

Hierarchical multi-scale modelling of the nonlinear deformation of fibre reinforced composites by means of general anisotropic constitutive models

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To my parents Bernice and Francis Bedzra

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Summary

Composite materials are made from a combination of two or more materials. Due to their high stiffness-to-weight ratio, they are highly desirable in lightweight construction. However, the effective use of these materials depends on the ability to predict the ultimate load and residual strength of the structures for which they are employed. To achieve this, an accurate representation of the constitutive response of the composite material is required. The present dissertation seeks to address some aspects of this issue by developing and implementing several constitutive models for various composite materials.

To this end, a multi-surface constitutive model is developed for woven tungsten fibre reinforced copper matrix composite. Plastic anisotropy is modelled based on the concept of structural tensors by employing three different yield functions for three different load scenarios in the plane of the composite sheet. A finite element model of a plain weave repeating unit cell is set-up for parameter identification and validation. The applicability of the constitutive model is demonstrated by performing a simulation of drawing a thin circular plate with a hole and a cylindrical roof subjected to a line load.

A second material model, based on the multi-surface constitutive model, is developed to model the in-plane anisotropic elastoplastic behaviour of paper and paperboard. The model is calibrated from a set of simple uniaxial tension tests carried out in various directions of the material and is validated against loading in other directions. The accuracy as well as the numerical performance of the constitutive model is accessed against a non-quadratic counterpart of the model.

Furthermore, a constitutive model for the unidirectional tungsten fibre reinforced copper matrix composite is also developed. The constitutive model employs a Hill type yield function as well as multiple hardening functions to describe the anisotropic hardening behaviour of the composite. A finite element model of the composite is set-up for parameter identification and validation.

Finally, a non-associative viscoelastic-viscoplastic constitutive model for unidirectional fibre reinforced polymer composites is developed. As a case study, flax fibre reinforced epoxy matrix is considered. The model adopts an anisotropic linear viscoelastic solid expressed in terms of Boltzmann hereditary form coupled with an anisotropic viscoplastic formulation to describe the deformation behaviour of the material. The yield surface of the model is constructed based on the concept of structural tensors. The anisotropic evolution of the yield surface is described by means of multiple non-linear isotropic and kinematic hardening functions. A finite element model of the unidirectional composite is also setup for calibration and validation. The

developed constitutive model is assigned to the tows of a plain weave flax fibre/epoxy composite and the deformation behaviour of the composite is studied as well as the identification of the composite yield surface through virtual experiments.

Zusammenfassung

Verbundwerkstoffe (auch Kompositwerkstoffe oder einfach Komposite genannt) werden aus einer Kombination von zwei oder mehr Materialien hergestellt. Aufgrund ihres guten Steifigkeits-Gewichtsverhältnisses werden sie häufig im Leichtbau verwendet. Ihre Effektivität hängt jedoch entscheidend von der Fähigkeit ab, die Tragfähigkeit und Restfestigkeit der Strukturen vorherzusagen, für die sie verwendet werden. Um dies zu erreichen, ist ein genaues konstitutives Modell des Kompositwerkstoffes erforderlich. In der vorliegenden Dissertation werden einige Aspekte dieses Themas behandelt, indem mehrere konstitutive Modelle für verschiedene Verbundwerkstoffe entwickelt und implementiert werden.

Es wird ein konstitutives Modell einer mit gewebten Wolframfasern verstärkten Kupfermatrix entwickelt, das auf einem „multi-surface“ Ansatz basiert. Plastische Anisotropie wird mittels Strukturtenoren und drei verschiedenen Fließfunktionen für drei unterschiedliche Lastszenarien in der Ebene des Verbundbleches realisiert. Ein Finite-Elemente-Modell einer sich wiederholenden „plain-weave“ Einheitszelle wird für die Parameteridentifikation und Validierung aufgesetzt. Die Anwendbarkeit des Modells wird durch die Ziehsimulation einer dünnen kreisförmigen Platte mit Loch und eine Zylindrische Dach unter belastung demonstriert.

Weiterhin wird ein drittes Materialmodell entwickelt, das auf dem konstitutiven Modell mit „multi-surface“ Ansatz basiert, um das in der Ebene vorhandene anisotrope elastoplastische Verhalten von Papier und Pappe zu modellieren. Das Modell wird mittels einer Reihe von einfachen einachsigen Zugversuchen in unterschiedliche Richtungen kalibriert und durch Belastungen in andere Richtungen validiert. Die Genauigkeit und das numerische Verhalten des Materialmodells wird mit einem nicht-quadratisches Gegenstück des konstitutiven Modells verglichen.

Zudem wird ein Materialmodell für einen unidirektionalen Kompositwerkstoff entwickelt. Das Modell verwendet eine Hill-Fließfunktion als auch mehrere Verfestigungsfunktionen zur Beschreibung des anisotropen Verfestigungsverhaltens des Verbundwerkstoffes. Ein Finite-Elemente-Modell einer sich wiederholenden Einheitszelle des Komposites wird für die Parameteridentifikation und Validierung aufgesetzt.

Zum Schluss wird ein nicht-assoziatives viskoelastisch-viskoplastisches Materialmodell für unidirektional faserverstärkte Polymerverbundwerkstoffe entwickelt. Als Fallstudie wird ein flachsfaserverstärktes Epoxidharz betrachtet. Das Modell verwendet einen anisotropen linearen viskoelastischen Feststoff, der an eine anisotrope viskoplastische Formulierung gekoppelt ist, um die Verformung des Materials zu beschreiben. Die Fließfläche des Modells wird auf Basis von Strukturtenoren konstruiert. Die anisotrope Entwicklung der Fließfläche wird durch

mehrere nichtlineare isotrope und kinematische Verfestigungsfunktionen beschrieben. Es wird ein Finite-Elemente-Modell einer sich wiederholenden Einheitszelle eines unidirektionalen Kompositwerkstoffes zur Kalibrierung und Validierung generiert. Das entwickelte konstitutive Modell wird den Fäden eines Komposits bestehend aus gewebten Flachsfasern in einer Epoxidmatrix zugeordnet und das Verformungsverhalten des Verbunds sowie die Identifizierung der Verbundfließfläche durch virtuelle Experimente untersucht.

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1 | Introduction

1.1. Motivation

Composite materials are made from a combination of two or more materials. They consist mainly of continuous fibres or textile fabrics which are embedded in a matrix material. Although the inclusions could be discontinuous fibres or particles, the main focus here is on continuous fibres. Due to their high stiffness-to-weight ratio, thus cost saving ability, they are highly desirable in lightweight construction where tailorable materials are gaining more importance. The effective use of these materials however depends on their ability to predict the ultimate load and residual strength of the structures for which they are employed. To achieve this, an accurate representation of the constitutive response of the composite material is required.

Modelling such materials can be very challenging due to the fact that different length scales have to be taken into account in order to capture the intrinsic microstructure of the composite in the computations on the structure scale (part or assembly). The typical scales encountered are the micro-scale which consist of continuous fibres embedded in a matrix material, the meso-scale which entails woven tows (composed of the micro-scale composite architecture) embedded in a matrix material and the macro-scale which may either be a single ply (of unidirectional composite or woven composite) or a sequence of plies with different orientations stacked together to form a laminate. In principle, it is possible to go beyond the micro-scale to consider the atomic scale where molecular dynamics simulations can be used to determine the material parameters of the micro-scale constituent materials. However in this work, the smallest scale is restricted to the micro-scale.

Structures designed from composite materials usually have very high fibre volume ratio, which makes accounting for each fibre in a finite element (FE) analysis virtually impossible due to the high computational effort and time required. Assuming the possibility even exist to simulate the full microscopic model of the structure, the data obtained will be redundant and complicated procedures will be required to extract the desired information. A way to overcome this challenge is by employing a multi-scale modelling approach. Such an approach seeks

to design combined macroscopic-microscopic computational methods which are sufficiently accurate and lead to a reduction in computational effort as well as computational time.

The objective of this dissertation is the development and implementation of anisotropic constitutive models for the unidirectional composite material (micro-scale) as well as the textile composite material (meso-scale) using a hierarchical multi-scale modelling approach. In particular, attention is placed on the modelling of tungsten fibre/copper metal matrix composite as well as flax fibre/epoxy matrix composite. Furthermore, the in-plane anisotropic macro response of paper and paperboard is also considered. Paper is a form of composite which is made up of a network of fibres. The fibres in turn are composed of microfibrils which are arranged in a lignin/hemicellulose matrix.

1.2. State-of-the-art in composite material modelling

There are several approaches in the literature for modelling and simulating composite materials. They can be divided into two main categories: single scale modelling approaches and multi-scale modelling approaches. This section provides a brief introduction to these approaches; more details are given in subsequent chapters.

1.2.1. Single-scale methods

The single-scale approach treats the composite as a homogeneous material with properties usually determined by actual experiments. Most analytical models as well as some phenomenological models fall under this category. The main advantage of this approach is its computational efficiency. The major drawback however, is the lack of adequate information regarding the behaviour of the micro- or meso-scale structure, due to the limitations imposed by actual experiments on the loads that can be subjected to the composite material. This leads to a reduction in the capability of these models to accurately predict the response of the composite, especially when nonlinear effects are taken into account. A review of some analytical models for modelling the elastic response of woven fibre reinforced composites can be found in Hallel et al. [2013]. Also phenomenological models for the plastic response and the damage response of unidirectional fibre reinforced composites as well as woven fibre reinforced composites can be found in Vogler et al. [2013]; Vyas et al. [2011]; Chung and Ryou [2009] and Miami et al. [2007*a,b*]; Barbero and Vivo [2001], respectively.

1.2.2. Multi-scale methods

Multi-scale methods can be divided into three categories: hierarchical, synergetic and concurrent method.

The hierarchical method is a two-step process. The first step deals with the generation of a representative volume element of the micro-structure, discretization of the volume element, assignment of constituent material models to the corresponding domains, application of periodic boundary conditions in order to reduce the size of the volume element and subsection of the micro-structure to various loads in order to obtain homogenized material response. The second step deals with the construction of a phenomenological model of the composite material, based on the knowledge gained through various loads subjected to the microstructure, some of which are impossible to undertake in actual experiments. The phenomenological model then serves as the material model of the composite which is employed for computations on the next scale. The main advantage of this method is the ability to take into account the microstructure while at the same time achieving a reduction in computational effort as well as time. It is fast compared to other multi-scale modelling approaches. However, the major drawback is the fact that very advanced constitutive models are required especially on the composite scale. In some cases the material models required on the micro-scale to describe the constituent materials may also be complex. For a few publications where this approach is employed, the reader is referred to Reese [2003]; Melro et al. [2012]; Bedzra et al. [2017a]; Sodhani et al. [2017].

The synergetic approach deals with the generation of a micro-structure of the composite material. The micro-structure then serves as the material model of the composite where in every integration point, the computed strain on the structure-scale is passed to the micro-scale and the effective stress as well as the tangent is in turn passed back to the integration point. The main advantage of this method is the fact that no complex constitutive models for the composite have to be developed. Furthermore, extremely accurate results are generated by this method. The drawback however is that it is computationally expensive and time consuming as compared to the hierarchical modelling approach. For publications where the finite element method is used on both the micro-scale and the structure-scale, the reader is referred to Kohlhaas and Klinkel [2015]; Schröder [2014]; Unger [2013], for an alternative approach such as the generalized method of cells (GMC), where the method relies on the semi-analytical solution of the micro-structure, the reader is referred to Aboudi et al. [2012].

The concurrent modelling approach deals with the coupling of different domains of the structure at different scales and considering them simultaneously. By employing this method, a critical region within a structure where a phenomenon such as damage occurs can be considered at an atomistic scale whilst the rest of the structure is considered at a continuum scale. A few of

the scale bridging methods used to couple the lower scale and the upper scale are the bridging domain method (BDM) Talebi et al. [2015] and the quasi-continuum method Amelang et al. [2015]. Although this method leads to some savings in time, it is still computationally expensive. The concurrent modelling approach is mainly used to analyse coupled atomistic-continuum scale problems, however the composites considered in this dissertation are limited to scales beyond the atomistic scale.

For a detailed literature review on other multi-scale modelling approaches, the reader is referred to Kanouté et al. [2009b].

1.3. Outline of the dissertation

The dissertation is organized as follows. The second, third and fourth chapters are published journal papers and a book chapter, respectively. The last two chapters are journal papers which are yet to be published.

In Chapter 2, an elastoplastic constitutive model for woven tungsten fibre reinforced copper composite is developed. The constitutive framework is based on multi-surface plasticity and is derived in a thermodynamically consistent manner. Plastic anisotropy is modelled based on the concept of structural tensors by developing three different yield functions and parameterized consistency conditions for three different loading scenarios in the plane of the composite sheet. Additionally, the evolution equations are integrated using the unconditionally stable backward Euler method. Also the commonly used elastic predictor-plastic corrector method is employed to update the internal variables. Furthermore, to determine the parameters of the constitutive model as well as for validation, a finite element model of a plain weave repeating unit cell is set-up. Finally, the applicability of the constitutive model is demonstrated by performing a simulation of drawing a thin circular plate with a hole and a cylindrical roof subjected to a line load.

Chapter 3 discusses a constitutive model, based on the multi-surface plasticity model developed in Chapter 2, for modelling the in-plane anisotropic elastoplastic response of paper and paperboard. The constitutive model is calibrated from a set of simple uniaxial tension test in various directions of the material and is validated against loading in other directions. Additionally, the predictive capability as well as the numerical performance of the constitutive model is accessed against a non-quadratic plasticity counterpart of the model. Finally, the applicability of the constitutive model is demonstrated by performing a tensile test on a paperboard with a hole.

Chapter 4 describes the derivation of an anisotropic elastoplastic constitutive model for

unidirectional tungsten fiber reinforced copper composite. The yield surface of the composite is identified by performing virtual experiments on a finite element model of the unidirectional composite. An anisotropic elastoplastic constitutive model based on the identified yield surface, which makes use of the concept of structural tensors, is developed. This material model serves as the material model for macro computations. To ensure a good agreement between the constitutive model and the computer model of the composite during plastic evolution, multiple hardening functions are employed. The parameters of the constitutive model are identified and validated against the response of the computer model of the unidirectional composite.

Chapter 5 and 6 presents a non-associative anisotropic viscoelastic-viscoplastic constitutive model for unidirectional fibre reinforced polymer composites. As a case study, flax fibre reinforced epoxy matrix is considered. The model is formulated in an infinitesimal strain framework. The model adopts an anisotropic linear viscoelastic solid expressed in terms of Boltzmann hereditary form, which is coupled to an anisotropic viscoplastic formulation to describe the deformation of the material. The yield surface of the model is constructed based on the concept of structural tensors. The anisotropic evolution of the yield surface is described by means of multiple non-linear isotropic and kinematic hardening functions. To calibrate the constitutive model as well as to validate the model, a finite element model of a unidirectional composite representative volume element is generated. The developed constitutive model is assigned to the tows of a plain weave flax fibre/epoxy composite repeating unit cell and the deformation behaviour of the composite is studied as well as the identification of the composite yield surface.

As a conclusion, the last chapter gives a summary of the results of the dissertation including an outlook into possible future research directions.

2 | Article 1:

Meso-macro modelling of anisotropic metallic composites within the framework of multi-surface plasticity

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R. Bedzra formulated the actual concept, realized and implemented the model, and wrote the article. J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice. All authors drafted the work for intellectual content and approved the publication of the final version of the manuscript.

