1) gives

$$\sum_{N=1}^{N_{\rm gr}} \int_{\Omega_N} \left(\operatorname{tr} \left(\nabla \times (\mathbf{G}\mathbf{F}) \right) + \left(\nabla \times \mathbf{G}^{\rm T} \right) \cdot \mathbf{F}^{\rm T} \right) \mathrm{d}v = 0 \,. \tag{4.22}$$

Applying the generalized divergence theorem for each grain separately then leads to

$$\sum_{N=1}^{N_{\rm gr}} \left[\sum_{\gamma=1}^{M_N} \operatorname{tr} \left(\int_{\Gamma_{N,\gamma}} \mathbf{n} \times (\mathbf{GF}) \, \mathrm{d}a \right) + \int_{\Omega_N} \left(\nabla \times \mathbf{G}^{\rm T} \right) \cdot \mathbf{F}^{\rm T} \mathrm{d}v \right] = 0 \,, \qquad (4.23)$$

where the linearity of the integration and trace operators was used to interchange their order.

The tensor-valued test function **G** is taken as the gradient of a vector-valued test function **w**, i.e., $\mathbf{G} = \nabla \mathbf{w}$. Consequently, $\nabla \times \mathbf{G}^{\mathrm{T}} = \nabla \times (\nabla \mathbf{w})^{\mathrm{T}} = \nabla (\nabla \times \mathbf{w})$. In general, this term is not zero, but for the choice of piece-wise linear test functions **w** introduced in (4.5), it follows that inside each grain N the tensor **G** is constant and therefore meets the relation $\nabla \times \mathbf{G}^{\mathrm{T}} = \mathbf{0}$. Correspondingly, the second term in (4.23) vanishes. Now, using the assumed fields (4.5) in (4.23) and in view of the identity tr $(\mathbf{n} \times (\mathbf{GF})) = (\mathbf{n} \times \mathbf{F}) \cdot \mathbf{G}$, the weak form of the kinematic compatibility equation becomes

$$\sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \left(\mathbf{n} \times \mathbf{F}_N \right) \cdot \mathbf{G}_I \mathrm{d}a = 0 , \qquad (4.24)$$

where G_I is given by (4.6), with $I = \hat{I}(N, \gamma)$.

The summation in (4.24) is carried out over all grains N and all interfaces γ , hence it includes surface integrals on both sides of each interface I. Correspondingly, using (4.6), the weak form (4.24) may be expressed as

$$\sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \frac{1}{2} \left(\mathbf{n} \times \mathbf{F}_N + \mathbf{n}' \times \mathbf{F}_{N'} \right) \cdot \mathbf{G}_N da$$

$$= \sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} \int_{\Gamma_{N,\gamma}} \frac{1}{2} \left(\mathbf{n} \times \left(\mathbf{F}_N - \mathbf{F}_{N'} \right) \right) \cdot \mathbf{G}_N da = 0 , \qquad (4.25)$$

where $\mathbf{n}' = -\mathbf{n}$ refers to the outward normal unit vector of face $\Gamma_{N',\gamma'}$.

The formulation (4.25), together with the constraint (4.9), leads to the following system of equations

$$A_{N,\gamma} \frac{1}{2} \mathbf{n} \times (\mathbf{F}_N - \mathbf{F}_{N'}) = \mathbf{0},$$

for all $N = 1, \dots, N_{\text{gr}}, \ \gamma = 1, \dots, M_N,$
subjected to:
$$\sum_{N=1}^{N_{\text{gr}}} V_N \left(\mathbf{F}_N - \bar{\mathbf{F}} \right) = \mathbf{0}.$$
(4.26)

Similar to the weak formulation of linear momentum presented in (4.18), the weak formulation (4.26) for the equation of kinematic compatibility leads to an over-determined system of equations, i.e., there are $N_{int} + 1$ distinct tensor-valued equations and only N_{gr} tensor-valued unknowns. Observe that a trivial solution to this system of equations corresponds to a uniform state of deformation, $\mathbf{F}_N = \bar{\mathbf{F}}$ in the grains N, reflecting the well-known Taylor bound. Note that the equilibrium and compatibility equations presented in Sections 4.1.2 and 4.1.3 have been consistently obtained using the *common assumption* (4.5) for the test functions w. This is particularly relevant in view of the framework presented in the section below, which combines both sets of equations.

4.1.4 Formulation of the constrained minimization problem

By assuming grain-wise constant deformation gradients, see expression (4.5), the discrete form of the balance of linear momentum (4.18) leads to the uniform stress solution (Sachs bound), whereas the discrete form of the kinematic compatibility equation (4.26) provides the state of a uniform deformation gradient or strain (Taylor bound). The GGCM consists of finding solutions that *simultaneously approximate* these two conditions. A simple combination of the formulations (4.18) and (4.26) results in $2N_{\text{int}} + N_{\text{gr}} + 1$ distinct tensor-valued equations. The unknown variables in these equations are (i) the deformation gradients of the cluster's grains, which can be collected in a set \mathcal{F} defined as

$$\mathcal{F} := \{\mathbf{F}_N\}_{N=1\dots,N_{\rm gr}} , \qquad (4.27)$$

and (ii) the Lagrange multiplier Σ . Correspondingly, there are $N_{\rm gr} + 1$ (tensor-valued) unknowns, resulting in an over-determined system of equations. This is a consequence of the simplifying assumption of a grain-wise constant deformation gradient, which does not provide sufficient degrees of freedom for finding a solution that simultaneously satisfies the weak forms of (4.7) and (4.20). Therefore, a compromise between these requirements needs to be found, which is accomplished by using a *minimization* formulation that approximates (4.18)_{1,2} and (4.26)₁ while enforcing the multiscale condition (4.18)₃ (which is the same as (4.26)₂). For this purpose, a weighted scalar functional *J* is defined that depends on the variables \mathcal{F} and Σ as follows:

$$J(\mathcal{F}, \mathbf{\Sigma}) := \alpha_1 J_1(\mathcal{F}) + \alpha_2 J_2(\mathcal{F}) + \alpha_3 J_3(\mathcal{F}, \mathbf{\Sigma}), \tag{4.28}$$

where α_i , with i = 1, 2, 3, are scalar weighting factors and

$$J_{1}(\mathcal{F}) := \frac{1}{2\beta^{2}A_{\text{int}}} \sum_{N=1}^{N_{\text{gr}}} \sum_{\gamma=1}^{M_{N}} A_{N,\gamma} \left\| \left(\mathbf{P}_{N} - \mathbf{P}_{N'} \right) \mathbf{n} \right\|^{2},$$

$$J_{2}(\mathcal{F}) := \frac{1}{2A_{\text{int}}} \sum_{N=1}^{N_{\text{gr}}} \sum_{\gamma=1}^{M_{N}} A_{N,\gamma} \left\| \mathbf{n} \times \left(\mathbf{F}_{N} - \mathbf{F}_{N'} \right) \right\|^{2},$$

$$J_{3}(\mathcal{F}, \mathbf{\Sigma}) := \frac{1}{2\beta^{2}V} \sum_{N=1}^{N_{\text{gr}}} V_{N} \left\| \left(\mathbf{P}_{N} - \mathbf{\Sigma} \right) \right\|^{2}.$$
(4.29)

Here, $\|\cdot\|$ refers to the norm of the corresponding vector or tensor, i.e., for a vector **a** with cartesian components a_i , $\|\mathbf{a}\| = \left(\sum_{i=1}^3 a_i^2\right)^{1/2}$ and for a second-order tensor **A** with

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components A_{ij} , $\|\mathbf{A}\| = \left(\sum_{i,j=1}^{3} A_{ij}^2\right)^{1/2}$.

The terms A_{int} and V denote the total interfacial area and the total volume of the cluster Ω , respectively, as expressed by

$$A_{\rm int} := \frac{1}{2} \sum_{N=1}^{N_{\rm gr}} \sum_{\gamma=1}^{M_N} A_{N,\gamma} , \quad V := \sum_{N=1}^{N_{\rm gr}} V_N .$$
(4.30)

For the numerical implementation of the GGCM it is convenient to warrant that the stressrelated terms, i.e., J_1 and J_3 , and the term directly related to the deformation gradients, i.e., J_2 , are of the same order of magnitude. Thus, a scaling factor β (units of stress) is introduced in (4.29)_{1,3} in order to non-dimensionalize the stress terms J_1 and J_3 and achieve a proper scaling. In principle, the same goal may be realized with the weighting factors α_i ; however, for presentation purposes it is convenient to work with nondimensional values for α_i .

The generalized grain cluster method can now be outlined as follows: For a given macroscopic deformation gradient $\bar{\mathbf{F}}$ applied to a cluster of $N = 1, \ldots, N_{\text{gr}}$ polyhedral grains, each with volume V_N and connected to adjacent grains N' through interfaces of area $A_{N,\gamma}$ with outward normal unit vectors $\mathbf{n} = \mathbf{n}(N,\gamma)$, find the collection of deformation gradients $\mathcal{F}^* = {\mathbf{F}_N^*}_{N=1,\ldots,N_{\text{gr}}}$ and the Lagrange multiplier $\boldsymbol{\Sigma}^*$ such that

$$J(\mathcal{F}^*, \mathbf{\Sigma}^*) = \min_{\mathcal{F}, \mathbf{\Sigma}} J(\mathcal{F}, \mathbf{\Sigma}) ,$$

subjected to $\mathbf{C} (\mathcal{F}, \bar{\mathbf{F}}) = \mathbf{0},$ (4.31)

with J given by (4.28) and (4.29) and the tensor-valued multiscale constraint C given by

$$\mathbf{C}\left(\mathcal{F},\bar{\mathbf{F}}\right) := \sum_{N=1}^{N_{\rm gr}} \frac{V_N}{V} \mathbf{F}_N - \bar{\mathbf{F}}.$$
(4.32)

The first Piola-Kirchhoff stress tensor \mathbf{P}_N in $(4.29)_{1,3}$ is assumed to be determined by a (path-dependent) constitutive model of grain N that depends on the deformation gradient \mathbf{F}_N and a set of internal variables characterizing the inelastic response.

The solution to the constrained minimization problem summarized by expressions (4.31) and (4.32) depends on the specific choice of the weighting factors α_i , i = 1, 2, 3. In general, a range of solutions may be obtained that is bounded by the limit cases of a uniform stress and a uniform deformation gradient in the grain cluster. Accordingly, the GGCM should be equipped with a *calibration procedure* for determining the specific combination of weighting factors for which a close approximation of an accurate reference solution or an experimental response is found. This procedure will be discussed in more detail in Section 4.3. The numerical implementation of the GGCM is discussed in Section 4.2 below.

4.2 Numerical implementation

If the microscopic material behavior in the grain cluster is inelastic and thus path-dependent, its effective macroscopic response can be computed by incrementally loading the cluster from an initial state to the final state of deformation $\bar{\mathbf{F}}$. Correspondingly, the loading process may be divided into discrete steps $s = 1, \ldots, N_{\text{steps}}$, where N_{steps} represents the total number of steps. The initial state (s = 0) typically corresponds to an unloaded configuration characterized by the macroscopic deformation gradient being equal to identity, $\bar{\mathbf{F}}^{s=0} = \mathbf{I}$. The loading process can be parameterized by a scalar t^s , which may be interpreted as the actual time for rate-dependent constitutive models, with $\bar{\mathbf{F}}^s = \bar{\mathbf{F}}(t^s)$ reflecting the macroscopic loading at time t^s in a quasi-static process. Consider a given macroscopic loading increment expressed by the change in the deformation gradient going from step s to step s + 1,

$$\left(\Delta \bar{\mathbf{F}}\right)^{s+1} := \bar{\mathbf{F}}^{s+1} - \bar{\mathbf{F}}^s \,. \tag{4.33}$$

Denote by $\{\mathcal{F}, \Sigma, \Xi\}$ a microscopic state, where $\Xi := \{\xi_N\}_{N=1...,N_{gr}}$ represents a collection of internal variables ξ_N of the inelastic constitutive model in grain N. Starting from the last converged state $\{\mathcal{F}^s, \Sigma^s, \Xi^s\}$ corresponding to the macroscopic deformation gradient $\overline{\mathbf{F}}^s$, the goal is to determine the state $\{\mathcal{F}^{s+1}, \Sigma^{s+1}, \Xi^{s+1}\}$ that minimizes J under the incremental deformation (4.33), subject to the multiscale constraint $\mathbf{C}(\mathcal{F}^{s+1}, \overline{\mathbf{F}}^{s+1}) = \mathbf{0}$. Since the internal variables Ξ^{s+1} are determined from a user-defined, constitutive model, the task is to calculate the Lagrange multiplier Σ^{s+1} and a collection of deformation gradients \mathcal{F}^{s+1} that minimize J. To this end, the gradients of J with respect to the Lagrange multiplier Σ and the deformation gradients \mathbf{F}_N (collected in the set \mathcal{F}) need to be computed, as described below.

4.2.1 Unconstrained gradient

For solving the constrained minimization problem (4.31), a simple constrained gradient descent method based on the computation of the gradient of the objective functional J is proposed. In this section the components of the unconstrained gradient of the objective functional are derived. Observe that, in view of (4.28) and (4.29), the symbolic expression for the unconstrained gradient is the same for all loading steps s, hence the superindex s will be suppressed for notational simplicity.