2.1. Abstract

This paper discusses a rate-independent elastoplastic constitutive model for fibre reinforced composite materials. The type of composite material considered here is tungsten fibre reinforced copper (W/Cu). The constitutive framework is based on multisurface plasticity and is derived in a thermodynamically consistent manner. Plastic anisotropy is modelled based on the concept of structural tensors by developing three different yield functions and parameterized consistency conditions for three different loading scenarios in the plane of the composite sheet. Additionally, the evolution equations are integrated using the unconditionally stable backward Euler method. Also the commonly used elastic predictor-plastic corrector method is employed to update the internal variables. Furthermore, to determine the parameters of the constitutive model as well as for validation, a finite element model of a plain weave repeating unit cell (RUC) is set-up. Finally, the applicability of the constitutive model is demonstrated by performing a simulation of drawing a thin circular plate with a hole and a cylindrical roof subjected to a line load.

2.2. Introduction

Composite materials are formed by a combination of two or more materials to achieve properties that are superior to those of its constituents. They consist mainly of unidirectional fibres or textile fabrics which are embedded in a matrix material. Although the inclusion could also be discontinuous fibres or particles, the main focus here is on continuous fibres. Depending on the application, there are a variety of fibre/matrix combinations. For lightweight constructions, composites made from a combination of glass fibre or carbon fibre and a thermoset or a thermoplastic matrix is employed because of their very high stiffness-to-weight ratio. Also metal matrix composites (MMCs) such as tungsten fibre reinforced composites, which is the material of interest, is being considered for use in high temperature propulsion environments due to their increased temperature capabilities and relatively low density Doychak [1992]; Sanfeliz [1993].

Modelling such a material requires the consideration of different length scales in order to capture the intrinsic microstructure of the composite material in the structure computation on the macro-level. To accomplish this, there exist several methodologies in the literature. Among them, the asymptotic homogenization method for periodic structures and the computational homogenization scheme are prominent. In the asymptotic homogenization method, physical fields such as the displacement of fibre or matrix are represented by multiple-scale asymptotic

expansions in power of a small dimensionless natural parameter which is defined as the ratio of the microscopic inhomogeneity to the macroscopic length scale of the composite. These physical fields are then substituted into a boundary value problem which describes the deformation of the composite and are integrated over a unit cell to obtain homogenized response of the composite. A detailed overview of this methodology can be found in Kalamkarov et al. [2009]. On the contrary, the computational homogenization scheme Miehe et al. [1999]; Kanouté et al. [2009a]; Geers et al. [2010] is based on the construction of a micro-scale boundary value problem that is used to determine the governing behaviour of the material at the macro-scale. If the macro-scale boundary value problem is solved simultaneously, a fully nested solution of two boundary value problem is obtained, often referred to as the FE^2 -method.

Despite the ability to assess the macroscopic influence on microscopic parameters in a rather straightforward manner for the case of the computational homogenization, these homogenization schemes are either limited due to their inability to capture complex phenomenon or are computationally costly and time consuming. An alternative approach is to develop a continuum mechanical material model on the macro-scale which takes into account the microscopic response of the individual constituents. In Reese [2003] this approach is exploited to model pneumatic membranes by constructing a computer model of the composite where the fibres and the matrix material are respectively modelled as an elastoplastic material exhibiting large deformation and an elastic rubber material which also exhibits large deformation. Based on the response of the composite, a finite strain anisotropic elastoplastic phenomenological constitutive model which makes use of the concept of structural tensors was derived on the macro-level. Recently, the same approach has been used in Stier et al. [2014] and Simon et al. [2015] for modelling layered fibre reinforced composites. This was done by considering the plies to be made up of textile reinforcements embedded in an epoxy resin. The global response of the plies were then modelled by a linearized version of the strain energy function proposed in Reese et al. [2001]. This strain energy function is also constructed on the basis of stress-strain curves generated from a computer model of the composite and it also makes use of the concept of structural tensors. In the following considerations, this homogenization approach is further exploited for the modelling of plain weave composites with tows as well as matrix that behave elastoplastically.

Anisotropic elastoplasticity has been investigated by various authors over the years, where the initial yield anisotropy is incorporated either through an empirical or phenomenological anisotropic yield surface whose coefficients are obtained from mechanical test, for pioneering works, see Ref. Hill [1948, 1979]; Barlat et al. [2005], and for more recent works, see Ref. Cazacu et al. [2006]; Plunkett et al. [2009]; Stoughton and Yoon [2008]. Another method is

to incorporate the initial yield anisotropy directly by means of crystallographic texture models Hill [1966]; Rice [1971]; Asaro [1983]. Furthermore, other authors account for the initial yield anisotropy by making use of the concept of structural tensors. These are second order tensors which are characterized by unit vectors pointing in a privileged direction of the material. The Structural tensors may be fixed Gaser and Holzapfe [2002]; Vladimirov et al. [2010]; Vogler et al. [2013] or may evolve with plastic flow Reese [2003]; Svendsen et al. [2006]; Noman et al. [2010]; Pietryga et al. [2012]. The present anisotropic yield surface falls under a phenomenological model and is constructed based on structural tensors. The difference here with respect to the crystallographic texture models is that the fiber orientations represent material directions instead of slip directions. Furthermore, the model proposed in this paper is an extension of the yield function derived in Reese [2003] for modelling pneumatic membranes in the context of large deformation but is limited to small strains.

The model is developed in three steps. The first step deals with setting up a finite element model of a repeating unit cell (RUC) of a plain weave composite. The tows are made of tungsten and the matrix of copper. It should be noted that the derived continuum material model is not restricted to this fibre/matrix combination but it is also applicable to any fibre which exhibits elastoplastic deformation. In step two, computational homogenization is performed on the plain weave RUC to obtain test data which is used to characterize the behaviour of the composite under consideration and is further used to validate the continuum phenomenological anisotropic yield function derived on the basis of this characterization.

Finally, step three deals with the incorporation of the model into a finite element formulation. This is done by integrating the constitutive model by means of the unconditionally stable backward Euler integration scheme at the Gauss point level. Furthermore, the internal variables are updated using a version of the elastic predictor/plastic corrector method for multisurface plasticity. Also, the consistent tangent operator is derived analogously to Simo et al. [1988] and Simo and Hughes [1998] but with some modification to the Jacobian matrix.

2.3. Textile model

In order to identify the yield surface of the composite as well as the material parameters of the continuum anisotropic constitutive model and for later validation of the constitutive model, virtual experiments are carried out on a finite element model of a plain weave repeating unit cell (RUC).

2.3.1. Geometry generation

A thorough description of the generation of the plain weave RUC has already been presented in Bednarczyk et al. [2015]. To enable a better understanding, the most important steps in the development process are outlined.

The idealized geometry of the plain weave RUC has a length of 3.8mm in both x-direction and y-direction and a thickness of 0.4mm in z-direction, see Figure 6.1. In idealized geometries, the tows are often assumed to be elliptic which leads to a relatively low tow-to-total-volume fraction (ca. 0.5 – 0.55) as a result of maintaining proper aspect ratios of the inter tow-matrix elements due to undulation of the tows. To overcome this problem, the cross-section of the undulating tows is varied along the length of the tows. As a result of this, a tow-to-total-volume fraction of 0.748 is achieved.

Also, since the repeating unit cell is assumed to be part of a much larger material specimen, periodic boundary conditions are applied through equation constraints in the ABAQUS/Standard software package Dessault systèmes [2014]. To accomplish this, the mesh needs to coincide on the opposite outer faces of the RUC. This is achieved readily for the tows through sweeping the mesh along the path of the tows. However, for the pure matrix region, only a free mesh generation is possible in ABAQUS. With a free mesh, the node positions can only be controlled on edges. Hence, the faces of the RUC are partitioned. Once the faces are subdivided into patches, the nodal position along the edges of the patches can be controlled. This way, a coinciding mesh is generated using the free mesh generator for the inter-tow matrix. For more details on the application of periodic boundary conditions via equation constraints in ABAQUS, see Ref. Barbero [2008].

For efficiency reasons, reduced integration eight node linear solid elements (C3D8R) are used to discretize the tow geometry. The surrounding matrix regions are discretised with linear tetrahedral elements. In total, the model is composed of 30,969 elements. A detailed representation of both the meshed tows and RUC is shown in Figure 6.1.

2.3.2. Tow and matrix material

The tows are modelled as General Electric 218CS (GE218CS) continuous tungsten wire, whereas the matrix is modelled as a cold worked oxygen free high conductivity copper (OFHC) material. Figure 3.2 shows real experimental results of uniaxial tensile test obtained from Sanfeliz [1993] for GE218CS and OFHC. In what follows, both materials are represented with a standard von Mises yield function Φ with isotropic hardening. Summarized in Table 5.2 are the equations of the constitutive model. Here, σ^D represents the deviatoric part of the Cauchy

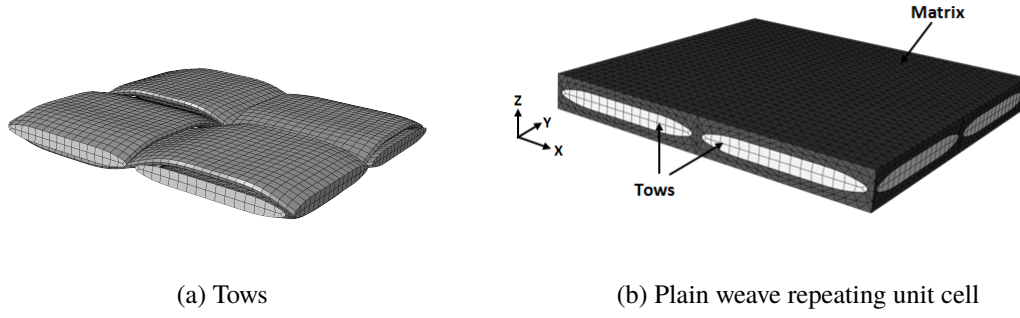


Figure 2.1.: Finite element mesh of the tows and the plain weave composite repeating unit cell

stress tensor $\boldsymbol{\sigma}$ which is related to the elastic part of the strain $\boldsymbol{\varepsilon}_e$ through the fourth-order isotropic elastic stiffness tensor $\mathbf{C}$ which is a function of the Poisson's ratio ν and the Young's modulus E , $\boldsymbol{\varepsilon}$ is the total strain which is additively decomposed into an elastic part $\boldsymbol{\varepsilon}_e$ and a plastic part $\boldsymbol{\varepsilon}_p$. The quantity $\dot{\lambda}$ represents the plastic multiplier. The expression for the isotropic hardening stress R is chosen according to Voce's exponential hardening function, where κ is the isotropic hardening variable. Also β and Q_0 together with the yield stress σ_Y are material parameters which are determined by fitting the yield function to uniaxial stress-strain data obtained from experiment. To complete the set of equations, the Kuhn Tucker (K.T) conditions for loading and unloading as well as the consistency condition are specified. Additionally, the material parameters used for the fit in Figure 3.2 for both the tow and the matrix material are given in Table 3.3.

Table 2.1.: Tow and matrix material model

Elastic law	$\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\varepsilon}_e$
Strain	$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$
Yield function	$\Phi = \sqrt{\boldsymbol{\sigma}^D \cdot \boldsymbol{\sigma}^D} - \sqrt{\frac{2}{3}}(\sigma_Y + R)$
Hardening law	$R = Q_0(1 - e^{-\beta\kappa})$
Flowrule	$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}, \quad \dot{\kappa} = \dot{\lambda} \frac{\partial \Phi}{\partial R}$
K.T conditions	$\dot{\lambda} \geq 0, \quad \Phi \leq 0, \quad \dot{\lambda}\Phi = 0$

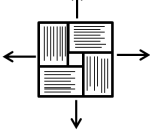
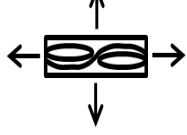
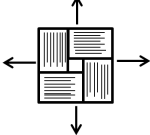
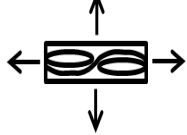
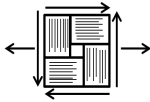
Table 2.2.: Tow and matrix material constants

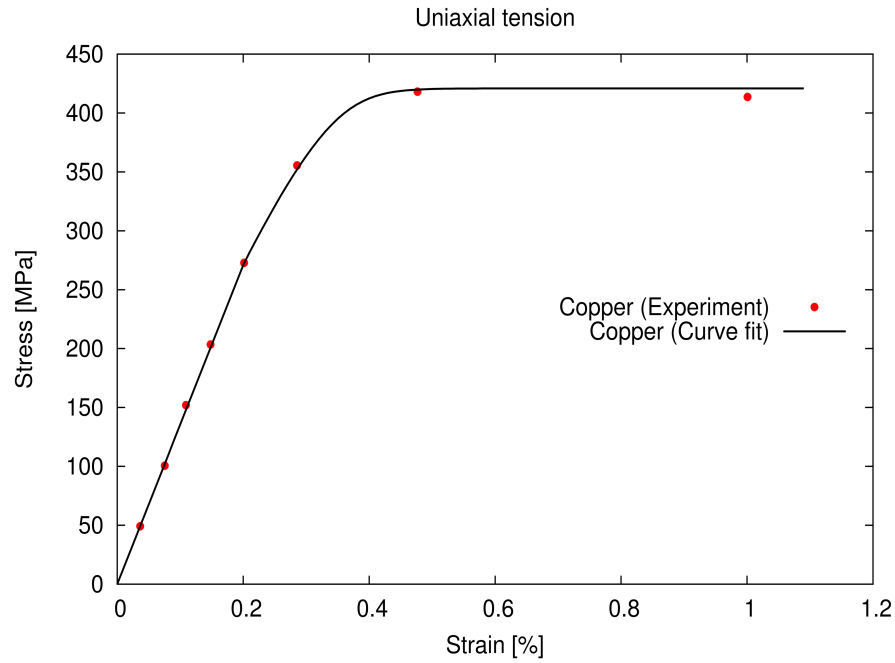
Fit	E[MPa]	ν [-]	σ_y [MPa]	Q_0 [MPa]	β [-]
Tungsten	677887	0.28	1368.87	987.20	52.60
Copper	135248	0.34	272.76	148.10	2994

2.3.3. Determination of composite yield surface

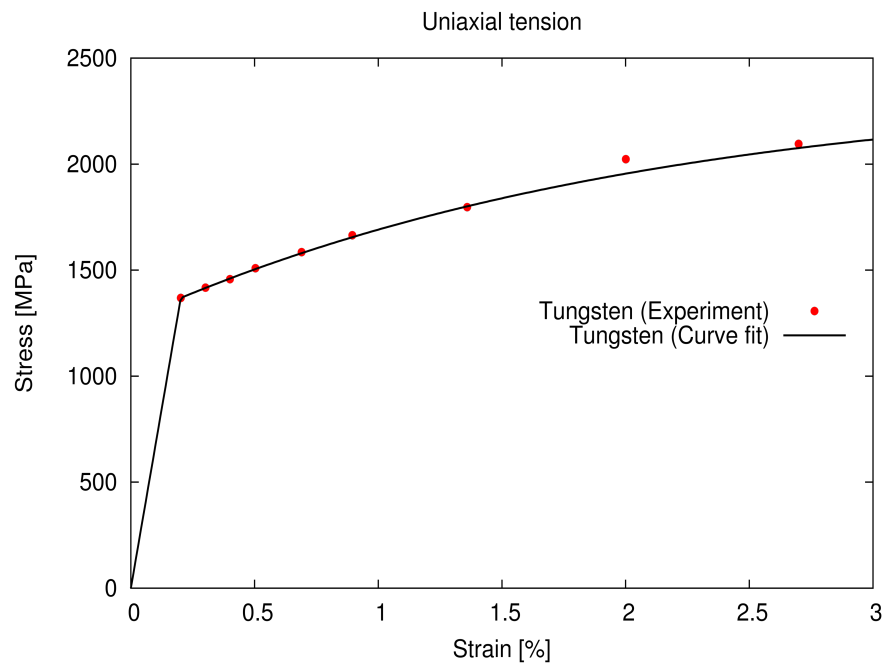
To establish the equations of the constitutive model, multi-axial experimental data is required to define the yield surface for the RUC under consideration. This is done by subjecting the RUC to various biaxial tensile tests as well as combined shear tension tests. The combinations of applied stresses, σ_{xx}/σ_{yy} , σ_{xy}/σ_{xx} and σ_{xx}/σ_{zz} , σ_{xz}/σ_{xx} subjected to the RUC to identify the yield surface in 11/22- and 11/33-principal stress space respectively are summarized in Table 2.3 with a two dimensional depiction of the RUC displayed in Figure 2.3. Additionally, it should be noted that, the RUC is further subjected to σ_{xy}/σ_{yy} and σ_{xz}/σ_{zz} combined shear tension test with the same load ratios as employed for σ_{xy}/σ_{xx} and σ_{xz}/σ_{xx} . Due to the geometry of the RUC under consideration and the fact that the tows have the same geometrical as well as material properties, it is not necessary to identify the yield surface in 22/33-principal stress space since it will be the same as the yield surface in 11/33-principal stress space. In Figure 2.4, the obtained yield surfaces in 11/22- and 11/33-principal stress space are displayed.