Consider a generic grain $K \in [1, ..., N_{gr}]$ and the corresponding deformation gradient \mathbf{F}_K with cartesian components $(F_K)_{mn}$. Henceforth, implicit summation on repeated cartesian components i = 1, 2, 3 will be assumed. The derivatives of the terms composing

J in (4.29) are as follows:

$$\frac{\partial J_1}{\partial (F_K)_{mn}} = \frac{2}{\beta^2 A_{\text{int}}} \sum_{\gamma=1}^{M_K} A_{K,\gamma} \times \left((P_K)_{ij} - (P_{K'})_{ij} \right) n_j \frac{\partial (P_K)_{ik}}{\partial (F_K)_{mn}} n_k ,$$

$$\frac{\partial J_2}{\partial (F_K)_{mn}} = \frac{2}{A_{\text{int}}} \sum_{\gamma=1}^{M_K} A_{K,\gamma} \times \left((F_K)_{ml} - (F_{K'})_{ml} \right) \left(\delta_{nl} - n_n n_l \right) ,$$

$$\frac{\partial J_3}{\partial (F_K)_{mn}} = \frac{V_K}{\beta^2 V} \left((P_K)_{ij} - \Sigma_{ij} \right) \frac{\partial (P_K)_{ij}}{\partial (F_K)_{mn}} ,$$

$$\frac{\partial J_3}{\partial \Sigma_{mn}} = -\frac{1}{\beta^2 V} \sum_{N=1}^{N_{gr}} V_N \left((P_N)_{mn} - \Sigma_{mn} \right) ,$$
(4.34)

where the identity $\epsilon_{ikl}\epsilon_{ipn} = \delta_{kp}\delta_{ln} - \delta_{kn}\delta_{lp}$ was used to derive $(4.34)_2$, with δ_{ij} representing the Kronecker delta symbol. Observe that the factor 2 in front of $\partial J_1/\partial (F_K)_{mn}$ and $\partial J_2/\partial (F_K)_{mn}$ is related to the contributions from grains K' that are adjacent to K. The tangential stiffness $\partial (P_K)_{ij}/\partial (F_K)_{mn}$ is obtained from the constitutive model of grain K, and can be calculated analytically and/or numerically, for example, through a numerical perturbation technique [62]. The constitutive model further provides the stress components $(P_K)_{ij}$ and the internal variables by means of an incremental-iterative update scheme, such as a return mapping algorithm commonly used for classical plasticity models. Henceforth, it is assumed that for an *arbitrary* deformation gradient $(F_K)_{mn}$ it is possible to compute $(P_K)_{ij}$ and $\partial (P_K)_{ij}/\partial (F_K)_{mn}$ from a user-defined constitutive model for grain K.

It is convenient to enforce the necessary condition for a minimum of the objective functional J with respect to the Lagrange multiplier Σ from the outset, i.e., the derivative of J with respect to Σ is set to zero. Consequently, in view of (4.34)₄, the Lagrange multiplier Σ that satisfies the necessary condition for a minimum of J is interpreted as the macroscopic stress, i.e.,

$$\boldsymbol{\Sigma} = \sum_{N=1}^{N_{\rm gr}} \theta_N \mathbf{P}_N , \qquad (4.35)$$

where the scalars θ_N correspond to the volume fractions of the grains:

$$\theta_N := \frac{V_N}{V} \quad N = 1, \dots, N_{\rm gr} .$$
(4.36)

It is worth pointing out that the Hill-Mandel condition, which refers to the consistency between the microscale power $\sum_{N=1}^{N_{\text{gr}}} \theta_N \mathbf{P}_N \cdot \dot{\mathbf{F}}_N$ and macroscale stress power $\boldsymbol{\Sigma} \cdot \dot{\mathbf{F}}$, is in general only approximately satisfied, since neither the kinematical compatibility relation nor the equilibrium condition are exactly met in the present framework. A consequence of this is that the spatial average of the energy dissipated at the microscale is not equal to the

energy dissipated in a material point at the macroscale, although the difference is expected to be small in general. In the limit cases of uniform deformation and uniform stress, the Hill-Mandel condition is satisfied, albeit at the expense of relaxing, respectively, the equilibrium condition and the kinematic compatibility relation.

Using (4.35) in (4.34) and in view of (4.28), the derivative of J with respect to the deformation gradient in a generic grain K becomes

$$\frac{\partial J}{\partial (F_K)_{mn}} = \frac{2\alpha_1}{\beta^2 A_{\text{int}}} \sum_{\gamma=1}^{M_K} A_{K,\gamma} \left((P_K)_{ij} - (P_{K'})_{ij} \right) n_j (\mathbb{A}_K)_{ikmn} n_k
+ \frac{2\alpha_2}{A_{\text{int}}} \sum_{\gamma=1}^{M_K} A_{K,\gamma} \left((F_K)_{ml} - (F_{K'})_{ml} \right) (\delta_{nl} - n_n n_l)
+ \frac{\alpha_3 \theta_K}{\beta^2} \left((P_K)_{ij} - \Sigma_{ij} \right) (\mathbb{A}_K)_{ijmn} ,$$
(4.37)

with Σ_{ij} given by (4.35) and the material tangent stiffness \mathbb{A}_K of the K-th grain defined in cartesian components as

$$(\mathbb{A}_K)_{ijmn} := \frac{\partial (P_K)_{ij}}{\partial (F_K)_{mn}} \,. \tag{4.38}$$

Observe that the tensor $\mathbf{I}-\mathbf{n}\otimes\mathbf{n}$ (in components: $\delta_{nl}-n_nn_l$) appearing in the second term on the right hand side of (4.37) represents a projection (of the microscopic deformation gradient) onto a grain boundary with normal vector **n**; hence this term measures the relative difference in deformation at grain boundaries. Furthermore, the first term in (4.37) reflects the traction discontinuity across a grain boundary and the third term represents the difference between the microscopic stress in a grain and the macroscopic stress.

In the gradient descent method, the estimate of the deformation gradient is modified by an incremental amount in the opposite direction of the derivative (4.37) in order to minimize the jumps in traction and displacement across grain boundaries, as well as the deviation of the microscopic stresses from the macroscopic stress. However, this modification cannot be performed arbitrarily, as it is required that the average microscopic deformation gradient remains unconditionally equal to the macroscopic deformation gradient, see expression $(4.31)_2$. Accordingly, in the next section a gradient descent direction is constructed that satisfies this multiscale constraint.

4.2.2 Constrained gradient

In view of the numerical implementation of the constrained gradient descent method, a matrix-vector notation is henceforth used, such that a single index Q is obtained from a

combination of a grain index K and two cartesian indices m and n, i.e.,

$$Q = Q(K, m, n) \text{ with } Q = 1, \dots, 9N_{\text{gr}},$$

for $K = 1, \dots, N_{\text{gr}}, m, n = 1, 2, 3.$ (4.39)

Similarly, two cartesian indices m and n are combined into a single index q such that

$$q = q(m, n)$$
 with $q = 1, \dots, 9$ for $m, n = 1, 2, 3$.

The index $Q = 1, ..., 9N_{gr}$ ranges over all degrees of freedom in the minimization problem while the index q = 1, ..., 9 ranges over all cartesian components of the deformation gradient. With this notational convention, the gradient of the objective functional can be collected in a vector **g**, for which the $9N_{gr}$ components \mathbf{g}_{Q} are given by

$$g_Q := \frac{\partial J}{\partial (F_K)_{mn}}$$
 with $Q = Q(K, m, n)$.

Similarly, denote as $\bar{\mathbf{f}}$ the vector representing the 9 components of the macroscopic deformation gradient $\bar{\mathbf{F}}$ and denote as \mathbf{x} the vector representing the $9N_{gr}$ components of all the microscopic deformation gradients \mathbf{F}_K in the set \mathcal{F} , i.e.,

$$f_q := F_{mn}$$
 and $x_Q := (F_K)_{mn}$,
with $q = q(m, n)$, $Q = Q(K, m, n)$. (4.40)

Accordingly, the multiscale constraint $(4.31)_2$ can be written as

$$\mathbf{L}\mathbf{x} = \bar{\mathbf{f}},\tag{4.41}$$

where **L** is a $9 \times 9N_{\text{gr}}$ (non-square) matrix composed of a collection of N_{gr} matrices, each of size 9×9 and arranged as follows:

$$\mathbf{L} := \begin{bmatrix} \theta_1 \mathbf{I} & \theta_2 \mathbf{I} & \dots & \theta_{N_{\rm gr}} \mathbf{I} \end{bmatrix} , \qquad (4.42)$$

where the scalars θ_N , with $N = 1, ..., N_{gr}$, are the grain volume fractions defined in (4.36) and I represents the 9×9 -identity matrix. The matrix L may be viewed as a "volume averaging" operator that maps *a* microscopic deformation state **x** to *the* macroscopic deformation state $\bar{\mathbf{f}}$.

Projecting the gradient **g** to the subspace characterized by the multiscale constraint (4.41) ensures that the gradient descent method preserves this constraint for all iterations at a given loading step. The projection may be achieved using a basis for the null space $\mathcal{N}(\mathbf{L})$ of the matrix \mathbf{L} . In view of (4.42), it can be shown that the null space $\mathcal{N}(\mathbf{L})$ has dimension $9N_{\rm gr} - 9$. The gradient descent direction is thus obtained by first computing the tangent **g** according to (4.37) and then projecting it onto $\mathcal{N}(\mathbf{L})$. However, instead of working with the null space directly, it is convenient to operate first in the subspace that

is the orthogonal complement of the null space, since this subspace has a dimension that is generally far less than the dimension of the null space itself, i.e., 9 instead of $9N_{\rm gr} - 9$. Because the projection has to be performed for every newly calculated tangent vector **g** in each iteration, for the efficiency of the computations it is preferable to first project the tangent vector **g** to the complementary subspace $\mathcal{N}(\mathbf{L})^{\perp}$ and then subtract this result from the tangent **g**. An orthonormal basis for $\mathcal{N}(\mathbf{L})^{\perp}$ can be constructed by taking the first nine left-singular vectors obtained from the singular value decomposition of $\mathbf{L}^{\rm T}\mathbf{L}$. Consequently, the projected gradient descent direction, denoted as $\mathbf{g}^{\rm p}$, is calculated in accordance with:

$$\mathbf{g}^{\mathrm{p}} := \mathbf{g} - \sum_{q=1}^{9} \left(\mathbf{g} \cdot \mathbf{u}_{q} \right) \mathbf{u}_{q} \,. \tag{4.43}$$

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Here, \mathbf{u}_q , with q = 1, ..., 9, are the first nine left-singular vectors of the matrix \mathbf{U} , as obtained from the singular-value decomposition of $\mathbf{L}^{\mathrm{T}}\mathbf{L}$, i.e.,

$$\mathbf{U}\mathbf{D}\mathbf{V}^{\mathrm{T}} = \mathrm{svd}\left(\mathbf{L}^{\mathrm{T}}\mathbf{L}\right)$$

with **D** being the diagonal matrix of singular values and **V** the matrix of right-singular vectors. Because the multiscale constraint (4.41) is linear, the unit vectors \mathbf{u}_q (q = 1, ..., 9) can be expressed in closed-form, such that the components of the projected gradient follow as:

$$\mathbf{g}_Q^{\mathbf{p}} = \frac{\partial J}{\partial \left(F_K\right)_{mn}} - \frac{\theta_K}{\hat{\theta}^2} H_{mn} \quad \text{with} \quad Q = Q(K, m, n), \tag{4.44}$$

where

$$H_{mn} := \sum_{N=1}^{N_{\rm gr}} \theta_N \frac{\partial J}{\partial (F_N)_{mn}} \quad \text{and} \quad \hat{\theta} := \left(\sum_{N=1}^{N_{\rm gr}} \theta_N^2\right)^{\frac{1}{2}} . \tag{4.45}$$

The tensor **H** with cartesian components H_{mn} defined in (4.45) represents the volume average of the gradient of J, while the factor $\hat{\theta}$ reflects the L_2 norm of the volume fractions of the grains.

4.2.3 Constrained gradient descent algorithm

Suppose that the converged state at loading step s has been determined and let \mathbf{x}^s denote the corresponding vector of deformation gradients in the grains. If the constitutive model of a grain uses internal variables, it is assumed that these were determined in the convergence process of the vector \mathbf{x}^s by means of an incremental (iterative) update algorithm at the grain level. This update algorithm also provides the converged stress \mathbf{P}_N^s in the grain, which, in view of (4.35), results in the update of the macroscopic stress Σ^s . In summary, \mathbf{x}^s may thus be formally interpreted as the vector with the main state variables in the grains of the cluster, for which the corresponding stress and history variables at

the grain level are computed through a user-defined constitutive model. To determine the converged state \mathbf{x}^{s+1} at loading step s + 1, the time-like parameter is incremented from t^s to t^{s+1} by a sufficiently small time step Δt^{s+1} , and the corresponding macroscopic deformation gradient is incremented from $\mathbf{\bar{f}}^s$ to $\mathbf{\bar{f}}^{s+1}$. Starting from an initial estimate $\mathbf{x}^{s+1,0}$, the vector of deformation gradients is updated from iteration *i* to iteration i + 1 by using the projected gradient \mathbf{g}^p as

$$\mathbf{x}^{s+1,i+1} = \mathbf{x}^{s+1,i} - \omega \left(\mathbf{g}^{\mathbf{p}}\right)^{i} \quad i = 0, 1, \dots$$
(4.46)

In (4.46), the scalar $\omega > 0$ is a suitably-chosen step size that, for simplicity, is assumed to be constant at a given loading step. The value of ω can be chosen such that the magnitude of $\omega (\mathbf{g}^{\mathbf{p}})^i$ is a fraction of the magnitude of \mathbf{x}^s . The projected gradient is given in components in (4.44), and is computed from the unconstrained gradient (\mathbf{g})^{*i*}, given in components in (4.37) and evaluated at $\mathbf{x}^{s+1,i}$.

The linearity of the constrained subspace characterized by (4.41) ensures that the projected gradient always lies within this subspace, and that all estimates $x^{s+1,i}$, with i = 0, 1, ..., satisfy the multiscale kinematic constraint (4.41), independent of the magnitude of the projected gradient or the value of the step size. The estimates are iteratively updated until a convergence criterion is satisfied, as represented by the objective functional J reaching a minimum within a prescribed tolerance ε :

$$\frac{|J^{i+1} - J^i|}{J^i} < \varepsilon . \tag{4.47}$$

Alternatively, or as a complementary check, the relative magnitude of the projected gradient can be monitored at a given iteration, where at a converged state it should be confirmed that

$$\frac{\left\| \left(\mathbf{g}^{\mathbf{p}} \right)^{i+1} \right\|}{\left\| \left(\mathbf{g}^{\mathbf{p}} \right)^{0} \right\|} \ll 1.$$
(4.48)

with $(\mathbf{g}^{\mathbf{p}})^0$ the projected gradient at the onset of the iterative process. If the convergence criterion (4.47) is not satisfied after a certain number of iterations, the time step Δt^s must be reduced and the update algorithm needs to be restarted at the last converged loading step.

The procedure indicated above is repeated for all loading steps *s* until the imposed macroscopic deformation gradient $\overline{\mathbf{f}}^s$ reaches its final value. To start the constrained gradient descent method at a new loading step s+1, it is required to specify an initial estimate $\mathbf{x}^{s+1,0}$ for the vector of microscopic deformation gradients. This issue deserves special attention and is discussed in the following section.

4.2.4 Loading step increment satisfying the multiscale kinematic constraint

Moving from loading step s to s + 1, an initial estimate $\mathbf{x}^{s+1,0}$ for the microscale deformation gradients needs to be specified, with the superscript '0' indicating the onset of the iterative process. This initial estimate should satisfy the multiscale kinematic constraint, i.e.,

$$\mathsf{L}\mathsf{x}^{s+1,0} = \bar{\mathbf{f}}^{s+1},\tag{4.49}$$

where $\bar{\mathbf{f}}^{s+1}$ represents the vectorized form of the macroscopic deformation gradient $\bar{\mathbf{F}}^{s+1}$ at time t^{s+1} . The system of equations (4.49) has more equations than unknown variables and lacks a unique solution. In order to find an accurate, approximate solution to this system of equations, the initial estimate for the microscopic deformation gradients is expressed as

$$\mathbf{x}^{s+1,0} = \mathbf{x}^s + \mathbf{d}^{s+1} \tag{4.50}$$

where \mathbf{x}^s denotes the converged solution at the previous loading step s and \mathbf{d}^{s+1} is a vector of $9N_{\rm gr}$ components representing an initial estimate for the incremental microscopic deformation gradients. Substituting (4.50) in (4.49) and using the fact that the converged solution \mathbf{x}^s at step s meets the constraint $\mathbf{L}\mathbf{x}^s = \mathbf{\bar{f}}^s$, it follows that

$$\mathbf{L}\mathbf{d}^{s+1} = \Delta \bar{\mathbf{f}}^{s+1} \quad \text{with} \quad \Delta \bar{\mathbf{f}}^{s+1} := \bar{\mathbf{f}}^{s+1} - \bar{\mathbf{f}}^s . \tag{4.51}$$

From (4.51), the solution \mathbf{d}^{s+1} may be generally expressed as

$$\mathbf{d}^{s+1} = \tilde{\mathbf{d}}^{s+1} - \mathbf{L}^+ \left(\mathbf{L} \tilde{\mathbf{d}}^{s+1} - \Delta \bar{\mathbf{f}}^{s+1} \right)$$
(4.52)

where $\tilde{\mathbf{d}}^{s+1}$ is an arbitrarily-chosen vector of $9N_{\rm gr}$ components and \mathbf{L}^+ is the (right) Moore-Penrose pseudo-inverse of \mathbf{L} . Since the *rows* of \mathbf{L} are linearly independent, the pseudo-inverse is given by

$$\mathbf{L}^{+} := \mathbf{L}^{\mathrm{T}} \left(\mathbf{L} \mathbf{L}^{\mathrm{T}} \right)^{-1} \,. \tag{4.53}$$

The averaging operator L presented in (4.42) has a relatively simple form, as a result of which the pseudo-inverse L^+ can be derived explicitly. This results in a $9N_{\rm gr} \times 9$ matrix composed of a collection of $N_{\rm gr}$ matrices, each of size 9×9 and arranged as follows:

$$\mathbf{L}^{+} = \frac{1}{\hat{\theta}^{2}} \begin{bmatrix} \theta_{1} \mathbf{I} \\ \theta_{2} \mathbf{I} \\ \vdots \\ \theta_{N_{\mathrm{gr}}} \mathbf{I} \end{bmatrix} , \qquad (4.54)$$

where, as before, the scalars θ_N are the grain volume fractions, I represents the 9 × 9identity matrix and $\hat{\theta}$ is given by (4.45)₂. It can be confirmed that inserting (4.52) into (4.50), followed by multiplying the result by **L** and invoking (4.53) and (4.51), indeed leads to the multiscale kinematic constraint (4.49) for the initial estimate $\mathbf{x}^{s+1,0}$ of the microscale deformation gradients.

In principle, one may choose any vector $\tilde{\mathbf{d}}^{s+1}$ in (4.52) to obtain an increment \mathbf{d}^{s+1} that can in turn be used in (4.50) to generate an initial estimate for $\mathbf{x}^{s+1,0}$ in the constrained minimization procedure. However, since the material response typically is path-dependent, it may be expected that the performance of the update algorithm will significantly depend on this initial estimate. Hence, it is critical to make a judicious choice for $\tilde{\mathbf{d}}^{s+1}$ in (4.52), such that the corresponding initial value $\mathbf{x}^{s+1,0}$ is located *close* to the final value obtained after reaching the convergence criterion (4.47). Accordingly, it is convenient to impose conditions on $\tilde{\mathbf{d}}^{s+1}$, under which at the grain boundaries the kinematic compatibility and/or traction continuity requirements are approximately satisfied, see Section 4.2.5 for examples. Furthermore, to effectively transfer the properties of $\tilde{\mathbf{d}}^{s+1}$ to \mathbf{d}^{s+1} , the term $\mathbf{L}\tilde{\mathbf{d}}^{s+1} - \Delta \tilde{\mathbf{f}}^{s+1}$ in (4.52) must be as small as possible, whereby $\mathbf{d}^{s+1} \approx \tilde{\mathbf{d}}^{s+1}$. This requirement can be satisfied by determining the vector $\tilde{\mathbf{d}}^{s+1}$ from a uniform scaling relation, i.e.,

$$\tilde{\mathbf{d}}^{s+1} = \eta^{s+1} \hat{\mathbf{d}}^{s+1} . \tag{4.55}$$

Here, η^{s+1} is a scaling factor and $\hat{\mathbf{d}}^{s+1}$ is an auxiliary vector, for which four specific options are discussed in Section 4.2.5. After inserting (4.55) in (4.52), it follows that the L_2 norm of the vector $\mathbf{L}\eta^{s+1}\hat{\mathbf{d}}^{s+1} - \Delta \bar{\mathbf{f}}^{s+1}$ needs to be minimized for meeting the condition $\mathbf{d}^{s+1} \approx \tilde{\mathbf{d}}^{s+1}$. This simply leads to the following expression for the scaling factor:

$$\eta^{s+1} = \frac{\left(\mathbf{L}\hat{\mathbf{d}}^{s+1}\right)^{\mathrm{T}} \Delta \bar{\mathbf{f}}^{s+1}}{\left(\mathbf{L}\hat{\mathbf{d}}^{s+1}\right)^{\mathrm{T}} \mathbf{L}\hat{\mathbf{d}}^{s+1}} \,.$$
(4.56)

A schematic representation of the above incremental/iterative method is shown in Fig. 4.3. Starting from the converged state \mathbf{x}^s at loading step *s* and a specific choice for the auxiliary vector $\hat{\mathbf{d}}^{s+1}$, the scaling factor η^{s+1} and the vector $\tilde{\mathbf{d}}^{s+1}$ are computed from (4.56) and (4.55), respectively, the vector \mathbf{d}^{s+1} containing the initial incremental deformation gradients is computed from (4.52) and the initial estimate $\mathbf{x}^{s+1,0}$ for the deformation gradients is determined from (4.50). Observe that $\mathbf{x}^{s+1,0}$ lies within the "feasible solution space", as characterized by the space containing the vectors \mathbf{x} that satisfy the multiscale kinematic constraint $\mathbf{L}\mathbf{x} = \bar{\mathbf{f}}^{s+1}$. Subsequently the constrained gradient is computed from (4.44) and the estimate is updated according to (4.46) until it converges to the final solution \mathbf{x}^{s+1} within the feasible solution space.



Figure 4.3: Schematic representation of the initial estimate $\mathbf{x}^{s+1,0}$ of the vector of deformation gradients at loading step s + 1, and the subsequent constrained gradient descent method. Points in the domain on the left represents schematically the collection of *microscale* deformation gradients for the grain cluster, which are mapped through the averaging operator **L** to the space of *macroscale* deformation gradients on the right.

4.2.5 Possible estimates for the initial deformation gradient increment

For an optimal performance of the constrained minimization algorithm visualized in Fig. 4.3, it is critical to choose an appropriate estimate for the vector containing the increments in the deformation gradient $\tilde{\mathbf{d}}^{s+1}$, which directly depends on the auxiliary vector $\hat{\mathbf{d}}^{s+1}$ through expression (4.55). Accordingly, four options for $\hat{\mathbf{d}}^{s+1}$ are discussed below.

Initial estimate based on uniform deformation gradient increment.

A possible choice for $\hat{\mathbf{d}}^{s+1}$ is to assume that all grains deform in accordance with the macroscopic increment of the deformation gradient from step s to step s + 1. In components, this choice is given by

$$\left(\hat{\mathsf{d}}^{s+1}\right)_Q = \Delta \bar{F}_{mn}^{s+1} \quad \text{with} \quad Q = Q(K, m, n), \quad K = 1, \dots, N_{\text{gr}}.$$
 (4.57)

With this particular choice it can be easily verified that

$$\mathbf{L}\hat{\mathbf{d}}^{s+1} - \Delta \bar{\mathbf{f}}^{s+1} = \mathbf{0} ,$$

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from which it follows from (4.56) that the scaling factor $\eta^{s+1} = 1$, and from (4.52) that the corresponding vector \mathbf{d}^{s+1} is given by

$$\mathbf{d}^{s+1} = \tilde{\mathbf{d}}^{s+1} = \hat{\mathbf{d}}^{s+1} .$$
(4.58)

The incremental estimate indicated in (4.57) and (4.58) is the *exact* incremental solution to the limit case of a *uniform deformation gradient* (Taylor bound), for which $\alpha_1 = \alpha_3 = 0$ in expression (4.28). Hence, it will serve as a good estimate for cases where the weighting factors α_1 and α_3 are relatively small compared to α_2 , but generally will not provide a suitable initial estimate if these weighting factors are relatively large and the limit case of uniform stress (Sachs bound) is approached.

Initial estimate based on uniform stress increment.

An alternative way to obtain an initial estimate for $\hat{\mathbf{d}}^{s+1}$ is to incrementally deform the grains in accordance with a uniform stress increment. This initial estimate satisfies the equilibrium conditions, and therefore would be particularly useful if the contribution to J by the equilibrium conditions (reflected by the weighting factors α_1 and α_3 in (4.28)) has a higher importance than the kinematic compatibility condition (reflected by the weighting factor α_2 in (4.28)). Suppose that from step s to step s + 1 the average stress tensor in the grain cluster increases from Σ^s to Σ^{s+1} . Although the stress Σ^{s+1} is unknown at the beginning of step s + 1, it can be *estimated* based on temporarily assuming that all grains are subjected to one and the same increment of the deformation gradient, $\Delta \bar{\mathbf{F}}^{s+1}$. For computing the corresponding increment in macroscopic stress, Σ^{s+1} , a frame-indifferent stress measure based on the Lie derivative of the first Piola-Kirchhoff stress is considered. The Lie derivative \mathbf{P} of the first Piola-Kirchhoff stress P is given as $\mathbf{P} = \mathbf{F}\mathbf{S}$, where $\mathbf{S} = \mathbf{F}^{-1}\mathbf{P}$ is the second Piola-Kirchhoff stress and \mathbf{S} denotes its invariant material time derivative. Correspondingly, the Lie derivative of \mathbf{P} may be formulated as

$$\ddot{\mathbf{P}} = \dot{\mathbf{P}} - \dot{\mathbf{F}}\mathbf{F}^{-1}\mathbf{P}, \qquad (4.59)$$

where the superimposed dot indicates a material time derivative. In analogy with this expression, for a sufficiently small load increment and under the assumption of an equal deformation increment in the grains, the initial estimate of the macroscopic stress increment from step s to step s + 1, denoted as $\Delta \Sigma^{s+1,0}$, may be computed as

$$\Delta \mathbf{\Sigma}^{s+1,0} := \bar{\mathbb{A}}^s \Delta \bar{\mathbf{F}}^{s+1} - \Delta \bar{\mathbf{F}}^{s+1} \left(\bar{\mathbf{F}}^{s+1} \right)^{-1} \mathbf{\Sigma}^s \quad \text{with} \quad \bar{\mathbb{A}}^s := \sum_{N=1}^{N_{\text{gr}}} \theta_N \mathbb{A}_N^s. \quad (4.60)$$

Here, $\overline{\mathbb{A}}^s$ is the volume average of the cluster's material tangent stiffness, \mathbb{A}_N^s is the material tangent stiffness of grain N and Σ^s is the macroscopic first Piola-Kirchhoff stress, all evaluated at the last converged step s. The estimate of the uniform stress increment,