Table 2.3.: Biaxial and combined shear-tension experiments

σ_{xx}/σ_{yy}	σ_{xx}/σ_{zz}								
		0/1	1/8	1/4	3/8	1/2	5/8	7/8	1/1
σ_{yy}/σ_{xx}	σ_{zz}/σ_{xx}								
		0/1	1/8	1/4	3/8	1/2	5/8	7/8	
σ_{xy}/σ_{xx}	σ_{xz}/σ_{xx}								
		1/1	2/3	1/2	0/1				



(a) Copper uniaxial tension



(b) Tungsten wire uniaxial tension

Figure 2.2.: Tungsten and copper experimental result from Sanfeliz [1993] and fit for uniaxial tension

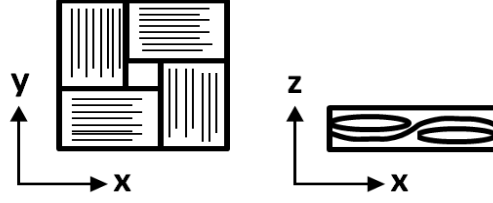


Figure 2.3.: Two dimensional depiction of the plain weave RUC

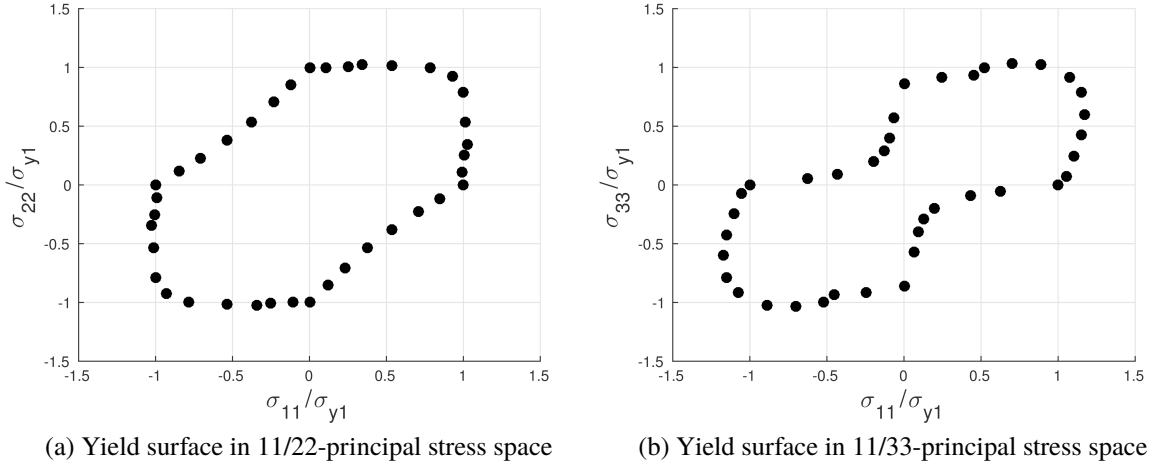


Figure 2.4.: Yield surface characterization in principal stress-space; (a) 11/22-principal stress space normalized by uniaxial yield stress in x-direction σ_{y1} ; (b) 11/33-principal stress space normalized by uniaxial yield stress in x-direction σ_{y1}

From these virtual experiments, both yield surfaces shown in Figure 2.4 are made of three subsurfaces which corresponds to the biaxial and combined shear-tension experiments summarized in Table 2.3. Furthermore, the subsurface obtained by applying σ_{xz}/σ_{xx} combined shear and tensile loading results in a non-convex yield surface which contradicts the normality condition for associative plasticity. Due to the aforementioned reason and reasons of simplicity, attention is restricted to the in-plane plastic behaviour of the plain weave RUC. The in-plane yield surface is idealized as shown in Figure 2.5, where each subsurface is described by a normal $\mathbf{V}^i$ ($i = 1, 2$) to the subsurface. Furthermore, the subsurface normal $\mathbf{V}^3$ is defined to account for shearing. As done in Xia et al. [2002], $\mathbf{V}^i$ here are second order tensors as opposed to unit vectors.

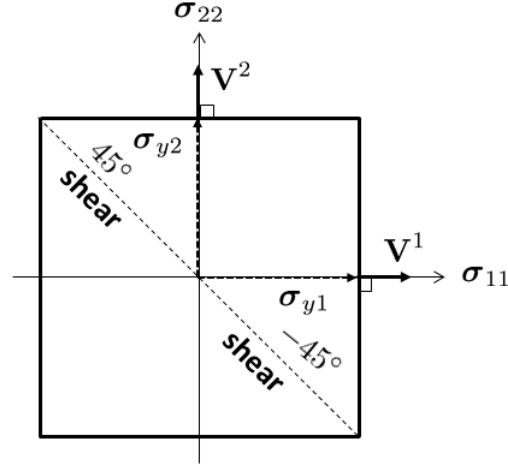


Figure 2.5.: Idealized representation of yield surface in 11/22 principal stress space

2.4. Material modelling

2.4.1. Helmholtz free energy

The Helmholtz free energy per unit undeformed volume decomposes additively into:

$$\psi = \psi_e(\boldsymbol{\varepsilon}_e, \mathbf{M}_1, \mathbf{M}_2) + \sum_{i=1}^n \psi_i^{iso}(\kappa). \quad (2.1)$$

The first part ψ_e represents the energy storage due to anisotropic elastic straining and is a function of the elastic part $\boldsymbol{\varepsilon}_e$ of the total strain tensor $\boldsymbol{\varepsilon}$ which is given by

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p. \quad (2.2)$$

Furthermore, $\mathbf{M}_1$ and $\mathbf{M}_2$ are second order tensors also called structural tensors, more details are given about them in subsequent sections. The terms $\psi_i^{iso}(\kappa)$ describe the additional amount of stored energy resulting from plasticity with isotropic hardening, where κ is the isotropic hardening variable (i.e. accumulated plastic strain) and the constant n depicts the total number of yield functions.

2.4.2. Derivation based on the Clausius-Duhem inequality

The constitutive model is derived in the context of small deformations. Also, viscous effects are not taken into account. The derivation is based on the Clausius-Duhem form of the entropy inequality for isothermal processes given as

$$-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0, \quad (2.3)$$

where $\boldsymbol{\sigma}$ is the second order Cauchy stress tensor. A dot between two second order tensors denotes their scalar product. Inserting the Helmholtz free energy (3.1) into the Clausius-Duhem inequality and differentiating with respect to time and taking (2.2) into account yields

$$-\left(\frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}} \cdot \dot{\boldsymbol{\varepsilon}} + \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}_p} \cdot \dot{\boldsymbol{\varepsilon}}_p + \sum_{i=1}^n \frac{\partial \psi_i^{iso}}{\partial \kappa} \dot{\kappa} \right) + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0. \quad (2.4)$$

By rearranging and grouping terms in (2.4), the final form of the Clausius-Duhem inequality is derived as

$$\left(\boldsymbol{\sigma} - \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}} \right) \cdot \dot{\boldsymbol{\varepsilon}} - \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}_p} \cdot \dot{\boldsymbol{\varepsilon}}_p - \sum_{i=1}^n \frac{\partial \psi_i^{iso}}{\partial \kappa} \dot{\kappa} \geq 0. \quad (2.5)$$

This inequality must be fulfilled for arbitrary thermodynamic processes, i.e. for arbitrary $\dot{\boldsymbol{\varepsilon}}$, $\dot{\boldsymbol{\varepsilon}}_p$ and $\dot{\kappa}$. This requirement leads to an expression for the Cauchy stress tensor $\boldsymbol{\sigma}$ given as

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}, \quad (2.6)$$

and the following inequality

$$\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}_p + \sum_{i=1}^n R_i \dot{\kappa} \geq 0. \quad (2.7)$$

$R_i = -\partial \psi_i^{iso} / \partial \kappa$ are stress like isotropic hardening variables. The inequality in (3.4) is sufficiently satisfied by the associative plastic flow rule for multisurface plasticity given as

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{i=1}^n \dot{\lambda}_i \frac{\partial \Phi_i}{\partial \boldsymbol{\sigma}}, \quad (2.8)$$

and the evolution equation for the multisurface plasticity counterpart of accumulated plastic strain given as

$$\dot{\kappa} = \sum_{i=1}^n \dot{\lambda}_i \frac{\partial \Phi_i}{\partial R_i}. \quad (2.9)$$

The evolution equations (3.6) and (3.7) are often referred to as Koiter's rule Koiter [1960]. The constant n represents the total number of yield functions Φ_i and their corresponding plastic multipliers $\dot{\lambda}_i$.

2.4.3. Description of plastic anisotropy

Based on the subsurface normals $\mathbf{V}^i$, three yield functions are defined as

$$\Phi_i = \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} - \sqrt{a_i}(\sigma_{yi} - R_i), \quad i = 1, 2, 3, \quad (2.10)$$

where σ_{y1} , σ_{y2} , and σ_{y3} represent the initial uniaxial yield stresses in 1- and 2-directions as well as the initial shear yield stress in 12-plane, respectively. The subsurface normals are given by

$$\mathbf{V}^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{V}^2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{V}^3 = \frac{1}{2} \begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (2.11)$$

In order to obtain the correct equivalent tensile stress for each of the three yield functions, the prefactors have to be set to $a_1 = 1$, $a_2 = 1$ and $a_3 = 2$. This can be verified by substituting the subsurface normals (2.11) into the yield functions (3.8).

In the following, the subsurface normals are rewritten making use of the concept of structural tensors as developed in Spencer [1971]; Boehler [1979] and Zhang and Rychlewski [1990]. A second-order structural tensor is defined as

$$\mathbf{M}_i = \mathbf{N}_i \otimes \mathbf{N}_i \quad i = 1, 2, 3, \quad (2.12)$$

where $\mathbf{N}_i$ are unit vectors pointing in privileged directions of the material. Additionally, these unit vectors $\mathbf{N}_i$ are orthogonal to each other, and hence the following relations hold:

$$\sum_{i=1}^3 \mathbf{M}_i = \mathbf{N}_1 \otimes \mathbf{N}_1 + \mathbf{N}_2 \otimes \mathbf{N}_2 + \mathbf{N}_3 \otimes \mathbf{N}_3 = \mathbf{1}, \quad \mathbf{N}_i \cdot \mathbf{N}_j = \delta_{ij}, \quad i, j = 1, 2, 3. \quad (2.13)$$

δ_{ij} refers to the Kronecker symbol and $\mathbf{1}$ is the second order identity tensor. Following this concept, the subsurface normals are rewritten as

$$\mathbf{V}^1 = \mathbf{M}_1, \quad \mathbf{V}^2 = \mathbf{M}_2, \quad \mathbf{V}^3 = \frac{\sqrt{2}}{2} (\mathbf{N}_1 \otimes \mathbf{N}_2 + \mathbf{N}_2 \otimes \mathbf{N}_1). \quad (2.14)$$

It is worth mentioning that, the 1- and 2-directions are associated with the fibre directions in

the later application.

2.4.4. Proof of convexity

A necessary condition to ensure maximum plastic dissipation is that the yield surface must be convex. For multisurface plasticity, the elastic domain which is defined as

$$\mathbb{E}_\sigma := \left\{ (\boldsymbol{\sigma}, \mathbf{V}^i, \sigma_{yi}, R_i) \mid \Phi_i < 0 \right\}, \quad (2.15)$$

is bounded by yield functions Φ_i intersecting possibly non-smoothly. As a result, the boundary $\partial\mathbb{E}_\sigma$ of $\mathbb{E}_\sigma$ is generally non-smooth and is given by

$$\partial\mathbb{E}_\sigma := \left\{ (\boldsymbol{\sigma}, \mathbf{V}^i, \sigma_{yi}, R_i) \mid \Phi_i = 0 \right\}. \quad (2.16)$$

To proof convexity, it has to be shown that the yield functions Φ_i are convex. A scalar valued function is said to be convex if the following definition

$$f(t\mathbf{X}_1 + (1-t)\mathbf{X}_2) \leq tf(\mathbf{X}_1) + (1-t)f(\mathbf{X}_2), \forall \mathbf{X}_1, \mathbf{X}_2 \in \mathbf{X}, \forall t \in [0, 1], \quad (2.17)$$

holds.

By taking into account (2.16), the functions for which convexity is to be proofed then reads

$$f_i(\mathbf{X}) = (\mathbf{X} \cdot \mathbf{V}^i)^2 = a_i (\sigma_{yi} - R_i)^2, \quad (2.18)$$

where $\mathbf{X}$ and $\mathbf{V}^i$ are second order tensors. Employing the definition of a convex function (2.17), (2.18) can be cast in the form

$$((t\mathbf{X}_1 + (1-t)\mathbf{X}_2) \cdot \mathbf{V}^i)^2 \leq t(\mathbf{X}_1 \cdot \mathbf{V}^i)^2 + (1-t)(\mathbf{X}_2 \cdot \mathbf{V}^i)^2. \quad (2.19)$$

The result in (2.19) can further be simplified as

$$(\mathbf{X}_1 \cdot \mathbf{V}^i - \mathbf{X}_2 \cdot \mathbf{V}^i)^2 \geq 0. \quad (2.20)$$

The final result obtained in (2.20) shows that the yield functions are convex.

2.4.5. Fulfilment of the Clausius-Duhem inequality

With this choice of yield functions, the derivatives with respect to R_i read $\partial\Phi_i/\partial R_i = \sqrt{a_i}$, which leads to the expression for $\dot{\kappa}$ as

$$\dot{\kappa} = \sum_{i=1}^3 \dot{\lambda}_i \sqrt{a_i}. \quad (2.21)$$

Also, the derivatives of the yield functions with respect to σ leads to the expression of $\dot{\epsilon}_p$ as

$$\dot{\epsilon}_p = \sum_{i=1}^3 \dot{\lambda}_i \frac{(\sigma \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\sigma \cdot \mathbf{V}^i)^2}}. \quad (2.22)$$

The set of constitutive equations is completed by the Kuhn-Tucker conditions $\dot{\lambda}_i \geq 0$, $\Phi_i \leq 0$, and $\dot{\lambda}_i \Phi_i = 0$.

To show that the above evolution equations actually fulfil the Clausius-Duhem inequality, consider the case when $\dot{\lambda}_i \geq 0$, substituting equation (2.21) and (2.22) into the Clausius-Duhem inequality (3.4) yields

$$\sigma \cdot \left(\sum_{i=1}^3 \dot{\lambda}_i \frac{(\sigma \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\sigma \cdot \mathbf{V}^i)^2}} \right) + \sum_{i=1}^3 R_i \dot{\lambda}_i \sqrt{a_i} \geq 0. \quad (2.23)$$

The result in (2.23) can be further simplified as

$$\sum_{i=1}^3 \dot{\lambda}_i \left(\sqrt{(\sigma \cdot \mathbf{V}^i)^2} + \sqrt{a_i} R_i \right) = \sum_{i=1}^3 \dot{\lambda}_i (\Phi_i + \sqrt{a_i} \sigma_{yi}) \geq 0. \quad (2.24)$$

Taking into account the Kuhn-Tucker conditions and considering the fact that $\sqrt{a_i} \sigma_{yi}$ is positive, it is obvious that the Clausius-Duhem inequality is satisfied.

The final form of the constitutive equations of the model is summarized below:

- Stress tensor

$$\sigma = \frac{\partial \psi_e}{\partial \epsilon}.$$

- Yield functions

$$\Phi_i = \sqrt{(\sigma \cdot \mathbf{V}^i)^2} - \sqrt{a_i} (\sigma_{yi} - R_i), \quad i = 1, 2, 3.$$

- Evolution equations

$$\dot{\epsilon}_p = \sum_{i=1}^3 \dot{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}, \quad \dot{\kappa} = \sum_{i=1}^3 \dot{\lambda}_i \sqrt{a_i}.$$

- Kuhn-Tucker conditions

$$\dot{\lambda}_i \geq 0, \quad \Phi_i \leq 0, \quad \dot{\lambda}_i \Phi_i = 0$$

2.4.6. Form of Helmholtz free energy functions

Till now, the relation for the stress $\boldsymbol{\sigma}$ has been derived without specifying the form of the Helmholtz free energy ψ_e , apart from the fact that it is a function of $\boldsymbol{\epsilon}_e$, $\mathbf{M}_1$, and $\mathbf{M}_2$. The strain energy function ψ_e due to elastic strain is represented by a linearized version of the strain energy function proposed for modelling bidirectional composite materials in Reese et al. [2001].

The energy terms ψ_e and ψ_{iso} are specified as

$$\begin{aligned} \psi_e(\boldsymbol{\epsilon}_e, \mathbf{M}_1, \mathbf{M}_2) &= 4K_1^{\text{iso}}(I_1)^2 + 4K_2^{\text{iso}}(I_2 + I_1) + 4K_1^{\text{ani1}}(I_4)^2 + 4K_2^{\text{ani1}}(I_5 + I_4) + 4K_1^{\text{ani2}}(I_6)^2 \\ &\quad + 4K_2^{\text{ani2}}(I_7 + I_6) + 4K^{\text{kop1}}(I_1)(I_4) + 4K^{\text{kop2}}(I_1)(I_6) + 4K^{\text{kop12}}(I_4)(I_6), \\ \psi_i^{\text{iso}} &= Q_i \left(\kappa + \frac{e^{-\beta_i \kappa} - 1}{\beta_i} \right), \quad i = 1, 2, 3, \end{aligned} \quad (2.25)$$

where I_1 and I_2 represent the first and second invariant of the elastic strain tensor. Additionally, I_4, I_5, I_6 and I_7 denote the first invariant of $\boldsymbol{\epsilon}_e \mathbf{M}_1, \boldsymbol{\epsilon}_e^2 \mathbf{M}_1, \boldsymbol{\epsilon}_e \mathbf{M}_2$, and $\boldsymbol{\epsilon}_e^2 \mathbf{M}_2$, respectively. Their full form is given by

$$\begin{aligned} I_1 &:= \text{tr} \boldsymbol{\epsilon}_e & I_2 &:= \frac{1}{2}[(\text{tr} \boldsymbol{\epsilon}_e)^2 - \text{tr}(\boldsymbol{\epsilon}_e^2)] & I_4 &:= \text{tr}(\boldsymbol{\epsilon}_e \mathbf{M}_1) & I_5 &:= \text{tr}(\boldsymbol{\epsilon}_e^2 \mathbf{M}_1) & I_6 &:= \text{tr}(\boldsymbol{\epsilon}_e \mathbf{M}_2) \\ I_7 &:= \text{tr}(\boldsymbol{\epsilon}_e^2 \mathbf{M}_2). \end{aligned} \quad (2.26)$$

The coefficients $K_1^{\text{iso}}, K_2^{\text{iso}}, K_1^{\text{ani1}}, K_2^{\text{ani1}}, K_1^{\text{ani2}}, K_2^{\text{ani2}}, K^{\text{kop1}}, K^{\text{kop2}}$ and K^{kop12} are related to the Young's moduli E_1, E_2, E_3 , the Poisson's ratios $\nu_{12}, \nu_{13}, \nu_{23}$, and the shear moduli G_{12}, G_{13}, G_{23} . For the relation between the coefficients and the engineering constants, see B.2.

The corresponding constitutive relation for the Cauchy stress σ is given as

$$\begin{aligned}\sigma &= \mathcal{C}_{\text{ani}} [\epsilon_e], \\ \mathcal{C}_{\text{ani}} &= \frac{\partial^2 \psi_e}{\partial \epsilon_e^2} = (8K_1^{\text{iso}} + 4K_2^{\text{iso}}) \mathbf{1} \otimes \mathbf{1} - 4K_2^{\text{iso}} \mathcal{I} + 8K_1^{\text{ani1}} (\mathbf{M}_1 \otimes \mathbf{M}_1) + 4K_2^{\text{ani1}} \mathcal{E}^1 \\ &\quad + 8K_1^{\text{ani2}} (\mathbf{M}_2 \otimes \mathbf{M}_2) + 4K_2^{\text{ani2}} \mathcal{E}^2 + 4K^{\text{kop1}} (\mathbf{1} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \mathbf{1}) \\ &\quad + 4K^{\text{kop2}} (\mathbf{1} \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{1}) + 4K^{\text{kop12}} (\mathbf{M}_1 \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{M}_1),\end{aligned}\quad (2.27)$$

where $\mathcal{I}$ represents the fourth-order identity tensor which in index notation reads

$$\mathcal{I}_{ijkl} = \delta_{ik} \delta_{jl}. \quad (2.28)$$

Furthermore, the fourth-order tensors $\mathcal{E}^1$ and $\mathcal{E}^2$ are given by

$$\mathcal{E}_{ijkl}^\alpha = \frac{1}{2} (M_{ik}^\alpha \delta_{jl} + M_{jl}^\alpha \delta_{ik} + M_{il}^\alpha \delta_{jk} + M_{jk}^\alpha \delta_{il}), \quad \alpha = 1, 2. \quad (2.29)$$

Also, the isotropic hardening stresses R_i are given by:

$$R_i = -\frac{\partial \psi_i^{\text{iso}}}{\partial \kappa} = -Q_i (1 - e^{-\beta_i \kappa}). \quad (2.30)$$

The form of R_i corresponds to Voce's exponential hardening function as given in Chaboche [2008]. Q_i and β_i are material parameters used to describe nonlinear isotropic hardening. In total, the material model has 18 material parameters which are summarized in Table 3.1.

2.5. Numerical aspects

2.5.1. Integration of the evolution equations

The evolution equations are discretized in time by means of the backward Euler integration scheme at the Gauss point level. In what follows, all variables without subscripts are assumed to be evaluated at time t_{n+1} . The final form of the discretized plastic evolution equation and

Table 2.4.: Material parameters

E_1	Young's modulus in 1- direction
E_2	Young's modulus in 2- direction
E_3	Young's modulus in 3- direction
ν_{12}	Poisson's ratio between 1 and 2- direction
ν_{13}	Poisson's ratio between 1 and 3- direction
ν_{32}	Poisson's ratio between 3 and 2- direction
G_{12}	Shear modulus in 12-plane
G_{13}	Shear modulus in 13-plane
G_{23}	Shear modulus in 23-plane
$\sigma_{yi} (i = 1, 2, 3)$	Initial yield stress of $\Phi_i (i = 1, 2, 3)$
$\beta_i (i = 1, 2, 3)$	Rate of change of elastic domain
$Q_i (i = 1, 2, 3)$	Maximum change in size of elastic domain

the yield functions is summarized below in a residuum format as ($\bar{\lambda}_i := \dot{\lambda}_i \Delta t$):

$$\begin{aligned} \mathbf{r}(\boldsymbol{\varepsilon}^p, \bar{\lambda}_i) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \left(\sum_{i \in \mathcal{J}_{act}} \bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \right) = \mathbf{0}, \\ r_i &= \Phi_i = 0. \end{aligned} \tag{2.31}$$

$\mathcal{J}_{act}$ is a set which contains active yield functions, i.e. $\Phi_i = 0$ ($i = 1, 2, 3$). Depending on $\mathcal{J}_{act}$, one may have to solve a system of 9 nonlinear scalar equations iteratively by means of Newton's method at each Gauss point. In order to employ Newton's method, the consistent linearization of C.8 with respect to $\boldsymbol{\varepsilon}_p$, $\bar{\lambda}_1$, $\bar{\lambda}_2$ and $\bar{\lambda}_3$ has to be carried out. For the linearization of the constitutive equations, the reader is referred to D.1.

The scalar evolution equation for isotropic hardening 3.7 is also discretized by means of the backward Euler integration method:

$$\kappa = \kappa_n + \sum_{i=1}^3 \bar{\lambda}_i \sqrt{a_i}. \tag{2.32}$$

The accumulated plastic strain κ is computed at the end of each local Newton iteration via the converged value of the plastic multipliers $\bar{\lambda}_i$, therefore κ only needs to be updated when the local Newton iteration has converged.

2.5.2. Stress update algorithm

Application of Newton's method to equation (C.8) is not straight forward, since the yield functions are more than one. To accomplish this, an elastic predictor/plastic corrector algorithm for multisurface plasticity based on Simo and Hughes [1998]; Simo et al. [1988]; Reese [2003]; Gaser and Holzapfe [2002] is derived. Additionally, the following eight cases have to be distinguished:

1. $\Phi_1 < 0, \Phi_2 < 0, \Phi_3 < 0$: no plastification;
2. $\Phi_1 = 0, \Phi_2 < 0, \Phi_3 < 0$: plastification in Φ_1 ;
3. $\Phi_1 < 0, \Phi_2 = 0, \Phi_3 < 0$: plastification in Φ_2 ;
4. $\Phi_1 < 0, \Phi_2 < 0, \Phi_3 = 0$: plastification in Φ_3 ;
5. $\Phi_1 = 0, \Phi_2 = 0, \Phi_3 < 0$: plastification in Φ_1 and Φ_2 ;
6. $\Phi_1 = 0, \Phi_2 < 0, \Phi_3 = 0$: plastification in Φ_1 and Φ_3 ;
7. $\Phi_1 < 0, \Phi_2 = 0, \Phi_3 = 0$: plastification in Φ_2 and Φ_3 ;
8. $\Phi_1 = 0, \Phi_2 = 0, \Phi_3 = 0$: plastification in Φ_1, Φ_2 and Φ_3 .

At the beginning of the iteration, if the trial stress σ_{trial} results in $\Phi_i^{\text{trial}} \leq 0$ ($i = 1, 2, 3$), the step is an elastic step and this results in case 1. On the contrary, if this condition is violated, one proceeds into the Newton loops for the cases 2 – 8 which involves the iterative solution of the active set. As already mentioned, the active set contains the yield functions which violate this condition. For an active set which contains more than one yield function, e.g. case 5, it is possible for either $\Delta\bar{\lambda}_1$ or $\Delta\bar{\lambda}_2$ to be negative during the iteration. Should $\Delta\bar{\lambda}_1$ be negative, the yield function Φ_1 is dropped from the active set and this results in case 3 ($\Phi_2 = 0$). The new active set is solved iteratively till the Newton method converges. During the iteration, the variables ϵ^p and $\bar{\lambda}_i$ have to be updated.

For the calculation of the tangential stiffness matrix in a finite element computation, the derivation of the consistent tangent operator is required. The consistent tangent operator $\mathcal{C}_{\text{cons}}$ represents a relation between $\Delta\sigma$ and $\Delta\epsilon$. For more details on this tensor, see A.2.

2.6. Results and discussions

In this section, the constitutive model is characterized and its ability to predict the response of the plain weave RUC is investigated. Additionally, finite element analysis of the drawing of a circular plate with a hole as well as a cylindrical roof under line load is presented to validate the finite element implementation. All finite element simulations are performed by means of the ABAQUS/Standard software package Dessault syst mes [2014], where the material model has been implemented as a user material subroutine UMAT.

2.6.1. Parameter identification

In order to identify the parameters of the constitutive model, four virtual experiments are performed on the RUC under investigation. The first two load cases are uniaxial tension in 1- and 3-directions, followed by shear loading in 12- and 23-plane. Due to the fact that the tows in 1- and 2-directions both have the same geometry as well as material properties, symmetry conditions can be applied. Hence, it is not required to further perform virtual experiments for uniaxial tension in 2-direction as well as shear in 13-plane. Based on the obtained stress-strain response, the elasticity constants $E_1 = E_2$, E_3 , G_{12} , $G_{13} = G_{23}$, $\nu_{12} = \nu_{21}$, $\nu_{13} = \nu_{23}$, and $\nu_{31} = \nu_{32}$ are identified. Also, the uniaxial yield stresses σ_{y1} , σ_{y2} in 1- and 2-direction, as well as the shear yield stress σ_{y3} in 12-plane are identified.

The constants of the three exponential hardening functions are identified by manually fitting the functions to the flow curves obtained from the virtual experiments. The constants Q_1 , β_1 are identified from the fit to the flow curve obtained from uniaxial tension in 1-direction. For the same reasons as mentioned earlier, the constants Q_2 , β_2 are equal to Q_1 , β_1 . Furthermore, the constants Q_3 and β_3 are identified from the fit to the flow curve obtained from shear loading in 12-plane. Finally to confirm the fit, simulations are conducted using the identified material constants and are compared to the stress-strain curves obtained from the virtual experiments conducted on the RUC. The plot of the fits are shown in Figure 3.3 and the constants are given in Tables 2.5 and 2.6. From the results obtained, the capability of the constitutive model to fit the stress-strain response generated from the plain weave RUC is demonstrated.