(4.60), can now be used to compute an initial estimate of the corresponding *non-uniform* increments in the deformation gradient of the grains, $\Delta \mathbf{F}_{K}^{s+1,0}$, by formulating a relation similar to (4.60) for each specific grain K:

$$(\mathbb{A}_{K}^{s}) \Delta \mathbf{F}_{K}^{s+1,0} - \Delta \mathbf{F}_{K}^{s+1,0} \mathbf{S}_{K}^{s} = \Delta \boldsymbol{\Sigma}^{s+1,0},$$

with $\mathbf{S}_{K}^{s} := (\mathbf{F}_{K}^{s})^{-1} \mathbf{P}_{K}^{s}$ $K = 1, \dots, N_{\text{gr}}.$ (4.61)

Observe that in the above expression the second Piola-Kirchhoff stress in the grains, \mathbf{S}_{K}^{s} , is known from the last converged loading step s. Hence, (4.61) represents a linear system of equations in terms of the initial values of the deformation gradients in the grains, $\Delta \mathbf{F}_{K}^{s+1,0}$, i.e., one set of 9 linear equations for each grain K. For computing the numerical solution of this system of equations, the vectors $\hat{\mathbf{d}}_{K}^{s+1}$ and $\mathbf{p}^{s+1,0}$ are invoked, each composed of 9 components. These vectors incorporate, respectively, the initial estimate of the incremental deformation gradient in grain K and the estimate of the increment in the macroscopic first Piola-Kirchhoff stress, i.e.,

$$\left(\hat{\mathsf{d}}_{K}^{s+1} \right)_{q} := \left(\Delta F_{K}^{s+1,0} \right)_{mn} ; \quad \left(\mathsf{p}^{s+1,0} \right)_{q} := \Delta \Sigma_{mn}^{s+1,0},$$
with $q = q(m,n)$, for $K = 1, \dots, N_{\text{gr}}$.
$$(4.62)$$

Similarly, define the 9×9 material tangent stiffness matrix \mathbf{A}_{K}^{s} of grain K (which corresponds to the converged solution at the previous step s) as

$$(\mathsf{A}_{K}^{s})_{pq} := (\mathbb{A}_{K}^{s})_{ijkl} - \delta_{ik} (S_{K}^{s})_{lj},$$

with $p = p(i, j), q = q(k, l)$ for $K = 1, \dots, N_{\text{gr}},$ (4.63)

where \mathbb{A}_{K}^{s} and \mathbf{S}_{K}^{s} are the material tangent stiffness and the second Piola-Kirchhoff stress in the *K*-th grain, respectively, and δ_{ik} reflects the Kronecker delta symbol. Employing the notation in (4.63), the system of equations (4.61) can be expressed in vector-matrix form as

$$\mathbf{A}_{K}^{s} \hat{\mathbf{d}}_{K}^{s+1} = \mathbf{p}^{s+1,0}$$
 for $K = 1, \dots, N_{\text{gr}}$ (no sum on K). (4.64)

The matrix \mathbf{A}_{K}^{s} is non-singular for the subspace of (vectorized) symmetric tensors but is singular for the subspace of (vectorized) skew-symmetric tensors. To circumvent this singularity, the general solution of (4.64) is formulated as

$$\hat{\mathbf{d}}_{K}^{s+1} = \tilde{\tilde{\mathbf{d}}}_{K}^{s+1} - \left(\mathbf{A}_{K}^{s}\right)^{+} \left(\mathbf{A}_{K}^{s}\tilde{\tilde{\mathbf{d}}}_{K}^{s+1} - \mathbf{p}^{s+1,0}\right)$$
(4.65)

where $(\mathbf{A}_{K}^{s})^{+}$ is the pseudo-inverse of \mathbf{A}_{K}^{s} and $\tilde{\mathbf{d}}_{K}^{s+1}$ is an arbitrarily-chosen vector of 9 components. For definiteness, the components of the vector $\tilde{\mathbf{d}}_{K}^{s+1}$ are chosen as zero, which simplifies (4.65) into

$$\hat{\mathbf{d}}_{K}^{s+1} = (\mathbf{A}_{K}^{s})^{+} \mathbf{p}^{s+1,0} .$$
(4.66)

The grain cluster vector $\hat{\mathbf{d}}^{s+1}$ of $9N_{\rm gr}$ components can now be straightforwardly assembled from the grain level vectors $\hat{\mathbf{d}}_{K}^{s+1}$ for the $K = 1, \ldots, N_{\rm gr}$ grains. Subsequently, the initial estimate of the deformation gradients $\mathbf{x}^{s+1,0}$ follows from (4.56), (4.55), (4.52) and (4.50). Clearly, the determination of the uniform stress initial increment is computationally more demanding than the computation of the uniform deformation gradient initial increment presented in Section 4.2.5. Nonetheless, as will be demonstrated in detail in Section 4.3, the uniform stress initial increment has the advantage that it provides an adequate prediction for a wide range of material responses and weighting factors α_i .

Initial estimate based on previous loading steps

Another option for the calculation of the initial estimate $\hat{\mathbf{d}}^{s+1}$ is to use the *history* of converged solutions at previous loading steps. Particularly, one could straightforwardly compute $\hat{\mathbf{d}}^{s+1}$ from the difference of the converged solutions at steps *s* and *s* - 1, i.e.,

$$\hat{\mathbf{d}}^{s+1} = \mathbf{x}^s - \mathbf{x}^{s-1} . \tag{4.67}$$

Substituting (4.67) in (4.56) and noting that $L(\mathbf{x}^s - \mathbf{x}^{s-1}) = \Delta \overline{\mathbf{f}}^s$, it follows that

$$\eta^{s+1} = \frac{\left(\Delta \bar{\mathbf{f}}^s\right)^{\mathrm{T}} \Delta \bar{\mathbf{f}}^{s+1}}{\left(\Delta \bar{\mathbf{f}}^s\right)^{\mathrm{T}} \Delta \bar{\mathbf{f}}^s} \quad \text{with} \quad \Delta \bar{\mathbf{f}}^{s+1} := \bar{\mathbf{f}}^{s+1} - \bar{\mathbf{f}}^s , \quad \Delta \bar{\mathbf{f}}^s := \bar{\mathbf{f}}^s - \bar{\mathbf{f}}^{s-1} .$$
(4.68)

The initial guess based on the loading history is proposed here because of its simplicity, and because it may provide an accurate and efficient prediction for material systems subjected to proportional loading. Under the latter condition the vectors $\Delta \bar{\mathbf{f}}^{s+1}$ and $\Delta \bar{\mathbf{f}}^s$ are parallel with respect to each other, whereby η^{s+1} in (4.68) becomes equal to the relative change in loading magnitude going from step *s* to step *s*+1. However, under strongly non-proportional loading the initial estimate (4.67) should be treated with care: Note that in the extreme case a load increment $\Delta \bar{\mathbf{f}}^{s+1}$ may be specified such that $(\Delta \bar{\mathbf{f}}^s)^T \Delta \bar{\mathbf{f}}^{s+1} = 0$, for which η^{s+1} becomes zero and the current estimate would not be applicable.

Initial estimate based on the null vector

The last option presented in this section is included for completeness, and corresponds mathematically to the most basic choice for $\hat{\mathbf{d}}^{s+1}$, namely the null vector. Although from (4.56) it may be concluded that for this case the scaling factor η^{s+1} is not defined, in view of (4.55) it follows that $\tilde{\mathbf{d}}^{s+1} = \mathbf{0}$. Correspondingly, from (4.52) the vector \mathbf{d}^{s+1} simply becomes

$$\mathbf{d}^{s+1} = \mathbf{L}^+ \Delta \bar{\mathbf{f}}^{s+1} \,. \tag{4.69}$$

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Using expression (4.54), expression (4.69) can be written in components as

$$\left(\mathsf{d}^{s+1}\right)_Q = \frac{\theta_K}{\hat{\theta}^2} \Delta \bar{F}_{mn}^{s+1} \quad \text{with} \quad Q = Q(K, m, n), \quad K = 1, \dots, N_{\text{gr}}, \qquad (4.70)$$

where $\hat{\theta}$ is given by $(4.45)_2$. Note that this initial estimate is based on the grain size only, i.e., the increment in the deformation gradient for a grain K scales proportionally with the grain volume fraction θ_K , see (4.70). Preliminary numerical tests not presented here have indicated that such an initial estimate, though simple to determine, may result in an inconvenient starting point for the incremental-iterative update algorithm, and therefore in a (very) poor convergence behavior.

4.2.6 Overview of GGCM algorithm

The incremental-iterative update algorithm for the generalized grain cluster method is summarized in Algorithm 1. The algorithm is based upon the uniform stress initial increment presented in Section 4.2.5; the implementations of the three alternative initial estimates presented in Section 4.2.5 occurs in a similar fashion, but are omitted here for brevity reasons. A detailed analysis of the performance of the different initial estimates is provided in Section 4.3.3.

It is worth pointing out that user-defined constitutive models may provide tangent stiffnesses based on stress and deformation measures different than the first Piola-Kirchhoff stress and the deformation gradient used in expression (4.38). However, these material tangent stiffnesses may be converted to this format using push-forward and pullbackward relations presented in the literature, see, e.g., [57, 62]. Furthermore, the parameters $\alpha_1, \alpha_2, \alpha_3, \beta, \omega$ and the time step Δt require a calibration procedure, such as that described in Section 4.3.5. Representative values of these parameters are used in the numerical examples treated in the section below.

4.3 Simulations of clusters of multiphase materials

4.3.1 Preliminaries

A series of simulations involving microstructures typically found in low-alloyed multiphase steels is presented in this section in order to illustrate important features of the generalized grain cluster method. These microstructures consist of an aggregate of ferritic grains (primary phase) and metastable retained austenitic grains (secondary phase). Under mechanical loading, the austenitic grains may partially or totally transform into a third phase, called martensite. The crystal plasticity model presented in [71] and extended in [70] is used to simulate the elasto-plastic deformation in the ferritic grains. For incorporating the crystal plasticity model in the GGCM, the deformation gradient \mathbf{F}_K , for each

Algorithm 1 Algorithm for GGCM

Pre-processing:

Generate cluster's microstructural geometry, e.g., using a (multilevel) Voronoi algorithm

Assign grain and surface indices $N = 1, \ldots, N_{gr}$ and $\gamma = 1, \ldots, M_N$

Construct global connectivity array $I = \hat{I}(N, \gamma)$

Compute volumes V_N and V, areas A_I and A_{int} and volume fractions θ_N and $\hat{\theta}$ from (4.30), (4.36) and $(4.45)_{2}$

Assemble averaging operator L from (4.42) and its pseudo-inverse L^+ from (4.54) (use compact storage) Select weighting parameters $\alpha_1, \alpha_2, \alpha_3$, scaling factor β and step size ω appearing in (4.28), (4.29) and (4.46)

Initialize (s = 0)

for $N = 1, \ldots, N_{gr}$ do

For an unloaded and unstressed initial state, construct \mathbf{x}^0 from $\mathbf{F}_N^0 = \mathbf{I}$ and set $\mathbf{P}_N^0 = \mathbf{0}$, $\mathbf{\Sigma}^0 = \mathbf{0}$ For inelastic constitutive models, initialize internal variables Ξ_N^0

Compute initial constitutive tangents \mathbb{A}^0_N (see (4.38)) from the given constitutive model(s) of grain N end for

Main loop $(s \ge 1)$

while $s + 1 \leq N_{\text{steps}}$ do

Store converged state at loading step s and increase the time-like process parameter $t^{s+1} = t^s + \Delta t^{s+1}$ Update externally-applied macroscopic deformation gradient $\mathbf{\bar{f}}^{s+1} = \mathbf{\bar{f}}^s + \Delta \mathbf{\bar{f}}^{s+1}$

Initial deformation gradient $x^{s+1,0}$

For the method shown in Section 4.2.5: (see Section 4.2.5 for other methods) Compute estimate of stress increment $\mathbf{p}^{s+1,0}$ from (4.62)₂ and (4.60)

for $N = 1, ..., N_{gr}$ do

Compute \mathbf{A}_N^s from (4.63) and (4.61)₂ and its pseudo-inverse $(\mathbf{A}_N^s)^+$

Compute grain-level increment $\hat{\mathbf{d}}_N^{s+1}$ from (4.66) and assemble in cluster-level vector $\hat{\mathbf{d}}^{s+1}$

end for

Compute scaled initial deformation gradient increment \tilde{d}^{s+1} from (4.56) and (4.55)

Compute projected initial deformation gradient increment d^{s+1} from (4.52)

Get initial estimate $\mathbf{x}^{s+1,0}$ from (4.50)

Constrained minimization

i = 0

while Not converged do

Compute $(\mathbf{P}_N, \mathbb{A}_N, \mathbf{\Xi}_N)^{s+1,i}$ for $N = 1, \dots, N_{\text{gr}}$ from the grains' constitutive model(s) Update the estimate of the macrostress $\mathbf{\Sigma}^{s+1,i}$ from (4.35) Compute unconstrained gradient $(\mathbf{g})^i$ from (4.37) Compute constrained gradient $(\mathbf{g}^{\mathbf{p}})^{i}$ from (4.44) and (4.45) Update estimate of deformation gradients $\mathbf{x}^{s+1,i+1}$ from (4.46) Check convergence $i \leftarrow i + 1$ end while $s \leftarrow s + 1$ end while

ferritic grain K, is decomposed as

$$\mathbf{F}_K = \mathbf{F}_K^{\mathrm{e}} \mathbf{F}_K^{\mathrm{p}}$$

where \mathbf{F}_{K}^{e} represents the elastic part of the deformation gradient and \mathbf{F}_{K}^{p} is the plastic part of the deformation gradient. The crystal plasticity model includes a so-called ferritic microstrain as an internal variable, which reflects the local elastic distortions in the crystalline lattice due to the presence of dislocations, see Section 3.1.2 and Section 2.1.6 (2.63) for more details. For the *K*-th ferritic grain, the microstrain is denoted as β_{K}^{F} , and the volume average over the ferritic grains is indicated as $\bar{\beta}^{F}$. The latter parameter will be used for characterizing the average plastic deformation in the ferritic grains in the simulation results presented in this section.