2.6.2. Validation of the constitutive model

To check the ability of the constitutive model to accurately describe the response of the RUC, an in-plane virtual biaxial tensile test is carried out on the RUC as well as loading in the direction 30° off-axis to 1-direction. The constitutive model is subjected to similar load conditions and

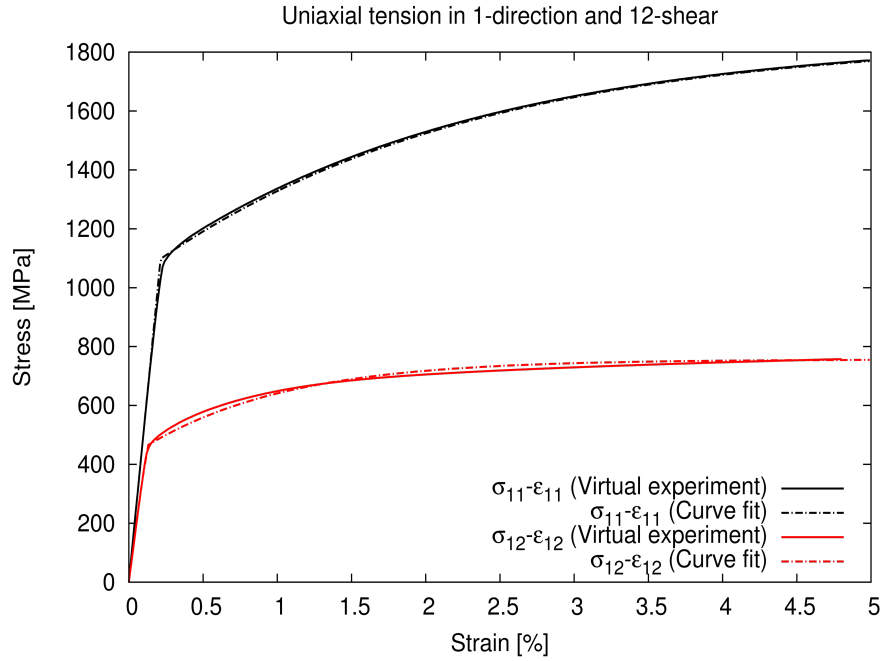


Figure 2.6.: A fit of the constitutive model to the RUC response

Table 2.5.: Elasticity constants

Youngs modulus [MPa]		Shear modulus [MPa]		Poisson's ratio [-]	
E_1	513,665	G_{12}	193,084	ν_{12}	0.275
E_2	513,665	G_{13}	142,084	ν_{13}	0.298
E_3	414,945	G_{23}	142,084	ν_{23}	0.240

Table 2.6.: Plasticity constants

	σ_{yi} [MPa]	Q_i [MPa]	β_i [-]
1-direction	1,097.71	745.00	49.86
2-direction	1,097.71	745.00	49.86
12-shear	463.13	293.00	56.00

the obtained results are compared. A plot showing the comparison between the stress-strain curves obtained from both models is shown in Figure 3.4.

From the plot, the stress-strain curve predicted by the constitutive model is in good agreement with the corresponding stress-strain curve predicted from the virtual experiment carried out on

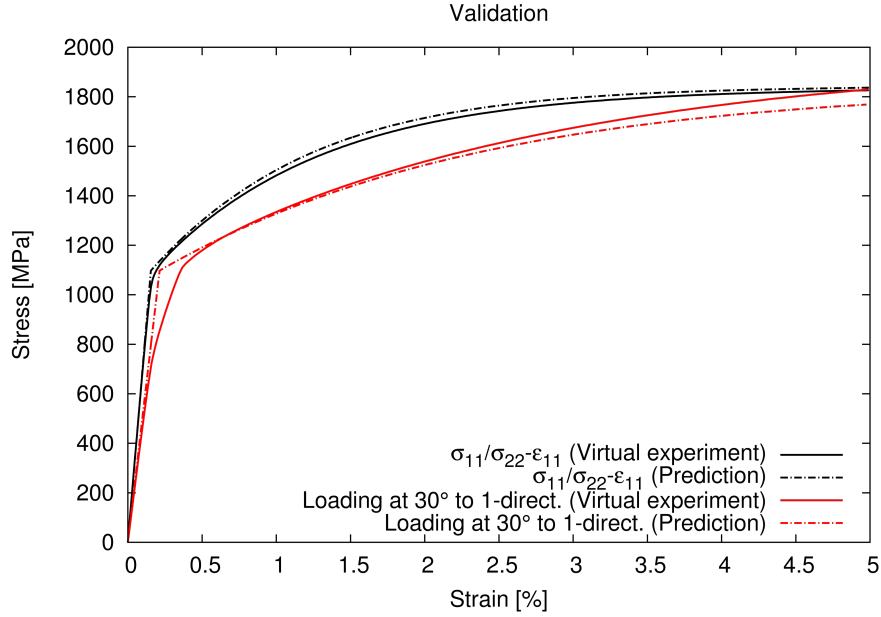


Figure 2.7.: Comparison between homogenized results from the RUC and the macro-model

the plain weave RUC, showing the ability of the constitutive model to capture other in-plane stress-strain response of the RUC.

2.6.3. Drawing of a thin circular plate

This example is concerned with drawing of a thin circular plate with a hole subjected to a radial load, see ref. Sansour et al. [2008] and Vladimirov et al. [2010]. It is a benchmark problem for the analysis of anisotropic elastoplastic response and it is based on a similar numerical problem as considered in Papadopoulos and Li [2001] and Miehe et al. [2002].

The initial geometry of the circular plate as discretized is shown in Figure 3.6. The plate is 10mm thick and has an outer and inner radius of 400mm and 200mm, respectively. The nodes at the inner radius of the plate are subjected to a pressure load of $q = 10,000$ MPa acting towards the centre of the plate. The simulation is load controlled. The lower and upper parts of the blank are simply supported in the vertical directions. This is to enable only planar deformation. Due to the geometrical and material symmetry, only a quarter of the structure is discretised and considered in the finite element analysis. It is meshed by 100 (radius $\times$ circumference $\times$ thickness = $10 \times 10 \times 1$) C3D8R reduced integration solid elements.

The material parameters determined from the fit are employed in the computation. Three different cases are considered. The first case is concerned with plastic isotropy. This is realized by employing a von Mises yield function with a Voce-type hardening function and taking into

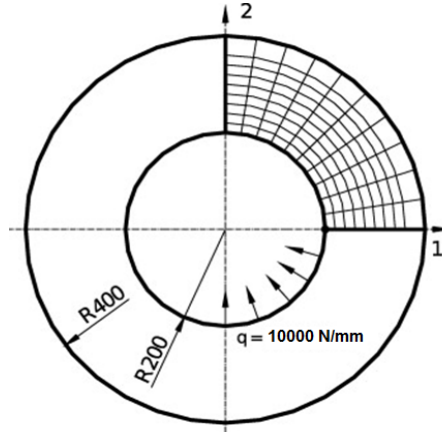


Figure 2.8.: Drawing of a circular plate: initial geometry and discretization, from Sansour et al. [2008]

account the following material parameters, initial yield stress $\sigma_y = 1097.71$ MPa, and the constants of the hardening function $Q = 745$ MPa and $\beta = 49.86$. In the second case it is assumed that the normal yield stresses dominate and the shear yield stress is twice as large as the isotropic case. This is obtained by choosing $\sigma_{y3} = 1097.71$ MPa. Also, the structure tensors $\mathbf{M}_i$ ($i = 1, 2$) are represented by the unit vectors $\mathbf{N}_1 = (1, 0, 0)^T$ and $\mathbf{N}_2 = (0, 1, 0)^T$, respectively, in a Cartesian reference frame, i.e. they form a $0^\circ/90^\circ$ ‘texture’. The last case is characterized by dominating shear yield stress which is achieved by again choosing $\sigma_{y3} = 1097.71$ MPa and the unit vectors $\mathbf{N}_1 = (1/\sqrt{2}, -1/\sqrt{2}, 0)^T$ and $\mathbf{N}_2 = (1/\sqrt{2}, 1/\sqrt{2}, 0)^T$ respectively in a Cartesian reference frame, i.e. they form a $-45^\circ/45^\circ$ ‘texture’.

Figure 3.7 shows the deformed configurations and the distribution of accumulated plastic strain. As expected, in the isotropic case, the plate retains its circular shape and the distribution of accumulated plastic strain is axisymmetric. In the second case, the plastic strains are mainly concentrated along the directions of the material 1- and 2-axes. However, there is some amount of yielding in the shear direction which results in some amount of plastic strain distribution along $-45^\circ/45^\circ$ orientation. In the third case, the concentration occurs along a direction oriented at an angle of $-45^\circ/45^\circ$. In both anisotropic cases, the outer and inner edges of the blank have lost their initial circular shape. This is in agreement with the result shown in Vladimirov et al. [2010].

2.6.4. Cylindrical roof under line load

The second example deals with the deformation behaviour of a cylindrical roof under line load, see ref. Sansour et al. [2008]. The initial geometry as well as its dimensions is shown in

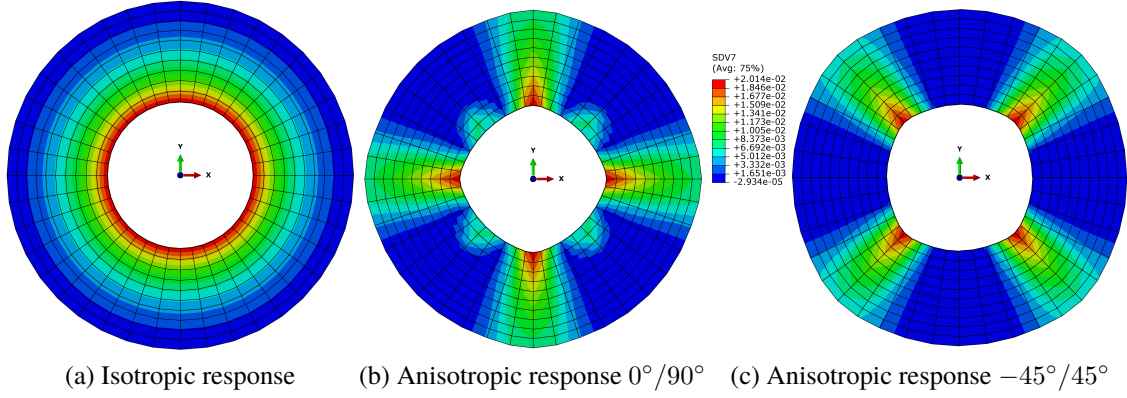


Figure 2.9.: Accumulated plastic strain

Figure 3.9. The cylinder is supported by rigid diaphragms along its curved boundaries. This implies displacement along the boundary in all three directions as well as rotation in z-x plane to be zero. It is meshed by 1296 (radius x depth x thickness = $36 \times 36 \times 1$) C3D8R reduced integration solid elements. The orientation of the material axes is chosen in such a way that for the computation defined by the angle 0° , the privileged directions of the material coincides with circumferential, axial and radial direction of the cylinder. In succeeding computations, the privileged directions are rotated at an angle 30° , 45° and 60° with respect to the previously mentioned initial position.

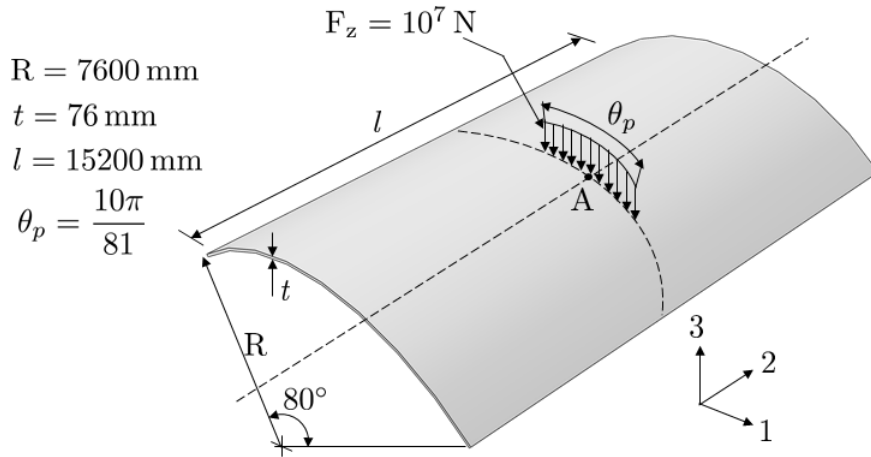


Figure 2.10.: Cylindrical roof under line load: initial geometry

The influence of the material directions on the response of the cylindrical roof is considered by comparing the force-displacement curve of the point A for the rotated principal axis. Figures 3.10, 2.12, and 2.13 show the force-displacement curves for point A, the Mises stress

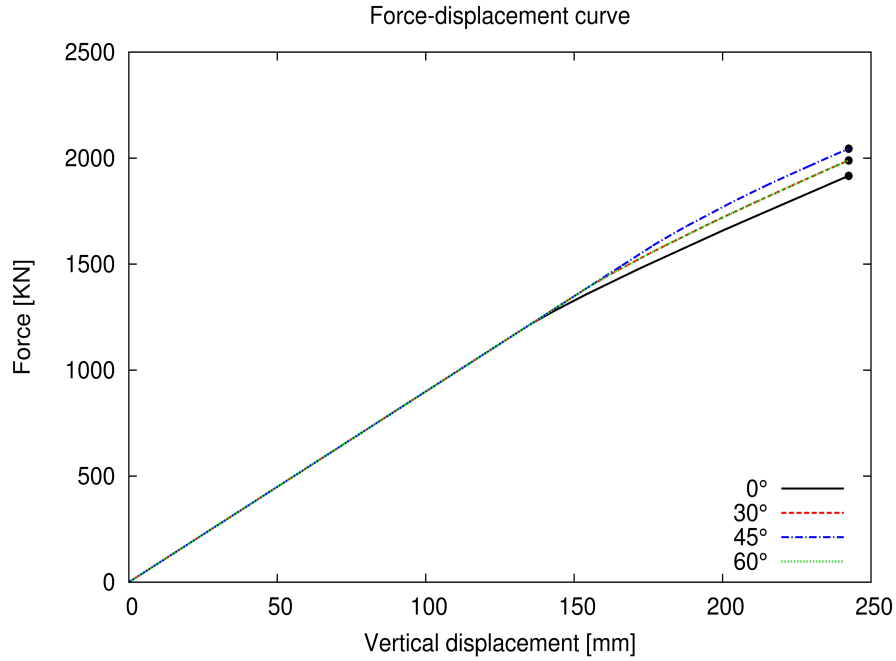


Figure 2.11.: Cylindrical roof: force-displacement curves for point A

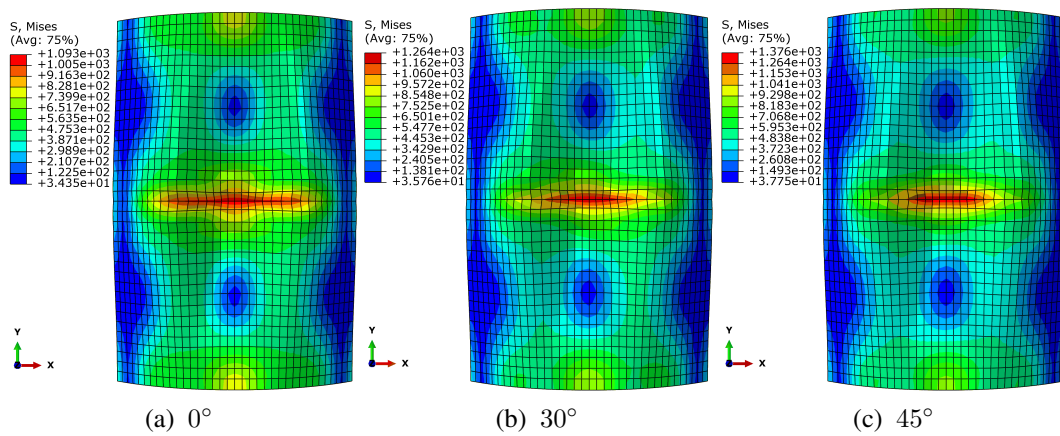


Figure 2.12.: Mises stress distribution for 0°, 30° and 45° counter-clockwise rotation of the privilege directions for the points marked on the force-displacement curves.

distribution, and the accumulated plastic strain distribution on the deformation profile of the cylindrical roof, respectively. As evident, the influence of the material direction on the deformation profile is observed. Furthermore, the force-displacement curves for 30° and 60° coincide. This is to be expected due to the shape of the yield surface, see Figure 2.5.

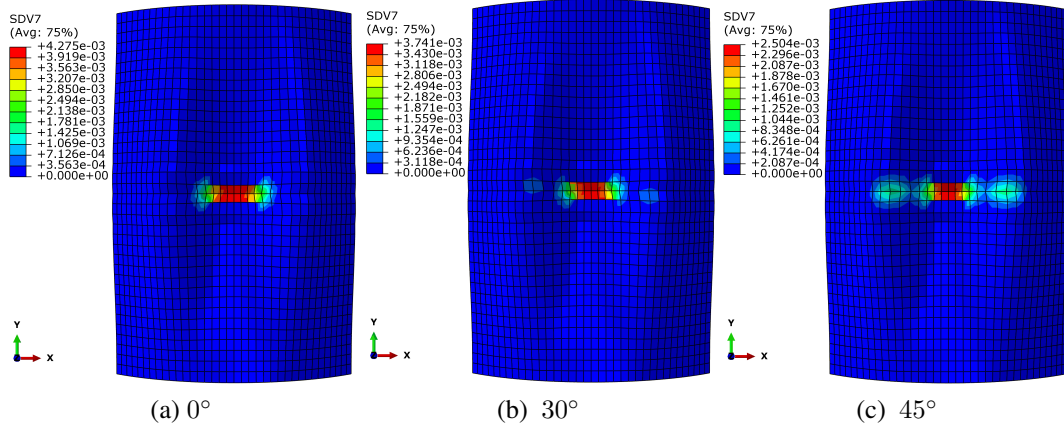


Figure 2.13.: Accumulated plastic strain distribution for 0° , 30° and 45° counterclockwise rotation of the privileged directions for the points marked on the force-displacement curves.

2.7. Conclusion and Outlook

The objective of this paper was to model anisotropic elastoplastic response of textile reinforced composite materials. In order to achieve this, a finite element model of a repeating unit cell of a plain weave composite was set up. Next, various biaxial tensile tests were carried out on the composite to determine the yield surface in principal stress space. To model the elastic response of the composite, an anisotropic strain energy function was adopted. The initial anisotropic yield behaviour of the composite was modelled by an initial yield surface constructed from subsurfaces which are defined by structural tensors pointing in privileged directions of the material. The strength of each of the yield surface was taken to harden with respect to the equivalent plastic strain, thus providing anisotropic strain hardening of the yield surface. The material parameters of the model were obtained by fitting the derived constitutive model to uniaxial stress-strain as well as shear stress-strain data generated from the finite element model of the composite. With the fitted parameters, the model was shown to be predictive of other in-plane stress-strain response of the composite material.

The integration of the evolution equations was efficiently achieved via a backward Euler scheme applied in the framework of a return-mapping algorithm. Finally, the numerical investigation of drawing a thin circular plate with a hole subjected to radial load and a cylindrical roof subjected to a line load was used to validate the finite element implementation of the constitutive model. From the obtained simulation results, it was shown that the fibre orientations played an important role in the deformation process.

It is aimed to further develop the constitutive model to take into account lateral contraction

during plastic flow which is not yet accounted for. Furthermore, the out of plane yield surface can be simplified in such a way that the non-convex subsurface is idealized as a convex subsurface.

3 | Article 2:

A comparative study of a multi-surface and a non-quadratic plasticity model with application to the in-plane anisotropic elastoplastic modelling of paper and paperboard

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Disclosure of the individual authors’ contributions to the article:

R. Bedzra formulated the actual concept, realized and implemented the model, and wrote the article. Y. Li conducted the experiments and post processed the experimental results and also came up with the example problem regarding uniaxial tension of paperboard with a hole. J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice. All authors drafted the work for intellectual content and approved the publication of the final version of the manuscript.

3.1. Abstract

In this paper, a three dimensional anisotropic multi-surface model for the in-plane elastoplastic deformation of paper and paperboard is developed. The model is based on the concept of structural tensors. It employs three different yield functions and parameterized consistency conditions for three different loading scenarios. The evolution of the yield surface with plastic strain is described by multiple hardening variables. Furthermore, the evolution equations are integrated using the unconditionally stable backward Euler method. Also, the internal variables are updated using a particular form of the elastic predictor/plastic corrector algorithm. The constitutive model is calibrated from a set of simple uniaxial tension test in various directions of the material and is validated against loading in other directions. Additionally, the predictive capability as well as the numerical performance of the constitutive model is accessed against an existing non-quadratic plasticity model. Finally, the applicability of the constitutive model is demonstrated by performing a tensile test on a paperboard with a hole

3.2. Introduction

Paper is a material formed from pressing together moist fibres of cellulose pulp derived from wood and drying them to form a sheet of pulp fibres. Depending on the application, it could be composed of only one sheet of pulp fibres or a layered sheet of pulp fibres bonded by starch or an adhesive material. Paper products are used in a wide range of applications, including writing, printing, and a number of industrial and construction processes. During the production of paper, fibres are primarily oriented in the plane of the sheet. The preferential fibre orientation results in a highly anisotropic mechanical behaviour, including anisotropic elasticity, initial yielding, strain hardening and tensile failure strength.

In order to take into account the anisotropic mechanical behaviour of paper, the elastoplastic deformation of the fibre network on the macroscopic length scale is described by means of phenomenological anisotropic material models. The fundamental framework for the phenomenological modelling of cellulose based materials was proposed by Xia et al. [2002]. In this work, the anisotropic elastoplastic behaviour of the material was described by a non-quadratic yield function which was constructed on the basis of a set of planes in stress-space. Furthermore to describe plastic evolution, the authors employed multiple hardening functions. Mäkelä and Östlund [2003] also proposed a model, based on the non-quadratic yield function proposed by Karafillis and Boyce [1993], which employs the concept of an isotropic plasticity equivalent material. In recent times, a lot of modification have been made to the model

proposed by Xia et al. [2002]. Borgqvist et al. [2014] modified the yield function to take into account the distortional hardening of the yield surface during plastic evolution. Furthermore, Tjahjanto et al. [2015] modified the yield function to take into account the stationary and the transient behaviour of the material in both the in-plane and out-of-plane deformation modes coupled with a kinematic hardening term to ensure a good prediction during cyclic loading. Li et al. [2016] also simplified the model by employing a single hardening function and a back-stress component to describe the in-plane anisotropic elastoplastic behaviour of the material. Most of the works mentioned thus far, apart from Tjahjanto et al. [2015], focus on the in-plane response of the material. Other works dealing with the out-of-plane elastoplastic deformation behaviour of paper can be found in Stenberg [2003], Nygård [2009], and Li et al. [2018]. In these works, it is assumed that the in-plane and out-of-plane stress components are only allowed to independently drive the in-plane and out-of-plane inelastic deformation, respectively. Also, some authors describe the response of the paper by continuum damage models, see Isaksson et al. [2006], Zechner et al. [2013], and Tryding et al. [2017]. A major drawback of the non-quadratic modelling approach is a slow rate of convergence as the edges of the yield surface becomes sharper. A possibility to overcome this problem is to describe the in-plane anisotropic behaviour of the material by means of a multi-surface plasticity model. One of the few models which employs a multi-surface approach to describe the in-plane anisotropic elastoplastic behaviour of paper material, which was used in the simulation of the deep drawing of paper, was proposed by Wallmeier et al. [2015].

Multi-surface plasticity is mostly prevalent in the context of crystal plasticity, where multiple yield functions are employed to model the onset of yielding on crystallographic slip planes. For details on the constitutive framework for crystal plasticity, refer to the classical works of Mandel [1972], Hill [1966], Rice [1971], and Asaro [1983]. For the computational aspects, see Cuitino and Ortiz [1992], Anand and Kothari [1996]. However, this modelling approach is seldomly used for describing the yield surface of other materials. In Bedzra et al. [2017a], a multi-surface plasticity model is developed, based on the concept of structural tensors, for modelling the anisotropic elastoplastic response of continuous tungsten fibre reinforced copper matrix composite. The aim of this contribution is to develop a multi-surface plasticity model for the in-plane elastoplastic response of paper and paperboard based on the aforementioned model and to compare it to the non-quadratic constitutive model proposed by Xia *et al.* Xia et al. [2002].

The paper begins by describing the constitutive framework of the multi-surface plasticity model. For completeness, the non-quadratic model is also described using the argument of thermodynamic consistency. Additionally, the integration of the evolution equations of both

constitutive models by means of the unconditionally stable backward Euler integration scheme including the linearization and the derivation of the consistent tangent operator is described. Finally, both models are fitted to experimental results and are compared to off-axis stress-strain responses as well as strain fields obtained from digital image correlation (DIC) experiments performed on a paperboard with a hole under uniform tension.

3.3. Multi-surface plasticity model

A thorough description of the constitutive framework of the multi-surface plasticity model has already been presented in Bedzra et al. [2017a]. In the following, only the important aspects of the constitutive model are discussed.

3.3.1. Derivation based on the Clausius-Duhem inequality

The Helmholtz free energy per unit undeformed volume is defined as

$$\psi = \psi_e(\boldsymbol{\varepsilon}_e, \mathbf{M}_1, \mathbf{M}_2) + \sum_{i=1}^n \psi_{iso}^i(\kappa), \quad (3.1)$$

where ψ_e represents the energy storage due to anisotropic elastic straining and $\boldsymbol{\varepsilon}_e$ is the elastic part of the total strain tensor $\boldsymbol{\varepsilon}$ which is defined as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p. \quad (3.2)$$

$\mathbf{M}_i = \mathbf{n}_i \otimes \mathbf{n}_i$ ($i = 1, 2, 3$) are second order tensors referred to as structural tensors and $\mathbf{n}_i$ are unit vectors pointing in designated directions of the material. Furthermore, the unit vectors $\mathbf{n}_i$ are orthogonal to each other. For more details on the theory of structural tensors, see Spencer [1971], Boehler [1979], and Zhang and Rychlewski [1990]. The terms $\psi_{iso}^i(\kappa)$ describe the additional amount of energy storage due to plasticity with isotropic hardening, where κ is the isotropic hardening variable (i.e. accumulated plastic strain) and the constant n represents the number of yield functions.

Substituting the Helmholtz free energy function (3.1) into the Clausius-Duhem form of the second law of thermodynamics, $-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0$, leads to a relation for the Cauchy stress tensor

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}, \quad (3.3)$$

and the following inequality

$$\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\epsilon}}_p + \sum_{i=1}^n R_i \dot{\kappa} \geq 0. \quad (3.4)$$

The stress-like isotropic hardening variables R_i is defined as:

$$R_i = -\frac{\partial \psi_{iso}^i}{\partial \kappa}. \quad (3.5)$$

The inequality in equation (3.4) is sufficiently satisfied by the associative plastic flow rule for multi-surface plasticity given as

$$\dot{\boldsymbol{\epsilon}}_p = \sum_{i=1}^n \dot{\lambda}_i \frac{\partial \Phi_i}{\partial \boldsymbol{\sigma}}, \quad (3.6)$$

and the evolution equation for the accumulated plastic strain

$$\dot{\kappa} = \sum_{i=1}^n \dot{\lambda}_i \frac{\partial \Phi_i}{\partial R_i}. \quad (3.7)$$

The evolution equations (3.6) and (3.7) are often referred to as Koiter's rule Koiter [1960]. Furthermore, $\dot{\lambda}_i$ are the plastic multipliers corresponding to the yield functions Φ_i .

3.3.2. Yield functions

The yield surface is described by a set of planes in three-dimensional stress space, where $\mathbf{V}^i$ ($i = 1, 2$) are subsurface normals defined in the material coordinates formed by the machine direction (MD), the cross direction or transverse direction (CD), and the out-of-plane direction (ZD). As opposed to the model proposed by Wallmeier *et al.* Wallmeier et al. [2015], the subsurface normals $\mathbf{V}^i$ ($i = 1, 2$) are dependent on both $\mathbf{M}_1$ and $\mathbf{M}_2$. To account for shearing, a third plane characterized by the subsurface normal $\mathbf{V}^3$ is defined. For simplicity, the yield strength is considered to be the same for both tension and compression. As a result, only three yield surfaces are required instead of six. This leads to three yield functions defined based on the subsurface normals $\mathbf{V}^i$ as

$$\Phi_i = \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2 - (r_i^0 - R_i^{mt})}, \quad i = 1, 2, 3, \quad (3.8)$$

where the yield surface parameters r_i^0 are defined in terms of the uniaxial yield stress in MD-direction σ_{y1} , CD-direction σ_{y2} , and 45° to MD-direction $\sigma_{y12}^{45^\circ}$, respectively, whereas the parameters R_i^{mt} are defined in terms of the hardening stress in MD-direction R_1 , CD-direction R_2 , and 45° to MD-direction R_{45° , respectively, see B.4 for details. The subsurface normals for

the case where the direction MD, CD, and ZD corresponds to the direction of the unit vectors $\mathbf{n}_1$, $\mathbf{n}_2$, and $\mathbf{n}_3$, respectively, are given by

$$\begin{aligned} \mathbf{V}^1 &= \frac{1}{\sqrt{1 + (\nu_{12}^p)^2}} (\mathbf{M}_1 + \nu_{12}^p \mathbf{M}_2), & \mathbf{V}^2 &= \frac{1}{\sqrt{1 + (\nu_{21}^p)^2}} (\nu_{21}^p \mathbf{M}_1 + \mathbf{M}_2), \\ \mathbf{V}^3 &= \frac{\sqrt{2}}{2} (\mathbf{n}_1 \otimes \mathbf{n}_2 + \mathbf{n}_2 \otimes \mathbf{n}_1). \end{aligned} \quad (3.9)$$

Furthermore, ν_{12}^p and ν_{21}^p are plastic strain ratios measuring the lateral contraction of the yield surface relative to axial strain during uniaxial tension in MD and CD directions respectively.

For proof that the yield functions are convex and the Clausius-Duhem inequality is fulfilled, the reader is referred to Bedzra et al. [2017a].

The final form of the constitutive equations is summarized below:

- Stress tensor

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}.$$

- Yield functions

$$\Phi_i = \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} - (r_i^0 - R_i^{mt}), \quad i = 1, 2, 3.$$

- Evolution equations

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{i=1}^3 \dot{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}, \quad \dot{\kappa} = \sum_{i=1}^3 \dot{\lambda}_i.$$

- Kuhn-Tucker conditions

$$\dot{\lambda}_i \geq 0, \quad \Phi_i \leq 0, \quad \dot{\lambda}_i \Phi_i = 0.$$

3.3.3. Numerical aspects

The numerical integration of the evolution equations is performed by means of the backward Euler integration scheme and the internal variables are updated by an elastic predictor/plastic corrector algorithm for multi-surface plasticity derived based on Simo et al. [1988]; Simo and Hughes [1998], Miehe and Schröder [2001], and Reese [2003]. For more details on this stress update algorithm as well as the linearization of the constitutive equations and the derivation of the consistent tangent operator, the reader is referred to Bedzra et al. [2017a].

3.4. Non-quadratic plasticity model

For the purpose of comparison, the non-quadratic plasticity model proposed by Xia et al. [2002] for the in-plane modelling of paper and paperboard is employed. For completeness, the model is described using the argument of thermodynamical consistency.

3.4.1. Derivation based on the Clausius-Duhem inequality

Making the same arguments as made in the derivation of the constitutive equations of the multi-surface plasticity model, one readily obtains the same relations for the Cauchy stress tensor $\boldsymbol{\sigma}$ (3.3) as well as the isotropic hardening stresses R_i (5.26).