The constitutive behavior of the austenitic grains is simulated using the model developed in [73, 75] and extended in [70]. This model is suitable for simulating single-crystal grains simultaneously undergoing a plastic deformation and a martensitic phase transformation from a face-centered cubic austenitic lattice structure into a body-centered tetragonal martensite upon mechanical and/or thermal loading. The model includes the possible transformation into crystallographically-distinct martensitic phases, referred to as *transformation systems*. For the implementation of the phase transformation model within the GGCM, the deformation gradient \mathbf{F}_K for each *austenitic* grain K is decomposed as

$$\mathbf{F}_K = \mathbf{F}_K^{\mathrm{e}} \mathbf{F}_K^{\mathrm{p}} \mathbf{F}_K^{\mathrm{tr}}$$

where, as before, \mathbf{F}_{K}^{e} and \mathbf{F}_{K}^{p} represent the elastic and plastic parts of the deformation gradient, respectively, and \mathbf{F}_{K}^{tr} corresponds to the transformation part. For the *K*-th austenitic grain, the total martensitic volume fraction is denoted as $\xi_{K}^{M} = \sum_{\alpha=1}^{N} \xi_{K}^{(\alpha)}$, which corresponds to the sum of volume fractions of the individual transformation systems, $\xi_{K}^{(\alpha)}$ ($\alpha = 1...N$). The volume average of the martensitic volume fraction over the austenitic grains is indicated as $\bar{\xi}^{M}$. This parameter will be used for quantifying the average martensitic transformation in the austenitic grains in the simulation results presented in this section. The material parameters used in the numerical simulations for the ferrite, austenite and martensite can be found in Table 2.1. The computation of the stress, tangential stiffness and internal variables in the individual grains is carried out by means of a fully implicit, incremental-iterative update algorithm formulated within a large deformation framework. The details of this numerical implementation, which includes a selection algorithm for the determination of the active transformation systems and slip systems, can be found in [62].

Using the constitutive models outlined above allows for testing the GGCM for relatively complex and challenging material systems, where a large number of internal variables at each material point inside a grain capture inelastic phenomena originating from the sub-grain length scale, i.e., plastic slip and phase transformation resolved in crystallographically-distinct planes. The periodic microstructures used in the simulations
Sample #	Total number	Austenitic grains	Ferritic grains	Volume frac-
	of grains			tion of austen-
				ite (%)
S1	8	1	7	12.0
S2	64	8	56	12.1
S3	100	12	88	12.2
S4	200	24	176	11.9
S5	450	56	394	12.0
S6	600	72	528	12.0

Table 4.1: Composition and volume fraction of different microstructural samples used in the GGCM simulations and the (finite element-based) DNS.

are constructed from a two-level Voronoi algorithm generating realistic (convex and nonconvex) polyhedral grains, see Section 3.2.1 for details. A randomly-chosen crystal orientation is assigned to each single-crystal grain in the cluster in order to approach a macroscopically isotropic material under an increasing number of grains. Representative pole figures for the orientation distributions of the samples analyzed in the present study can be found in Section 3.2.2. All grain clusters were macroscopically loaded under *simple shear* according to

$\bar{\mathbf{F}} = \mathbf{I} + \bar{\gamma} \mathbf{e}_1 \otimes \mathbf{e}_2 \,,$

where $\bar{\gamma}$ is the amount of shear and \mathbf{e}_1 and \mathbf{e}_2 are orthonormal unit vectors perpendicular to the external faces of the cubic grain cluster. The imposed macroscopic shear rate was $\dot{\bar{\gamma}} = 10^{-4} \mathrm{s}^{-1}$, which is in the range of quasi-static loading, i.e., it was confirmed that the inertial terms in the balance of linear momentum can be neglected. The samples were deformed up to a final value of $\bar{\gamma} = 0.2$. Unless indicated otherwise, the step size for the constrained gradient descent method equals $\omega = 20$ and the convergence criterion used is provided by expression (4.47), with the tolerance prescribed a priori as $\varepsilon = 10^{-3}$. It is emphasized that the simple shear deformation mode was chosen for reasons of simplicity, such that the basic characteristics of the GGCM can be demonstrated in a consistent and unequivocal fashion. The computation of sample responses under alternative, more complex deformation modes falls beyond the scope of this study, although it may be reasonably expected that these will expose similar characteristics of the GGCM as for the simple shear mode.

The performance of the GGCM is demonstrated by considering six microstructures, each composed of a different number of grains, see Table 4.1. Note that for all these microstructures the initial volume fraction of the secondary austenitic phase is approximately 12 %, which is within the range of experimental values observed in multiphase TRIP steels [60, 35, 58]. A parametric study is carried out using a wide range of values of the weighting factors α_i , with i = 1, 2, 3, see Table 4.2. In accordance with (4.28) and (4.29), in the solution procedure the weighting factors α_1 and α_3 determine the rel-

Set #	$\alpha_1 = \alpha_3$	α_2	Ratio α_2/α_1
W1	1.0×10^{-7}	1.0×10^{0}	1.0×10^7
W2	5.0×10^{-6}	2.0×10^{-2}	4.0×10^3
W3	1.0×10^{-5}	1.0×10^{-2}	1.0×10^3
W4	2.0×10^{-5}	5.0×10^{-3}	2.5×10^2
W5	1.0×10^{-4}	1.0×10^{-3}	1.0×10^{1}

Table 4.2: List of distinct weighting factors used in the GGCM simulations. In all cases, α_1 and α_3 were chosen equal to each other. Set W1 approximates the *Taylor bound* where the deformation gradient is uniform across the grains, while set W5 tends to the *Sachs bound*, for which the stress in the grains is uniform, within the tolerance provided by the kinematical multiscale constraint. Sets W2-W4 represent intermediate cases.

ative importance of the equilibrium conditions at the grain boundaries and within each grain, respectively, while the weighting factor α_2 sets the relevance of kinematical compatibility across grain boundaries. The scaling factor β that appears in (4.29) was kept fixed, by setting it equal to $\beta = 1$ (units of stress). The performance of the GGCM is demonstrated by considering six microstructures, each composed of a different number of grains, see Table 4.1. Note that for all these microstructures the initial volume fraction of the secondary austenitic phase is approximately 12 %, which is within the range of experimental values observed in multiphase TRIP steels [60, 35, 58]. A parametric study is carried out using a wide range of values of the weighting factors α_i , with i = 1, 2, 3, see Table 4.2. In accordance with (4.28) and (4.29), in the solution procedure the weighting factors α_1 and α_3 determine the relative importance of the equilibrium conditions at the grain boundaries and within each grain, respectively, while the weighting factor α_2 sets the relevance of kinematical compatibility across grain boundaries. The scaling factor β that appears in (4.29) was kept fixed, by setting it equal to $\beta = 1$ (units of stress).

For each grain cluster, the results from a direct numerical simulation (DNS) performed with an accurate finite element model were used as a benchmark. The term DNS is borrowed from its classical context in fluid mechanics to reflect the analogy between resolving the spatial scales of turbulence and resolving the micromechanical scales; it thus represents the full-field numerical solution obtained from determining the balance of linear momentum at each microscopic material point. Details of the finite element-based DNS simulations can be found in Chapter 3. Unless indicated otherwise, all DNS calculations were performed using a regular $30 \times 30 \times 30$ mesh (27000 hexahedral elements with a reduced integration scheme) with pointwise periodic boundary conditions, resulting in 81021 displacement degrees of freedom. This mesh size is based on a convergence study where the relative error in the effective main shear stress is less than 2% of the value found for a (substantially) finer $40 \times 40 \times 40$ mesh, see also [84]. The maximum time step in the DNS was determined as $\Delta t = 3.2$ s, since larger time steps typically triggered numerical convergence problems. All other parameters used in the DNS are identical to those in the simulations performed with the GGCM.



Sample S4, weighting W2

Figure 4.4: Average (macroscopic) Cauchy shear stress \overline{T}_{12} (a), stress component \overline{T}_{11} (b), martensitic volume fraction $\overline{\xi}^{\mathrm{M}}$ (c) and microstrain in the ferrite $\overline{\beta}^{\mathrm{F}}$ (d), all plotted as a function of the applied amount of shear $\overline{\gamma}$, for three distinct time steps in the GGCM: $\Delta t = 1.0$, 5.0 and 25.0 s. The sample used is S4 with 200 grains in total, see Table 4.1, and the set of weighting factors equals W2, see Table 4.2. The dashed lines represent the corresponding DNS responses, obtained from an accurate $30 \times 30 \times 30$ finite element model.

4.3.2 Influence of time step size

In order to examine the influence of the size of the time step on the accuracy and stability of the numerical results computed with the GGCM, the response of a microstructural sample loaded under simple shear is analyzed considering three distinct time steps, namely $\Delta t = 1$ s, 5s and 25s. The sample is composed of 24 grains of austenite and 176 grains of ferrite (sample S4 in Table 4.1). The corresponding response curves are shown in Fig. 4.4, which include the main Cauchy shear stress component \bar{T}_{12} averaged over the whole cluster (Fig. 4.4a), the average normal stress component \bar{T}_{11} (Fig. 4.4b), the average martensitic volume fraction $\bar{\xi}^{\rm M}$ (Fig. 4.4c) and the average microstrain in the ferrite $\bar{\beta}^{\rm F}$ (Fig. 4.4d), all plotted as a function of the macroscopic amount of shear $\bar{\gamma}$. The GGCM curves were computed using calibrated weighting factors $\alpha_1 = \alpha_3 = 5.0 \times 10^{-6}$ and $\alpha_2 = 2.0 \times 10^{-2}$ (set W2 in Table 4.2) and an initial estimate for the deformation gradient based on a uniform stress increment. As shown in the figure, for the largest time step, $\Delta t = 25$ s, the GGCM response shows significant fluctuations and deviates strongly from the DNS response represented by the dashed line. In contrast, the GGCM responses for $\Delta t = 1$ s and $\Delta t = 5$ s are relatively smooth and remain close to each other over the whole deformation range, thereby approaching the DNS response closely. Hence, it may be concluded that a specific minimum time step is required for obtaining a GGCM solution of satisfactory accuracy. Using an L_2 norm of the main shear stress along the complete deformation path (see also Section 4.3.5, expression (4.71)), the relative difference between the responses for $\Delta t = 1$ s and $\Delta t = 5$ s is calculated as 2.5%. Correspondingly, the results obtained with the time step $\Delta t = 5$ s were considered as sufficiently accurate, and forthcoming results were computed using this value.

From the aspect of stability, no specific conclusions on the maximum time step size can be drawn from the GGCM simulations, since for all three time steps considered the response remains bounded within the range analyzed. Conversely, as already indicated in the previous section, the DNS calculation did encounter convergence problems for time steps larger than $\Delta t = 3.2$ s; hence the DNS is characterized by a smaller maximum time step than the GGCM simulations.

4.3.3 Influence of initial estimate of the deformation gradients

In Section 4.2.5 several options were described for estimating the *initial* incremental microscale deformation gradients $\hat{\mathbf{d}}^{s+1}$ required at the onset of each new loading step s+1 of the constrained minimization algorithm. Due to the loading path dependency of inelastic material models, this initial estimate may affect the accuracy and efficiency of the generalized grain cluster method. Since GGCM has the general aim of closely approximating accurate DNS response curves at (much) lower computational cost, it needs to be examined in detail what the effect of this estimate is on the numerical accuracy and efficiency of three different initial estimates of $\hat{\mathbf{d}}^{s+1}$ are compared, as based upon (i) a uniform deformation gradient initial increment (Section 4.2.5), (ii) a uniform stress initial increment (Section 4.2.5) and (iii) previously converged loading steps (Section 4.2.5). The initial estimate based upon the null vector (Section 4.2.5) is left out of consideration in this comparison, since preliminary computations (not presented here) clearly indicated a deficient performance with respect to the other three approaches.