As opposed to the multi-surface model, the evolution equations for the plastic flow rule $\dot{\boldsymbol{\varepsilon}}_p$ and the accumulated plastic strain $\dot{\kappa}$ are specified as:

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\mathbf{K}}{\|\mathbf{K}\|} \quad \text{where} \quad \mathbf{K} = \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}, \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}_p\| = \dot{\lambda}. \quad (3.10)$$

3.4.2. Yield function

The non-quadratic yield function proposed by Xia et al. [2002] is here written as

$$\Phi = \sum_{i=1}^3 \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k} - 1, \quad (3.11)$$

where $2k$ is an even integer and $\mathbf{V}^i$ are the subsurface normals already defined in (3.9). The yield surface parameters s_i^0 and R_i^{nq} are defined in terms of the yield stresses σ_{y1} , σ_{y2} , $\sigma_{y12}^{45^\circ}$, and the hardening stresses R_1 , R_2 , R_{45° , for details see B.4. For a graphical interpretation of both the multi-surface yield function and the non-quadratic yield function, see Figure 3.1.

For a proof that the non-quadratic constitutive model fulfils the Clausius-Duhem inequality, the reader is referred to B.1.

The final form of the constitutive equations of the non-quadratic plasticity model is summarized below:

- Stress tensor

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}.$$

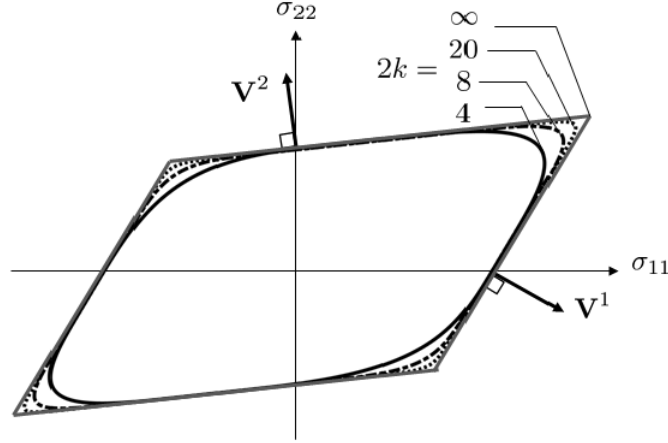


Figure 3.1.: Comparison between multi-surface ($2k = \infty$) and non-quadratic yield surface for different values of the parameter $2k$.

- Non-quadratic yield function

$$\Phi = \sum_{i=1}^3 \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k} - 1.$$

- Evolution equations

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\mathbf{K}}{\|\mathbf{K}\|} \quad \text{where} \quad \mathbf{K} = \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} = \sum_{i=1}^3 \frac{2k}{(s_i^0 - R_i^{nq})} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-1} \mathbf{V}^i, \quad \dot{\kappa} = \dot{\lambda}.$$

- Kuhn-Tucker conditions

$$\dot{\lambda} \geq 0, \quad \Phi \leq 0, \quad \dot{\lambda} \Phi = 0.$$

3.4.3. Numerical aspects

The evolution equations are discretized by means of a standard backward Euler integration scheme. In the following, all variables without subscripts are assumed to be evaluated at time t_{n+1} . The discretized evolution equation together with the yield function is summarized in a residuum format as ($\bar{\lambda} := \dot{\lambda} \Delta t$):

$$\begin{aligned} \mathbf{r}(\boldsymbol{\varepsilon}^p, \bar{\lambda}) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda} \frac{\mathbf{K}}{\|\mathbf{K}\|} = \mathbf{0}, \\ r &= \Phi = 0. \end{aligned} \tag{3.12}$$

Due to the symmetry of the internal variables, the symmetric tensor $\boldsymbol{r}$ can be represented in Voigt form as a six dimensional array. Thus, the resulting system of equations consists of 7 nonlinear scalar equations which have to be solved iteratively by means of e.g. Newton's method at each Gauss point. This iteration is performed in every time step until the root mean square value of the total residuum becomes smaller than a prescribed tolerance. In order to employ Newton's method, the consistent linearization of (C.8) with respect to $\boldsymbol{\varepsilon}^p$ and $\bar{\lambda}$ has to be carried out. The linearized system of equations is shown in B.2.

The scalar evolution equation for accumulated plastic strain (3.10) is also described by means of the backward Euler integration scheme as:

$$\kappa = \kappa_n + \bar{\lambda}. \quad (3.13)$$

The accumulated plastic strain κ is computed at the end of each local Newton iteration via the converged value of the plastic multiplier $\bar{\lambda}$. Therefore, κ is only updated when the local Newton iteration has converged.

In order to determine the tangential stiffness matrix in a finite element analysis, the derivation of the consistent tangent $\mathcal{C}_{\text{nonq}}$ is required, for details see B.3.

3.4.4. Form of Helmholtz free energy functions

The relation for the stress $\boldsymbol{\sigma}$ and the isotropic hardening stresses R_i have been derived without specifying the form of the Helmholtz free energy terms ψ_e and ψ_{iso}^i , respectively. The strain energy function ψ_e due to elastic strain is represented by a linearized version of the strain energy function proposed for modelling bidirectional composite materials by Reese et al. [2001] whereas the energy term ψ_{iso}^i is of the form

$$\psi_{iso}^i = Q_i \left(\kappa + \frac{e^{-\beta_i \kappa} - 1}{\beta_i} \right), \quad i = 1, 2, 3. \quad (3.14)$$

Making use of the elastic strain energy function ψ_e , the constitutive relation for the Cauchy stress $\boldsymbol{\sigma}$ is obtained as

$$\boldsymbol{\sigma} = \mathcal{C}_{\text{ani}} [\boldsymbol{\varepsilon}_e], \quad (3.15)$$

where the fourth-order anisotropic elastic stiffness tensor $\mathcal{C}_{\text{ani}}$ is expressed as:

$$\begin{aligned} \mathcal{C}_{\text{ani}} = \frac{\partial^2 \psi_e}{\partial \boldsymbol{\epsilon}_e^2} = & (8K_1^{\text{iso}} + 4K_2^{\text{iso}}) \mathbf{1} \otimes \mathbf{1} - 4K_2^{\text{iso}} \mathcal{I} + 8K_1^{\text{ani1}} (\mathbf{M}_1 \otimes \mathbf{M}_1) + 4K_2^{\text{ani1}} \boldsymbol{\mathcal{E}}^1 \\ & + 8K_1^{\text{ani2}} (\mathbf{M}_2 \otimes \mathbf{M}_2) + 4K_2^{\text{ani2}} \boldsymbol{\mathcal{E}}^2 + 4K^{\text{kop1}} (\mathbf{1} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \mathbf{1}) \\ & + 4K^{\text{kop2}} (\mathbf{1} \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{1}) + 4K^{\text{kop12}} (\mathbf{M}_1 \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{M}_1). \end{aligned} \quad (3.16)$$

$\mathcal{I}$ represents the fourth order identity tensor and the coefficients K_1^{iso} , K_2^{iso} , K_1^{ani1} , K_2^{ani1} , K_1^{ani2} , K_2^{ani2} , K^{kop1} , K^{kop2} , and K^{kop12} are related to the Young's moduli E_1, E_2, E_3 , the Poisson's ratios $\nu_{12}, \nu_{13}, \nu_{23}$, and the shear moduli G_{12}, G_{13}, G_{23} . For the relation between the coefficients and the engineering constants, see Bedzra et al. [2017a]. Furthermore, the fourth-order tensors $\boldsymbol{\mathcal{E}}^1$ and $\boldsymbol{\mathcal{E}}^2$ are given by

$$\mathcal{E}_{ijkl}^\alpha = \frac{1}{2} (M_{ik}^\alpha \delta_{jl} + M_{jl}^\alpha \delta_{ik} + M_{il}^\alpha \delta_{jk} + M_{jk}^\alpha \delta_{il}), \quad \alpha = 1, 2. \quad (3.17)$$

In the same manner, by employing the energy function due to isotropic hardening ψ_i^{iso} , the isotropic hardening stress R_i is obtained as:

$$R_i = -\frac{\partial \psi_i^{\text{iso}}}{\partial \kappa} = -Q_i (1 - e^{-\beta_i \kappa}), \quad i = 1, 2, 45^\circ. \quad (3.18)$$

The form of R_i corresponds to Voce's exponential hardening function as given in Chaboche [2008] where Q_i and β_i are material parameters used to describe nonlinear isotropic hardening.

In total, both constitutive models have 20 material parameters which are summarized in Table 3.1.

3.5. Results and discussion

This section deals with characterization of both the multi-surface and the non-quadratic constitutive models. Furthermore to validate the multi-surface model, it was compared to off-axis tensile tests as well as the non-quadratic constitutive model. Additionally, the multi-surface constitutive model and the non-quadratic constitutive model were employed in a finite element analysis of a paperboard with a hole under tension and the results were compared with experimental results. Also, the convergence behaviour of the multi-surface constitutive model was assessed against the non-quadratic constitutive model by employing a standalone stress driven algorithm implemented in FORTRAN 95. All finite element analyses were undertaken by means of ABAQUS/Standard software Dessault syst mes [2014] where both material models

Table 3.1.: Material parameters of both constitutive models

E_{MD}	Young's modulus in MD direction
E_{CD}	Young's modulus in CD direction
E_{ZD}	Young's modulus in ZD direction
ν_{12}	Poisson's ratio between MD and CD direction
ν_{13}	Poisson's ratio between MD and ZD direction
ν_{23}	Poisson's ratio between CD and ZD direction
G_{12}	Shear modulus in MD-CD plane
G_{13}	Shear modulus in MD-ZD plane
G_{23}	Shear modulus in CD-ZD plane
ν_{12}^p	Plastic strain ratio during uniaxial tension in MD-direction
ν_{21}^p	Plastic strain ratio during uniaxial tension in CD-direction
$\sigma_{yi} (i = 1, 2), \sigma_{y12}^{45^\circ}$	Initial yield stresses
$\beta_i (i = 1, 2, 45^\circ)$	Rate of change of elastic domain
$Q_i (i = 1, 2, 45^\circ)$	Maximum change in size of elastic domain

have been implemented as a user material subroutine UMAT.

3.5.1. Parameter identification

To identify the parameters of both constitutive models, uniaxial tensile tests were carried out in MD-, CD-, and 45° to MD-direction. For the calibration process, the material directions MD and CD were assumed to coincide with the 1- and 2-directions of the cartesian coordinate system. Also the parameter $2k$ of the non-quadratic yield function was set to $2k = 20$. For a detailed overview on the test procedure as well as the apparatus, the reader is referred to Li et al. [2016]. Based on the stress-strain curves obtained from the experiments, the in-plane elasticity constants E_{MD} , E_{CD} , G_{12} , and ν_{12} were identified. The elasticity constants E_{ZD} , G_{13} , and G_{23} , which describe the out-of-plane elastic response of the material were obtained from Li et al. [2018]. Furthermore, ν_{13} and ν_{23} were assumed to be zero since the main focus here is on the in-plane response of the paperboard. Additionally, due to the small thickness of the paperboard samples, it is a challenging task to measure ν_{13} and ν_{23} .

The plastic strain ratios ν_{12}^p and ν_{21}^p , which are related to the unit normals $\mathbf{V}^i (i = 1, 2)$, were obtained from the fit of both constitutive models to lateral strain versus axial strain curves obtained from uniaxial tension in MD and CD directions, respectively. The uniaxial yield stresses σ_{y1} , σ_{y2} , $\sigma_{y12}^{45^\circ}$, as well as the hardening parameters Q_1 , β_1 , Q_2 , β_2 and Q_{45° , β_{45° were

identified, using a least squares fit, by fitting the following equations

$$\sigma_{11} = \sigma_{y1} - R_1, \quad \sigma_{22} = \sigma_{y2} - R_2, \quad \sigma_{45^\circ} = \sigma_{y12}^{45^\circ} - R_{45^\circ}, \quad (3.19)$$

to the flow curves obtained from uniaxial tension in MD-, CD-, and 45° to MD-direction, respectively. To ensure a good fit, the plastic strains in MD ε_{11}^p , CD ε_{22}^p , and shear in MD-CD plane ε_{12}^p have to be converted to accumulated plastic strain κ using the following relations

$$\kappa = \sqrt{1 + (\nu_{12}^p)^2} \varepsilon_{11}^p, \quad \kappa = \sqrt{1 + (\nu_{21}^p)^2} \varepsilon_{22}^p, \quad \kappa = \sqrt{2} \varepsilon_{12}^p. \quad (3.20)$$

To confirm the fit, simulations were conducted using the identified material constants and the results were compared to the experimental results. The fit of both plasticity models to uniaxial tensile test conducted in MD-, CD-, 45° to MD-direction and the fit for the plastic Poisson's ratios are shown in Figure 3.2 and Figure 3.3, respectively. Also, the identified material parameters are summarized in Table 5.2 and Table 3.3. From the plot, both models yield the same result and are in a good agreement with the experimental results. This is to be expected since the yield surface parameters of both constitutive models are defined in terms of the plastic Poisson's ratios, the yield stresses, and the isotropic hardening stresses identified from the least squares fit.

Table 3.2.: Elasticity constants for both constitutive models

	Young's modulus [MPa]		Shear modulus [MPa]		Poisson's ratio [-]
E_{MD}	5542.55	G_{12}	984.36	ν_{12}	0.435
E_{CD}	1933.20	G_{13}	20.25	ν_{13}	0
E_{ZD}	2.76	G_{23}	15.15	ν_{23}	0

Table 3.3.: Plasticity constants for both constitutive models

	Plastic strain ratio, $d\varepsilon_{\perp}^p/d\varepsilon_{\parallel}^p$		Yield stress [MPa]	Q_i [MPa]	β_i [-]
ν_{12}^p	-0.62	MD	19.90	22.21	326.5
ν_{21}^p	-0.14	CD	10.23	11.93	99.4
		45°	13.45	15.78	172.2

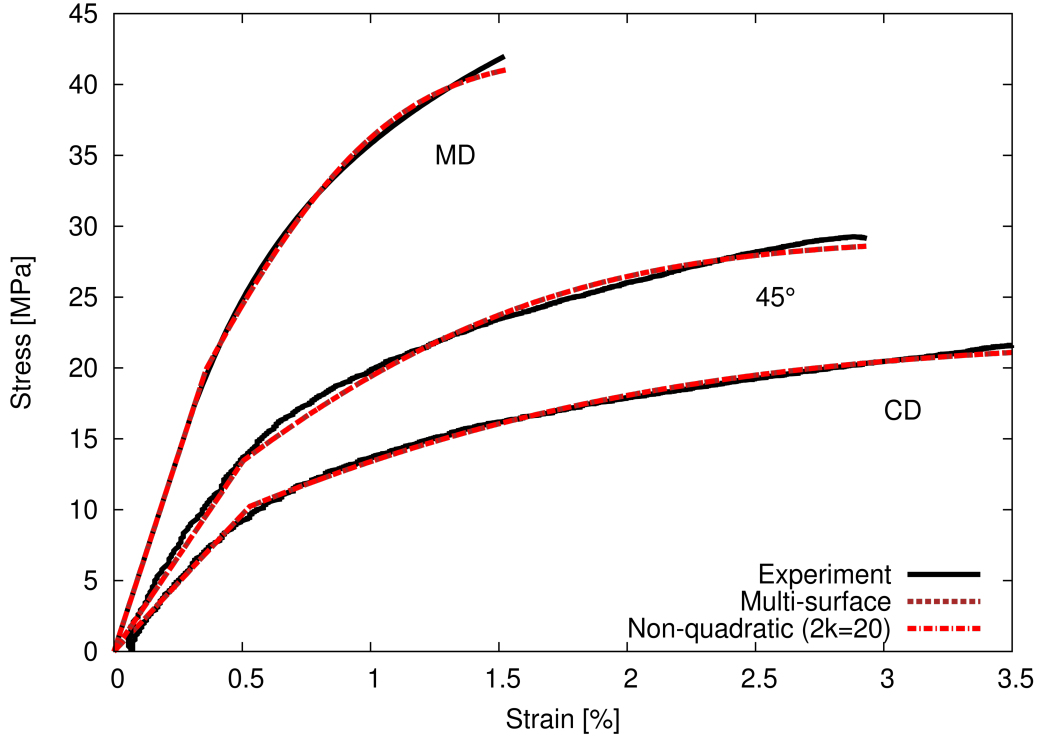


Figure 3.2.: Fit of both constitutive models to experimental stress-strain curves for MD, CD, and 45° uniaxial tension.