In the analysis a sample consisting of 8 grains of austenite and 56 grains of ferrite (set S2 in Table 4.1) is subjected to simple shear, where the GGCM responses calculated with the three initial estimates of $\hat{\mathbf{d}}^{s+1}$ are compared against the response of the accurate benchmark FEM model described in Section 4.3.1. In the GGCM the weighting factors are $\alpha_1 = \alpha_3 = 5.0 \times 10^{-6}$ and $\alpha_2 = 2.0 \times 10^{-2}$ (set W2 in Table 4.2) and the time step equals $\Delta t = 5$ s. The results of the simulations are shown in Fig. 4.5 in terms of the main Cauchy shear stress \overline{T}_{12} (Fig. 4.5a), the stress component \overline{T}_{11} (Fig. 4.5b), the martensitic volume fraction $\overline{\xi}^{\mathrm{M}}$ (Fig. 4.5c) and the microstrain in the ferrite $\overline{\beta}^{\mathrm{F}}$ (Fig. 4.5d). All



Sample S2, weighting W2

Figure 4.5: Average (macroscopic) Cauchy shear stress \overline{T}_{12} (a), stress components \overline{P}_{11} (b), martensitic volume fraction $\overline{\xi}^{M}$ (c) and microstrain in the ferrite $\overline{\beta}^{F}$ (d) as a function of the applied amount of shear $\overline{\gamma}$ for distinct initial estimates of the deformation gradient at the beginning of each GGCM loading step. The three initial estimates for the vector of deformation gradients within the grains, $\hat{\mathbf{d}}^{s}$, are based on (i) a uniform deformation gradient increment, (ii) a uniform stress increment, and (iii) previously converged loading steps. The sample used is S2 with 64 grains in total, see Table 4.1, and the set of weighting factors is W2, see Table 4.2. The dashed lines represent the corresponding DNS responses, obtained from an accurate $30 \times 30 \times 30$ finite element model.

quantities are displayed as a function of the macroscopic amount of shear $\bar{\gamma}$. It can be observed that the simulations based on a uniform deformation gradient initial increment and a uniform stress initial increment are relatively smooth and remain close to each other. The method based on a uniform deformation gradient increment predicts a slightly stiffer response for the main Cauchy shear stress \bar{T}_{12} compared to the simulation based on a uniform stress increment, while the opposite occurs for the stress \bar{T}_{11} , see Fig. 4.5a,b. For the present choice of weighting factors W2 both methods approach the solution obtained with DNS closely, although the method based on a uniform stress initial increment appears to be slightly more accurate. The response of the secondary phase, expressed in terms of the martensitic phase transformation, is somewhat underpredicted by both methods at larger deformation, $\bar{\gamma} > 0.1$, see Fig. 4.5c, while the microstrain $\bar{\beta}^{\rm F}$ in the ferrite

Initial estimate microscopic defor-	Section	Sample	Weighting	CPU
mation gradient				time
				(hours)
Uniform deformation gradient ini-	4.2.5	S2	W2	8
tial increment				
Uniform stress initial increment	4.2.5	S2	W2	17
Initial increment by previously con-	4.2.5	S2	W2	9
verged loading steps				

Table 4.3: Computational times of GGCM with distinct initial estimates of the microscopic deformation gradient at the onset of each incremental loading step. The sample is loaded under simple shear.

is predicted accurately over the whole deformation range, see Fig. 4.5d. In contrast, the simulation based on an initial estimate obtained from previously converged loading steps is characterized by significant fluctuations in the stress components and a relatively large over-prediction of the volume fraction of martensite. Moreover, the step size in the constrained minimization algorithm had to be reduced here from $\omega = 20$ to $\omega = 10$ in order to circumvent convergence problems. Consequently, the initial estimate based on extrapolating previously converged loading steps was deemed sub-optimal compared to initial estimates based upon an increment of a uniform deformation gradient and a uniform stress.

The computational times for the three initial estimates of $\hat{\mathbf{d}}^{s+1}$ are compared in Table 4.3. It is noted that in Section 4.3.6 the computational times of simulations performed with the GGCM will be also compared objectively to those of finite element-based DNS. The table shows that the simulations with a uniform deformation gradient initial increment and an initial increment based on previously converged loading steps are characterized by similar computational times, which are about half of the computational time obtained for a uniform stress initial increment. Nonetheless, additional simulations (not shown here) have indicated that the numerical results computed with the uniform deformation gradient initial increment may substantially loose their accuracy under conditions approaching the uniform stress limit case (i.e., set W5 in Table 4.2). Conversely, the numerical results obtained with the uniform stress initial increment proved to be accurate for *both* the uniform stress limit case (set W5) and the uniform deformation gradient limit case (set W1). Hence, despite its higher computational cost, from the viewpoint of accuracy all GGCM simulations discussed in the subsequent sections were carried out using a uniform stress initial increment. Note, however, that the method based on a uniform deformation gradient initial increment remains an attractive alternative under conditions generating negligible to moderate differences between the deformations in individual grains i.e., sets W1 to W3 in Table 4.2.



Figure 4.6: Shear stress distribution P_{12} across sample S2 at a macroscopic shear deformation $\bar{\gamma} = 0.2$ for weighting factors representing (a) the uniform deformation gradient limit case (set W1), (b) an intermediate case (set W2) and (c) the uniform stress limit case (set W5).

4.3.4 Influence of weighting factors α_i and sample composition

In this section the effects on the GGCM response by the weighting factors, α_i with i = 1, 2, 3, see (4.28), and the sample composition are demonstrated. For this purpose, a sample subjected to simple shear deformation, up to $\bar{\gamma} = 0.2$, is analyzed for five different sets of weighting factors, W1-W5, as listed in Table 4.2, and two different microstructural compositions, S1 and S4 (of 8 grains and 200 grains in total, respectively), see Table 4.1. The samples S1-S6 presented in Table 4.1 were recently subjected to an extensive convergence study using an accurate finite element model of $30 \times 30 \times 30$ elements, which demonstrated that sample S4 represents a lower bound for the number of grains required for reaching a macroscopic representative volume element (RVE), see [84] for more details. Accordingly, by comparing the response of the "minimal" RVE sample S4 to the response of the "small sample" S1, the influence by the discreteness of the microstructure on the overall response can be highlighted. A detailed analysis of the convergence behavior of the GGCM responses, including all samples S1-S6 summarized in Table 4.1, will be presented in Section 4.3.5.

In order to clearly illustrate some essential features of the weighting factors, first for sets W1, W2, and W5 the main Piola-Kirchhoff shear stress distribution \bar{P}_{12} in sample S2 is considered at the final state of deformation $\bar{\gamma} = 0.2$, see Fig. 4.6. As can be observed from Fig. 4.6a, in the limit of a uniform deformation gradient (set W1) the kinematic compatibility between individual grains is preserved, which occurs at the expense of violating the equilibrium requirements for the grains, i.e., the shear stress P_{12} jumps significantly in value across grain boundaries. The response shown in Fig. 4.6c for the limit case of uniform stress (set W5) indeed satisfies the equilibrium requirements, but clearly violates kinematic compatibility between grains. The intermediate case (set W2) shown in Fig. 4.6b corresponds to a compromise solution that partially satisfies both the kinematic compatibility and equilibrium requirements.

In Fig. 4.7 the evolutions of macroscopic state and internal variables of the samples S1 and S4 are compared. The figure illustrates the main Cauchy shear component, \bar{T}_{12} ,

(Fig. 4.7a,b) and the stress component \overline{T}_{11} (Fig. 4.7c,d), i.e., grain cluster averages, of the two samples, as a function of the applied macroscopic shear deformation $\overline{\gamma}$. It further shows the evolutions of the effective martensitic volume fraction $\overline{\xi}^{\mathrm{M}}$ in the secondary, austenitic phase (Fig. 4.7e,f) and the effective microstrain $\overline{\beta}^{\mathrm{F}}$ in the ferritic matrix (Fig 4.7g,h), with the latter parameter being a measure for the amount of plastic deformation generated. For both samples the GGCM responses for the five different sets of weighting factors W1-W5 are plotted together with the response obtained from an accurate finite element-based DNS described in Section 4.3.1. As mentioned before, the GGCM simulations were carried out with a uniform stress initial increment.

Both for samples S1 and S4 the limit cases of a uniform deformation gradient (set W1) and a uniform stress (set W5) provide relatively smooth response curves, which, as may be expected from basic homogenization principles, respectively overpredict and underpredict the DNS response. For the intermediate sets with weighting factors W2 to W4 the closest resemblance with the DNS response is realized by set W2, although for the small sample S1 some distinctive drops in stress are observed, see Fig. 4.7a,c. These stress drops result from a competition between the two opposing terms in the objective functional J given by (4.28), which are the compatibility term, $\alpha_2 J_2$, and the equilibrium term, $\alpha_1 J_1 + \alpha_3 J_3$. During the minimization procedure both terms occasionally fluctuate strongly in magnitude, thereby showing a tendency of compensating each other. Whenever the minimization of the functional J was dominated by the derivative of the force equilibrium term (i.e., the term $\partial(\alpha_1 J_1 + \alpha_3 J_3)/\partial (F_K)_{mn}$ following from (4.37) and (4.34)), the force equilibrium term $\alpha_1 J_1 + \alpha_3 J_3$ decreased while the compatibility term $\alpha_2 J_2$ increased. In contrast, this process was reversed when the compatibility term $\alpha_2 J_2$ became dominant. As demonstrated by the shear stress response in figure 4.7a, this bifurcation-type behavior is more apparent for the small sample S1, and thus can be associated to the level of discreteness of the microstructure. More discussion on the bifurcation sensitivity of the microstructural responses can be found in Section 4.4.

Under a stepwise change of the sets of weighting factors from W1 to W5 the corresponding Cauchy shear stress responses \overline{T}_{12} decrease monotonically, see Fig. 4.7a,b. A similar order in the responses for the different sets of weighting factors can be observed for the ferritic microstrain $\overline{\beta}^{\rm F}$, see Fig. 4.7g,h. In contrast, the responses of the stress component \overline{T}_{11} and the martensitic volume fraction $\overline{\xi}^{\rm M}$ do not follow this regular order, see Fig. 4.7c,d,e,f. This difference can be explained as follows. Under the applied isochoric shear deformation $\overline{\gamma}$ the secondary austenitic phase transforms into martensite, whereby the resulting volumetric expansion is compensated for by the surrounding ferritic matrix under the generation of normal stresses. Since the number of austenitic grains in samples S1 and S4 is relatively low (i.e., 1 grain and 24 grains, respectively, see Table 4.1), the resulting predictions for the effective stress component \overline{T}_{11} , and the martensitic volume fraction, $\overline{\xi}^{\rm M}$ occasionally are sensitive to inaccuracies, and therefore do not provide the regular order in responses mentioned above. Despite this aspect, for sample S4 all 4 response curves computed with the set of weighting factors W2 follow the corresponding



(g) (h) Figure 4.7: Average (macroscopic) Cauchy shear stress \overline{T}_{12} (a),(b), stress component \overline{T}_{11} (c),(d), martensitic volume fraction $\overline{\xi}^{M}$ (e),(f) and microstrain in the ferrite $\overline{\beta}^{F}$ (g),(h) in samples S1 and S4, respectively, plotted as a function of the applied amount of shear $\overline{\gamma}$ for different sets of weighting factors W1-W5, see Table 4.2. The dashed lines represent the corresponding DNS responses, obtained from an accurate $30 \times 30 \times 30$ finite element model.

DNS response curves reasonably well, see Fig. 4.7b,d,f,h.

The computational times of the numerical simulations presented in Fig. 4.7 are summarized in Table 4.4. All simulations were carried out with the uniform stress initial increment method, since this initial estimate leads to a good balance between computational accuracy and efficiency, see Section 4.3.3. It can be observed that the computational times are the largest for the uniform deformation gradient limit case W1. This is, because the initial estimate provides a deformation state that is incompatible at the grain boundaries, as a result of which in W1 the most dominant term, $\alpha_2 J_2$, representing kinematic compatibility, see (4.34) and (4.37), initially is relatively far off its minimum. Consequently, the number of iterations required for finding a converged state that satisfies kinematic compatibility is relatively large. Obviously, the application of the uniform deformation gradient initial increment method will reduce the number of iterations for set W1, since it matches the kinematic compatibility requirement and also satisfies the multiscale kinematic constraint given by (4.9). Recall, however, that this initial estimate may become inaccurate and inefficient under conditions approaching the limit case W5 of a uniform stress in the sample, see Section 4.3.3.

Table 4.4 shows that the computational time decreases when the set of weighting factors is changed stepwisely from W1 to W4. In accordance with this trend and the discussion presented above, it is somewhat counterintuitive to observe that the computational time for the uniform stress limit case W5, instead of being the lowest, is significantly higher than that of sets W2, W3 and W4. This can be explained, however, from the correction step that projects the uniform stress initial estimate for the deformation gradient, $\hat{\mathbf{d}}^{s+1}$, given by (4.66), within the feasible solution space that satisfies the multiscale kinematic constraint (4.9), leading to the projected initial deformation gradient increment \mathbf{d}^{s+1} , see (4.52) and (4.55) as well as Fig. 4.3. Accordingly, for step s+1 the starting values for the local deformation gradients in the minimization algorithm $x^{s+1,0} = x^s + \mathbf{d}^{s+1}$, see (4.50), *do not fully reflect a state of uniform stress*. This makes the minimization process for reaching the uniform stress limit case W5 computationally more demanding than for the "intermediate" sets W2, W3 and W4 for which the stress distribution in the sample is (far) less uniform.

4.3.5 Calibration procedure

From the results presented in Section 4.3.4 it became clear that the weighting factors α_1, α_2 and α_3 and the sample size play a major role in i) the accuracy and (ii) the computational efficiency of the generalized grain cluster method. If the analyst wants to adequately account for these two aspects in the calibration of the weighting factors, a parametric analysis similar to that presented in Section 4.3.4 needs to be performed. By inspection of Fig. 4.7 it was concluded that the set W2 provides the best agreement with the DNS response; therefore the parameters α_i (with i = 1, 2, 3) of set W2 may be referred to as the "calibrated weighting factors". A sensitivity analysis of these weighting

Weighting	CPU	time	CPU	time
	sample	S 1	sample	S4
	(hours)		(hours)	
W1 (\approx uniform deformation gradient)	13		244	
W2	3		39	
W3	1.5		16	
W4	0.5		7	
W5 (\rightarrow uniform stress)	4.75		91	

Table 4.4: Computational times (sample loaded under simple shear) of GGCM for distinct weighting factors, using a uniform stress initial increment and two different samples, S1 and S4 (Note: decimals refer to fractions of 60 minutes).

factors has indicated that differences in GGCM responses become significant only when the ratio α_2/α_1 is modified by *at least* a factor of 2. For example, Table 4.2 illustrates that the change in α_2/α_1 in the transition of set W2 to set W3 equals a factor of 4. As further shown in this table, the method becomes rather insensitive to changes in the ratio α_2/α_1 close to the uniform deformation gradient limit case W1 (α_2/α_1 approaches infinity) or the uniform stress limit case W5 (α_2/α_1 approaches zero). If the experimental data required for calibration is not readily available or if the analyst wants to "design" a material starting from its microstructural features, the relation between the microscopic behavior and the effective macroscopic response may be initially estimated using "default" weighting factors in the range of set W2.

In principle, the calibration procedure should be carried out with a grain cluster corresponding to a macroscopic representative volume element (RVE). Similar to common procedures used for multiscale simulations based on the finite element method, the minimally required size of an RVE for the GGCM may be established from a convergence analysis of the macroscopic response on grain clusters of increasing size. As mentioned before, the microstructures S1-S6 presented in Table 4.1 were recently subjected to such a convergence study, performed with an accurate finite element model of $30 \times 30 \times 30$ elements [84]. The results of this convergence study are here compared to that of a convergence study carried out with the GGCM, by computing the relative difference in macroscopic response for the individual samples S1-S6. The macroscopic response is reflected by two distinct macroscopic variables, which are the main Cauchy shear stress \overline{T}_{12} and the martensitic volume fraction $\bar{\xi}^{M}$. The main shear stress is representative of the whole grain cluster whereas the martensitic volume fraction reflects the average value in the secondary (austenitic/martensitic) phase. As indicated byFig. 4.8a, for both macroscopic variables the relative difference in response is based on an L_2 norm, which is taken over the complete deformation path from $\bar{\gamma} = 0$ to $\bar{\gamma} = 0.2$. For an arbitrary scalar function



Figure 4.8: (a) Relative differences in responses (to simple shear) computed by the GGCM and DNS, plotted as a function of the total number of grains in the sample. The GGCM computation of the macroscopicCauchy shear stress \overline{T}_{12} and martensitic volume fraction $\overline{\xi}^{M}$ was performed using the set of weighting factors W2, see Table 4.2. (b) Computational times (in CPU hours) of grain clusters S1-S6 subjected to simple shear ($\overline{\gamma} = 0.2$), together with a linear approximation (dashed line) in terms of the total number of grains in the sample. The microstructural characteristics of samples S1-S6 are listed in Table 4.1.

 $\bar{f} = \bar{f}(\bar{\gamma})$, this norm thus may be expressed as

$$\|\bar{f}\|_{L_2} = \left(\int_{\bar{\gamma}=0}^{\bar{\gamma}=0.2} \bar{f}^2 \mathrm{d}\bar{\gamma}\right)^{1/2} \,. \tag{4.71}$$

The GGCM response to simple shear for all samples S1-S6 was computed using the same set of weighting factors W2. As shown in Fig. 4.8a, the shear stresses predicted by GGCM and the accurate finite element-based DNS simulation remain within 5% difference when the number of grains grows. Furthermore, the difference between the martensitic volume fractions calculated by the GGCM and DNS simulations oscillates around 15% at a larger number of grains. Hence, the predictions by the GGCM and DNS simulations appear to have similar rates of convergence, from which it can be concluded that the minimal macroscopic RVE for the two methods is identical, i.e., the "minimal" RVE sample S4 with 200 grains in total. An additional observation from Fig. 4.8a is that, once a set of weighting parameters has been calibrated for a small sample, it can be subsequently used for an alternative, larger sample without significantly compromising to the accuracy of the results. Accordingly, the calibrated weighting factors appear as "objective", in a sense that they do not need to be modified when analyzing alternative microstructures. In addition, by using a sample that is smaller than the minimal RVE sample, this characteristic leads to a quick and straightforward calibration of the weighting factors. For example, in the present study sample S2 was used for a quick calibration of the weighting factors W2, see Section 4.3.3, which is composed of about three times fewer grains than the minimal RVE sample S4, see Table 4.1.

4.3.6 Performance assessment of GGCM in comparison to DNS

Fig. 4.8b illustrates the overall computational performance of the GGCM by depicting the CPU time for samples S1-S6 versus the corresponding number of grains in the sample. All computations were carried out on the same single-processor computer, using the uniform stress initial increment method and the set of weighting factors W2. The six data points depicted are approximated by a linear relation (dashed line) up to an R^2 -value of 0.8743 calculated by a least squares regression. The linear relation between the GGCM computational time and the total number of grains N_{ar} in the sample results from solving the local deformation gradient *per grain*, whereby the average computational effort per grain (i.e., the update of the stress, internal variables and tangential stiffness) is *nearly* independent of the total number of grains N_{qr} . In contrast, the computational time associated to a finite element calculation typically scales with the power n of the number of elements, where n > 1. Hence, it depends on the number of grains indirectly by means of the number of elements per grain required for achieving a converged solution to within a specific tolerance. Since the finite element models of the samples S1 to S6 use comparable $30 \times 30 \times 30$ meshes, they are characterized by similar computational times, in the range of 220 ± 30 CPU hours.

For an objective evaluation of the computational cost of the GGCM, its computational time should be compared against that of a finite element model of the same accuracy. As pointed out in Section 4.3.3, the calibration procedure of the GGCM under simple shear was efficiently performed using a relatively small sample S2 (64 grains in total), which led to the set of weighting factors W2. With these weighting factors the shear response of the "minimal RVE sample" S4 (200 grains in total) was computed, see Fig. 4.7 in Section 4.3.4. The accuracy of this GGCM solution will now be quantified with respect to a reference DNS solution, calculated using a finer finite element mesh of $40^3 = 64000$ hexahedral elements. Subsequently, the computational speed of this GGCM solution will be compared against that of a DNS solution with the same accuracy. This DNS solution can be traced back from FEM responses obtained for distinct finite-element meshes of 8^3 , 15^3 , 20^3 and 30^3 hexahedral elements (equipped with a reduced integration scheme), by evaluating their accuracies measured with respect to the reference DNS solution obtained for the mesh of 40^3 elements. The accuracies of these distinct FEM solutions are plotted in Fig. 4.9a by means of the error in the main Cauchy shear stress $\overline{T}_{12}^{\text{DNS}}$, measured with respect to the main Cauchy shear stress \overline{T}_{12} computed with the accurate FEM model of 40^3 elements in terms of an L_2 norm.

The figure also shows the relative L_2 error of the GGCM, which is slightly below 2%. It can be observed that the errors of the FEM calculations range from about 6% for a coarse 8³ element mesh to about 1% for a fine 30³ element mesh. By means of straightforward interpolation, the FEM model with the same 2% error as the GGCM turns out to consist of about 24³ elements, see Fig. 4.9a. The computational times for the various FEM discretizations are shown in Fig. 4.9b. For comparison purposes, the simulations with coarser meshes (8³, 15³ and 20³ elements) were carried out with the same time step

as applied in the GGCM, namely $\Delta t = 5$ s. As already indicated in Section 4.3.1, the time step used for the 30³ element mesh had to be reduced to $\Delta t = 3.2$ s to avoid convergence problems. The GGCM requires 39 CPU hours to complete a simulation for sample S4. In contrast, through a simple interpolation it can be estimated that a finite element simulation with a 24³ element mesh requires about 160 CPU hours for completing this task, which thus is about 4 times more CPU time than the GGCM.

It is worth pointing out that by using the uniform deformation gradient increment method (Section 4.2.5) instead of the uniform stress increment method (Section 4.2.5), an additional decrease in the GGCM computational time of about a factor of 2 can be expected, see Table 4.3, which then makes the GGCM about 8 times faster than the FEM simulation with 24^3 elements. Obviously, for accomplishing this result a recalibration of the weighting factors is required.

The part of the CPU time spent on iteratively solving the mathematical equations of the GGCM can be globally subdivided into (i) the time required at the local level of an integration point by the implicit update algorithms (for crystal plasticity and crystallographic phase transformations) to compute the stress and consistent tangent stiffness in each grain, and (ii) the time required at the global (system) level by the constrained gradient descent algorithm for minimizing the objective potential reflecting the equilibrium conditions and kinematic compatibility conditions of *all* grains. The update algorithms used at the integration point level are the same as used in the integration points of a finite element-based DNS, where, for the incremental step size and specific crystallographic models used in the current simulations, convergence is typically reached within 10 iterations. Note that the GGCM only uses the equivalent of one integration point per grain, while a representative DNS with a sufficiently fine mesh of $24 \times 24 \times 24$ elements on average uses 70 integration points per grain when computing the response for the minimal RVE size of 200 grains in total (Sample S4, Table 1). The resulting gain in computational efficiency by the GGCM is partly lost at the system level due to the relatively large (100 to 200) iterations required for convergence of the constrained gradient descent algorithm. Hence, for further increasing the efficiency of the GGCM it is worthwhile investigating the application of faster numerical algorithms at the system level. This remains a topic for future studies. +

4.4 Concluding remarks

The generalized grain cluster method presented in this communication can be used for the efficient and accurate simulation of advanced multiphase microstructures composed of a large number of grains of arbitrary shape. It was demonstrated that an accurate calibration of the GGCM can be performed relatively quickly by using samples smaller than the "minimal RVE sample". For samples subjected to simple shear deformation, a comparison of the computational results with those obtained from finite element-based direct numerical simulations indicated that, for a given accuracy, the computational speed of



Figure 4.9: (a) Relative error of the main macroscopic Cauchy shear stress $\overline{T}_{12}^{\text{DNS}}$ of sample S4 under simple shear ($\overline{\gamma} = 0.2$), computed for different FEM mesh sizes M corresponding to 8^3 , 15^3 , 20^3 and 30^3 elements in total. The DNS reference value \overline{T}_{12} characterizing the relative L_2 error was computed using a fine FEM mesh of 40^3 elements. For comparison, the relative error for the GGCM simulation of sample S4 (also measured with respect to the DNS reference value \overline{T}_{12}) is specified by the dashed line. The GGCM simulation uses the set of weighting factors W2, see Table 4.2. (b) Computational time (in CPU hours) of sample S4 for different mesh sizes of the DNS. For comparison, the GGCM computational time of sample S4 is indicated by the dashed line.

the GGCM may be up to almost an order of magnitude lower, i.e., a factor of 8. This motivates the application of the GGCM in multiscale analyses of large-scale engineering problems, whereby the solution to the macroscale problem is calculated by the finite element method, and the material response at the microscale is computed by the GGCM. The coupling between the two methods is rather straightforward; since the GGCM uses the macroscopic deformation gradient as input for solving the microscale response of a multiphase material, it can be naturally included in commercial finite element codes as a *user-supplied subroutine* at the integration point level, where the effective stress and the effective constitutive tangent stiffness calculated for the multiphase material are returned by the GGCM to the finite element model. Obviously, the gain in computational time compared to a multiscale FE^2 approach will be considerable for large-scale engineering problems, since with the GGCM a relative decrease in computational time up to almost an order of magnitude is obtained for *every* macroscopic integration point in the FEM model.

Due to the overdetermined system of equations that characterizes the GGCM, the collection of possible microscale solutions contains numerous local minima. Accordingly, under an incremental macroscopic deformation, a stationary point may jump from one local minimum to another local minimum. These fluctuations may be activated by numerical inhomogeneities such as the value of the incremental step size, the convergence criterion applied or the initial estimates used in the iterative solution procedure. In the simulation results presented in this communication, the bifurcation sensitivity of the solution became manifest through local variations in some of the responses computed, as observed in the variation studies on the time step (see Fig. 4.4a,b), the initial estimate for the incremental deformation gradient (see Fig. 4.5a,b,c), and the GGCM weighting factors (see Fig. 4.7a,c,e). In addition, the oscillatory convergence behavior of microstructural samples under an increasing number of grains (see Fig. 4.8a) also implies a bifurcation sensitivity of the response. However, the numerical results in Fig. 4.4, 4.5, 4.7 and 4.8 also show that fluctuations due to bifurcations (substantially) diminish once (the size of) the numerical parameters and the size of the RVE are adequately determined. A further reduction of the fluctuations may be obtained by applying numerical regularization techniques in the iterative update algorithm applied at the system level, which is a topic for future research.

5

Challenges and future developments

In chapter 2, a thermodynamically-consistent model was developed in order to study the thermomechanical response of multiphase steels at the mesoscopic length scale. In particular, the coupling between the entropy and the deformation gradient was rigorously established under the assumption that the deformation gradient depends on the reversible entropy (2.12). Through the integration of the equations obtained from the Coleman-Noll procedure $(2.23)_{1.2}$, it was shown that the two thermal and mechanical state variables are not completely independent of each other. In particular, a change in the thermal entropy necessarily induces a deformation according to the classical thermomechanical coupling and, conversely, a deformation generates a change in the reversible entropy. When applying the Coleman-Noll procdure, which is meant to guarantee that the dissipation is always non-negative, it is routinely assumed that the thermal and mechanical variables may be modified independently, which, in view of the coupling, is generally not a valid assumption. In order to enforce the non-negativity of the dissipation under coupled conditions, it was concluded that the entropy should depend on the elastic deformation field. An open issue would be the experimental verification of this theoretical result for multiphase steels. A challenging aspect are the relatively small length scales at which the model parameters would need to be measured, which would require carefully designed and controlled experiments.

In **chapter 3**, the FEM package Abaqus was used for the thermomechanical simulations of microstructural samples. The numerical implementation of the mesoscale thermomechanical model required the use of two user-defined subroutines, namely UMAT and UMATHT, which may be compiled with the main code. Due to current limitations in the

code, only hexahedral elements are available with a combination of the aforementioned subroutines. A consequence of this limitation is that arbitrary grain-like shapes generated from an arbitrary Voronoi tesselation are difficult to mesh with hexahedral elements, which meant that grains had to be approximated with irregular boundaries. An improvement would be to create a custom-made tetrahedral element (using the UEL subroutine in Abaqus) to more accurately reproduce the grains shapes. This, however, requires a careful derivation of the coupled thermomechanical element stiffness and extensive numerical testing to validate the robustness of the new element.

From the point of view of multiscale analysis, an open issue is the homogenization of thermomechanical problems. For purely mechanical problems, the scale transition requires controlling the average value of the deformation gradient in a representative volume element. The average value of the displacement field is not required since constitutive relations do not depend on this parameter. However, the scale transition for thermomechanical problems requires controlling the average value of the deformation gradient, the temperature and the temperature gradient. This is due to the fact that constitutive relations may depend on both the temperature and the temperature gradient. The difficulty in this approach arises since commonly-used periodic boundary conditions do not allow to simultaneously control the average temperature and the average temperature gradient. The challenge is to establish an algorithm and/or special boundary conditions that would circumvent this problem.

In chapter 4, an algebraic approach, termed the generalized grain cluster method (GGCM), was developed for estimating the macroscale response of a aggregate of single-crystal grains. The purpose of this method is to provide a computationally-efficient alternative to a direct numerical simulation (DNS). It was shown that the GGCM provides results with equivalent accuracy as the DNS at a significantly lower computational cost. However, to carry out multiscale simulations on relatively large macroscopic samples (e.g., during a forming process), it is required to further improve the efficiency of the method. To this end, two approaches may be explored, namely (i) the improvement of the GGCM and (ii) the use of an model adaptation multiscale method. For the first point, it is suggested to develop an efficient line search algorithm to find an improved step size in the minimization algorithm, which would reduce the number of iterations required for convergence. For the second point, it is advisable to implement a concurrent model adaptation algorithm coupled to a hierarchical mesoscale approach to create an efficient multiscale computational environment for accurately representing the material behavior in large scale simulations. An interesting challenge in that context is to develop reliable error indicators from which a sufficiently accurate and computationally-efficient model can be chosen at various spatial locations. In particular, in regions where the deformation localizes, it is generally expected that detailed models are required whereas in regions experiencing smaller deformations a coarser model may be used.



A.1 Non-redundant periodic boundary conditions

In order to have a consistent transition between two different scales, the volume average of the deformation gradient in a given microstructural volume element should be equal to the prescribed deformation gradient $\bar{\mathbf{F}}$ from the upper scale, i.e.,

$$\langle \mathbf{F} \rangle := \frac{1}{|\Omega|} \int_{\Omega} \mathbf{F} \mathrm{d}v = \bar{\mathbf{F}},$$
 (A.1)

where $|\Omega|$ denotes the volume of the microstructural domain. Since $\overline{\mathbf{F}}$ is constant over the domain, (A.1) can be written as

$$\int_{\Omega} \nabla \left(\mathbf{u} - \left(\bar{\mathbf{F}} - \mathbf{I} \right) \mathbf{x} \right) dv = \mathbf{0}, \tag{A.2}$$

with \mathbf{u} being the displacement field, \mathbf{I} the identity tensor and \mathbf{x} a material point in the reference configuration. A straightforward application of the divergence theorem results in the following expression:

$$\int_{\partial\Omega} \mathbf{n} \otimes \left(\mathbf{u} - \left(\bar{\mathbf{F}} - \mathbf{I} \right) \mathbf{x} \right) dv = \mathbf{0}, \tag{A.3}$$

where $\partial\Omega$ is the external surface of the domain and n is the outward unit normal vector. Henceforth, it is assumed that the microstructural domain Ω is a cube of edge length h and the edges are aligned with a global basis \mathbf{e}_i , i = 1, 2, 3, as shown in Figure Fig. A.1.



Figure A.1: Labeling convention for (a) external faces and corners and (b) edges of the computational domain.

Sufficient conditions for (A.1) to hold can be inferred from (A.3) in terms of the relative displacements of parallel faces of the cube, i.e.,

$$\begin{aligned} \mathbf{u}_{F1} - \mathbf{u}_{F2} &= \mathbf{a}_1 \coloneqq \left(\bar{\mathbf{F}} - \mathbf{I}\right) h \mathbf{e}_1, \\ \mathbf{u}_{F3} - \mathbf{u}_{F4} &= \mathbf{a}_2 \coloneqq \left(\bar{\mathbf{F}} - \mathbf{I}\right) h \mathbf{e}_2, \\ \mathbf{u}_{F5} - \mathbf{u}_{F6} &= \mathbf{a}_3 \coloneqq \left(\bar{\mathbf{F}} - \mathbf{I}\right) h \mathbf{e}_3, \end{aligned}$$
(A.4)

where \mathbf{u}_{Fi} , with i = 1, ..., 6, denote the surface displacement for points on the *i*-th surface of the cube (see Figure A.1). The vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 , defined in (A.4), are assumed to be known. While equations (A.4) are sufficient for satisfying the periodicity condition on the external boundary of the domain, this system of equations contains redundant information for points on the external corners and edges of the cube, which may potentially cause problems in numerical implementations. To avoid this redundancy, one has to establish the minimum number of independent relations (corner-to-corner and edge-to-edge relations) that preserve periodicity.

For the corner points, there are twelve relations that can be obtained from (A.4), namely

with other relations between corner points obtained in a similar fashion. In (A.5), \mathbf{u}_{Ci} , with i = 1, ..., 8, denotes the displacement of the *i*-th corner point. This system of equations has a rank deficiency of five (only seven independent corner-to-corner relations can be described). A non-redundant set of relations can be established by solving (A.5)

in terms of the displacement of a given corner point. Choosing corner C1 as a reference point yields the following solution:

Observe that the value of the displacement u_{C1} of corner C1 can be chosen arbitrarily as the material response is invariant under a rigid body translation. Consequently, choosing $u_{C1} = 0$, the displacement of all corner points can be obtained from (A.6).

For the edges of the cube, equations (A.4) are used again to write twelve displacement constraints between periodic edges. The resulting system has a rank deficiency of three (only nine independent edge-to-edge relations can be described). One possible solution is to solve the system in terms of u_{E7} , u_{E8} and u_{E9} , the displacement fields of points along edges E7, E8 and E9, respectively (see Figure A.1). This yields the following set of relations for the edges of the cube:

$$\mathbf{u}_{E1} = \mathbf{u}_{E7} + \mathbf{a}_1 - \mathbf{a}_3,$$

$$\mathbf{u}_{E2} = \mathbf{u}_{E8} + \mathbf{a}_2 - \mathbf{a}_3,$$

$$\mathbf{u}_{E3} = \mathbf{u}_{E7} - \mathbf{a}_3,$$

$$\mathbf{u}_{E4} = \mathbf{u}_{E8} - \mathbf{a}_3,$$

$$\mathbf{u}_{E5} = \mathbf{u}_{E7} + \mathbf{a}_1,$$

$$\mathbf{u}_{E6} = \mathbf{u}_{E8} + \mathbf{a}_2,$$

$$\mathbf{u}_{E10} = \mathbf{u}_{E9} + \mathbf{a}_2,$$

$$\mathbf{u}_{E11} = \mathbf{u}_{E9} + \mathbf{a}_2 - \mathbf{a}_1,$$

$$\mathbf{u}_{E12} = \mathbf{u}_{E9} - \mathbf{a}_1.$$

$$(A.7)$$

In summary, a set of non-redundant periodic boundary conditions may be prescribed using Equations (A.6) to fully specify the displacements of the corner points, Equations (A.7) to constrain the displacements of points on the edges (excluding corner points) and finally Equations (A.4) to constrain the displacements of points on the external faces (excluding the edges).

APPENDIX A.

B

B.1 Trace of the curl of the composition of two tensorvalued functions

To derive the weak formulation of the compatibility equation, it is required to integrate by parts the curl of the composition of two tensor-valued functions. A useful formula for this purpose is derived in this appendix. Let $\mathbf{G} = \mathbf{G}(\mathbf{x})$ and $\mathbf{F} = \mathbf{F}(\mathbf{x})$ be two tensorvalued functions of a vector \mathbf{x} . The cartesian components of these functions are denoted as G_{ij} and F_{ij} , with i, j = 1, 2, 3. Let tr be the trace operator and $\nabla_{\mathbf{x}} \times (\cdot)$ be the curl with respect to \mathbf{x} . Consider the term tr $(\nabla_{\mathbf{x}} \times (\mathbf{GF}))$, which can be written in cartesian components as

$$\operatorname{tr}\left(\nabla_{\mathbf{x}} \times (\mathbf{GF})\right) \longrightarrow \varepsilon_{kij} \left(G_{mn} F_{nj}\right)_{i} \delta_{km}, \tag{B.1}$$

where $(\cdot)_{\cdot,i}$ denotes partial differention with respect to x_i and implicit summation is assumed on repeated indices (see also Section 4.1.3 for additional notation). This term can be expanded as

$$\varepsilon_{kij} \left(G_{mn} F_{nj} \right)_{,i} \delta_{km} = \varepsilon_{kij} \left(G_{mn,i} F_{nj} + G_{mn} F_{nj,i} \right) \delta_{km}$$

= $\varepsilon_{mij} G_{mn,i} F_{nj} + \varepsilon_{mij} G_{mn} F_{nj,i}$. (B.2)

Using the properties of the alternator (permutation) tensor, the first term on the right hand side of (B.2) can be written as

$$\varepsilon_{mij}G_{mn,i}F_{nj} = -\varepsilon_{jim}G_{nm,i}^{\mathrm{T}}F_{nj} ,$$

which can be expressed in direct notation as

$$-\varepsilon_{jim}G_{nm,i}^{\mathrm{T}}F_{nj} \longrightarrow -\left(\nabla_{\mathbf{x}}\times\mathbf{G}^{\mathrm{T}}\right)\cdot\mathbf{F}^{\mathrm{T}}.$$
(B.3)

The second term on the right hand side of (B.2) can be expressed in direct notation as

$$\varepsilon_{mij}G_{mn}F_{nj,i} \longrightarrow (\nabla_{\mathbf{x}} \times \mathbf{F}) \cdot \mathbf{G}$$
. (B.4)

Combining (B.1)-(B.4) yields the following relation

$$\operatorname{tr}\left(\nabla_{\mathbf{x}} \times (\mathbf{G}\mathbf{F})\right) = -\left(\nabla_{\mathbf{x}} \times \mathbf{G}^{\mathrm{T}}\right) \cdot \mathbf{F}^{\mathrm{T}} + (\nabla_{\mathbf{x}} \times \mathbf{F}) \cdot \mathbf{G} . \tag{B.5}$$

B.2 Averaging matrix and pseudoinverse.

The cluster's averaging operator L defined in (4.42) has the following explicit form:

	θ_1	0	0	0	0	0	0	0	0		$\theta_{N_{\rm gr}}$	0	0	0	0	0	0	0	0
	0	θ_1	0	0	0	0	0	0	0		0	$\theta_{N_{\rm gr}}$	0	0	0	0	0	0	0
	0	0	θ_1	0	0	0	0	0	0		0	0	$\theta_{N_{ m gr}}$	0	0	0	0	0	0
	0	0	0	θ_1	0	0	0	0	0		0	0	0	$ heta_{N_{ m gr}}$	0	0	0	0	0
L =	0	0	0	0	θ_1	0	0	0	0	• • •	0	0	0	0	$ heta_{N_{ m gr}}$	0	0	0	0
	0	0	0	0	0	θ_1	0	0	0	• • •	0	0	0	0	0	$ heta_{N_{ m gr}}$	0	0	0
	0	0	0	0	0	0	θ_1	0	0	• • •	0	0	0	0	0	0	$ heta_{N_{ m gr}}$	0	0
	0	0	0	0	0	0	0	θ_1	0	• • •	0	0	0	0	0	0	0	$\theta_{N_{ m gr}}$	0
	0	0	0	0	0	0	0	0	θ_1	• • •	0	0	0	0	0	0	0	0	$\theta_{N_{ m gr}}$

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The right pseudo-inverse L^+ defined in (4.53) can be expressed explicitly as

	θ_1	0	0	0	0	0	0	0	0]
	0	θ_1	0	0	0	0	0	0	0
	0	0	θ_1	0	0	0	0	0	0
	0	0	0	θ_1	0	0	0	0	0
	0	0	0	0	θ_1	0	0	0	0
	0	0	0	0	0	θ_1	0	0	0
	0	0	0	0	0	0	θ_1	0	0
	0	0	0	0	0	0	0	θ_1	0
1	0	0	0	0	0	0	0	0	θ_1
$L^+ = \frac{1}{\hat{\rho}_2}$	÷	÷	÷	÷	÷	:	÷	:	:
U	$ heta_{N_{ m gr}}$	0	0	0	0	0	0	0	0
	0	$ heta_{N_{ m gr}}$	0	0	0	0	0	0	0
	0	0	$ heta_{N_{ m gr}}$	0	0	0	0	0	0
	0	0	0	$\theta_{N_{ m gr}}$	0	0	0	0	0
	0	0	0	0	$\theta_{N_{ m gr}}$	0	0	0	0
	0	0	0	0	0	$ heta_{N_{ m gr}}$	0	0	0
	0	0	0	0	0	0	$ heta_{N_{ m gr}}$	0	0
	0	0	0	0	0	0	0	$ heta_{N_{ m gr}}$	0
	0	0	0	0	0	0	0	0	$\theta_{N_{\rm gr}}$

where $\hat{\theta}$ is given by (4.45)₂.

APPENDIX B.

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Curriculum vitae

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List of publications

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APPENDIX B. CURRICULUM VITAE