3.5.2. Validation of the multi-surface model against experimental results and the non-quadratic model

To validate the multi-surface constitutive model, it was compared to experimental stress-strain curves obtained from loading in directions 30° and 60° off-axis to MD direction as well as axial versus lateral plastic strain curves obtained from tension in an orientation 45° to MD-direction. Additionally, it was compared to the non-quadratic plasticity model subjected to the same load conditions.

A plot comparing both constitutive models to off-axis experimental results for different values of the parameter $2k$ is shown in Figure 3.4. From the plot, it is observed that the plasticity models are in good agreement with the experimental results, although the multi-surface model slightly over predicts the stress-strain response for 60° off-axis to MD direction. Also, it can be observed that the parameter $2k$ in the considered regime does not significantly affect the obtained stress-strain response. A plot comparing both constitutive models to experimental result for lateral plastic strain versus axial plastic strain in 45° off-axis tension to MD-direction is shown in Figure 3.5. It can be observed that the curves obtained for lateral versus axial

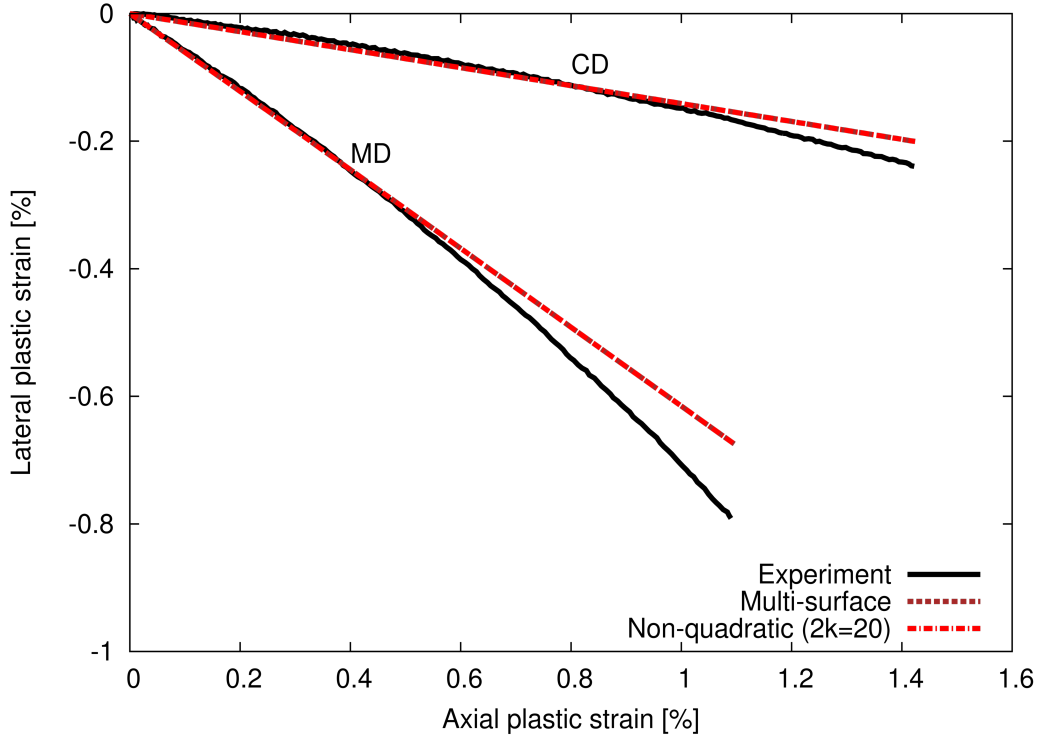


Figure 3.3.: Comparison of experimental and simulated lateral plastic strain vs. axial plastic strain curves for MD and CD uniaxial tension.

plastic strain using the multi-surface plasticity model and the non-quadratic plasticity model differ significantly from the experimental result. This is as a result of lack of coupling between the in-plane shear and the in-plane normal stress. As such, both constitutive models yield a pure shear plastic deformation mode under off-axis tension which results in a lateral strain versus axial plastic strain ratio of $\nu_{45^\circ}^p = -1$ upon continual loading. A similar observation was reported by Tjahjanto et al. [2015] for the non-quadratic plasticity model.

3.5.3. Paperboard with a hole under uniform tension

This example is concerned with the experimental and numerical investigation of a paperboard sheet with a circular hole under uniform tension. A similar analysis has been performed by Borgqvist et al. [2014], where a plain stress finite element model of the problem was considered. In the present case, a three dimensional finite element analysis of the problem is undertaken. This is needed because both plasticity models are fully three dimensional material models although the out-of-plane behaviour of the material is treated as elastic.

The experimental setup for this problem includes a Zwick Z5 universal testing machine em-

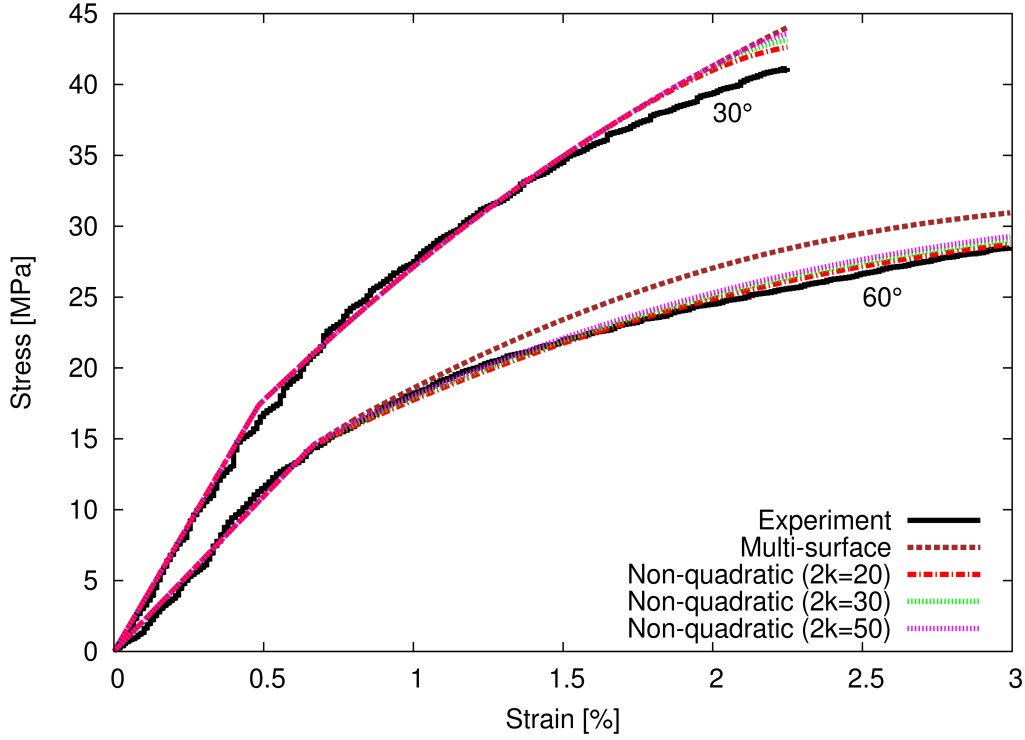


Figure 3.4.: Comparison of both models' prediction to experimental stress-strain curves for off-axis tension in 30° and 60° directions.

ployed for tensile loading of the material specimen and an Aramis 4M digital image correlation (DIC) system for synchronously recording force, displacement, and the corresponding strain field. The paper samples used for the test have a thickness of 0.362 ± 0.007 mm, a length of 200 mm, a width of 20 mm and a central hole with a diameter of 5 mm. The length of the paper samples were chosen as 200 mm to ensure a uniform strain distribution around the region close to the hole thus avoiding the effect of the clamps on the strain field. The tests were conducted along CD direction at a crosshead speed of 5 mm/min until fracture.

The geometry of the finite element model has a length of 50 mm and a thickness of 0.36 mm apart from which all other geometrical features are the same as the paper samples. Due to the geometrical and material symmetry, only a quarter of the structure is discretized and considered in the finite element analysis. It is meshed with a total of 8316 (ca. $\text{length}^2 \times \text{thickness} = (0.29)^2 \times 0.18$) eight node solid elements (C3D8) available in ABAQUS/Standard with 2 elements across the thickness direction. The initial geometry of the paperboard with a hole including boundary conditions and the discretized finite element model are shown in Figure 3.6.

In Figure 3.7, the global force-displacement data obtained from experiment and the simula-

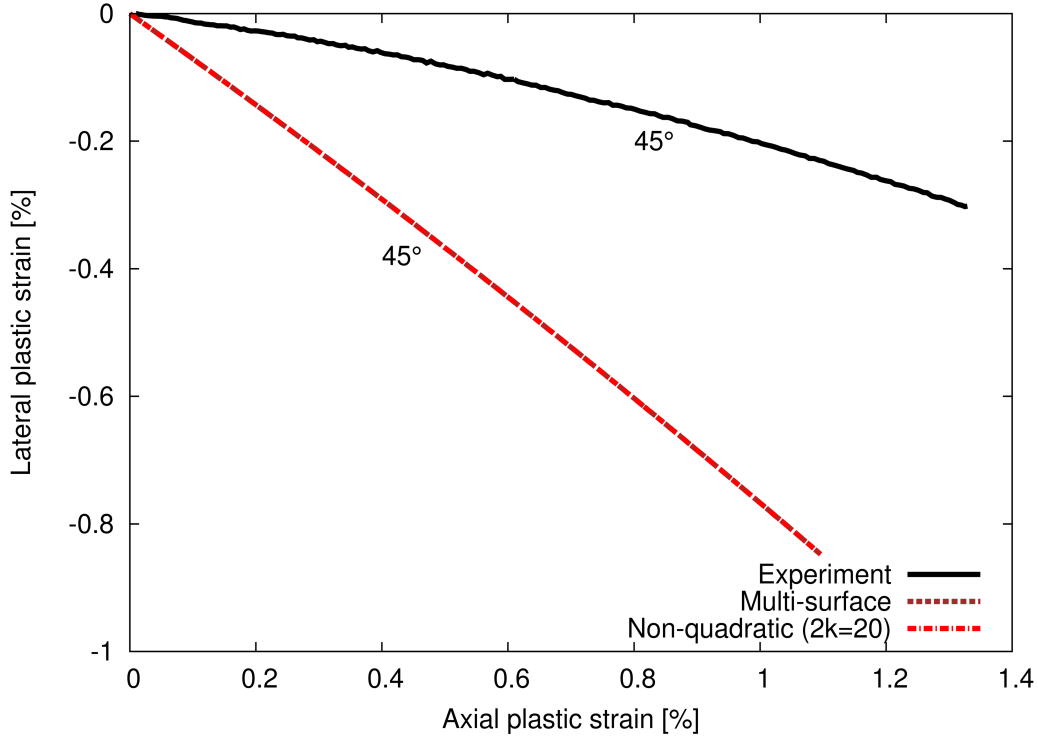


Figure 3.5.: Comparison of experimental and simulated lateral plastic strain vs. axial plastic strain curves for off-axis tension in 45° direction.

tions are compared. From the result, the multi-surface plasticity model and the non-quadratic plasticity model agree very well with the experimental results. Furthermore for a better insight into both model predictions, a relative difference plot based on the following definition

$$\epsilon_{rel} = \left| \frac{F_{mult} - F_{nonq}}{F_{mult}} \right|, \quad (3.21)$$

where F_{mult} and F_{nonq} are the force obtained from the multi-surface and non-quadratic plasticity models, respectively, is obtained and given in Figure 3.8. From the magnitude of the relative difference, both model predictions do not differ from each other significantly. Also, an increase of the parameter $2k$ results in the reduction of the relative difference between both models.

In Figures 3.9 and 3.10, the corresponding strain fields in CD and MD directions, respectively, obtained from both the finite element simulations and the DIC images are shown for the two points marked with 1 and 2 on the force displacement curve (Figure 3.7). It can be observed that the numerical predictions for the local strain fields are in agreement with the experimental data. Due to the similarity in the logarithmic strain distribution, only the strain fields obtained from the multi-surface model in comparison with the DIC images are shown.

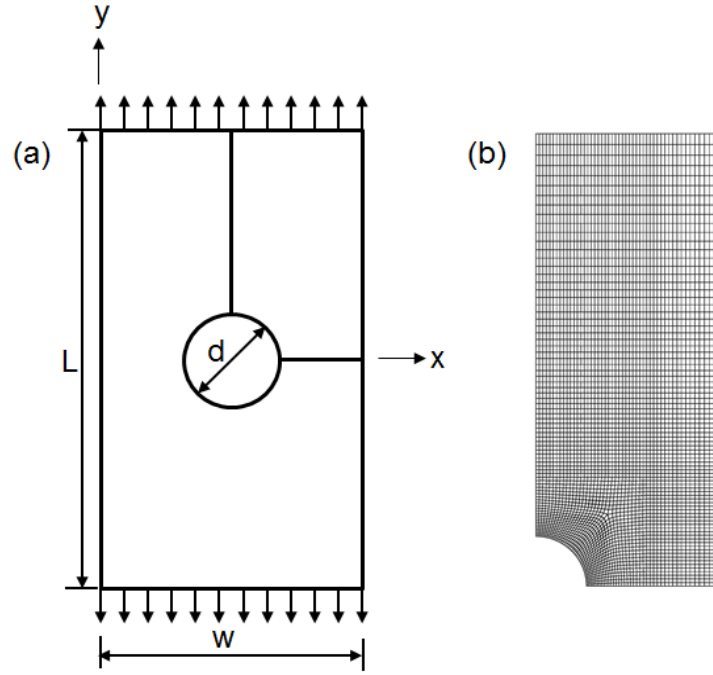


Figure 3.6.: Initial geometry of experimental specimen together with finite element discretization.

3.5.4. Global and local convergence behaviour of multi-surface and non-quadratic plasticity model

To study the convergence behaviour of the multi-surface model in comparison to the non-quadratic model, a stress driven standalone algorithm detailed in Algorithm 1 is implemented. For the input, a stress of $\Delta\sigma_{11} = 2\text{MPa}$ which corresponds to a uniaxial tension in CD direction is prescribed and applied in 20 load steps. Furthermore, a tolerance of 10^{-8} is specified for the convergence of the global and local iterations. Summarized in Tables 3.4 and 3.5 are the global and local residual norms of the last load step. From Table 3.4, the multi-surface plasticity model achieves global convergence after 5 iterations whereas the two variants of the non-quadratic plasticity model require an additional iteration to achieve global convergence.

Also a look at Table 3.5 reveals that by increasing the parameter $2k$, the non-quadratic plasticity model requires a significantly higher number of iterations to achieve local convergence for the first two global iterations as compared to the multi-surface plasticity model. This leads to a slower rate of convergence for the non-quadratic plasticity model. This can be attributed to an increase in the local residual norm at the beginning of the local iteration due to the increase of $2k$.

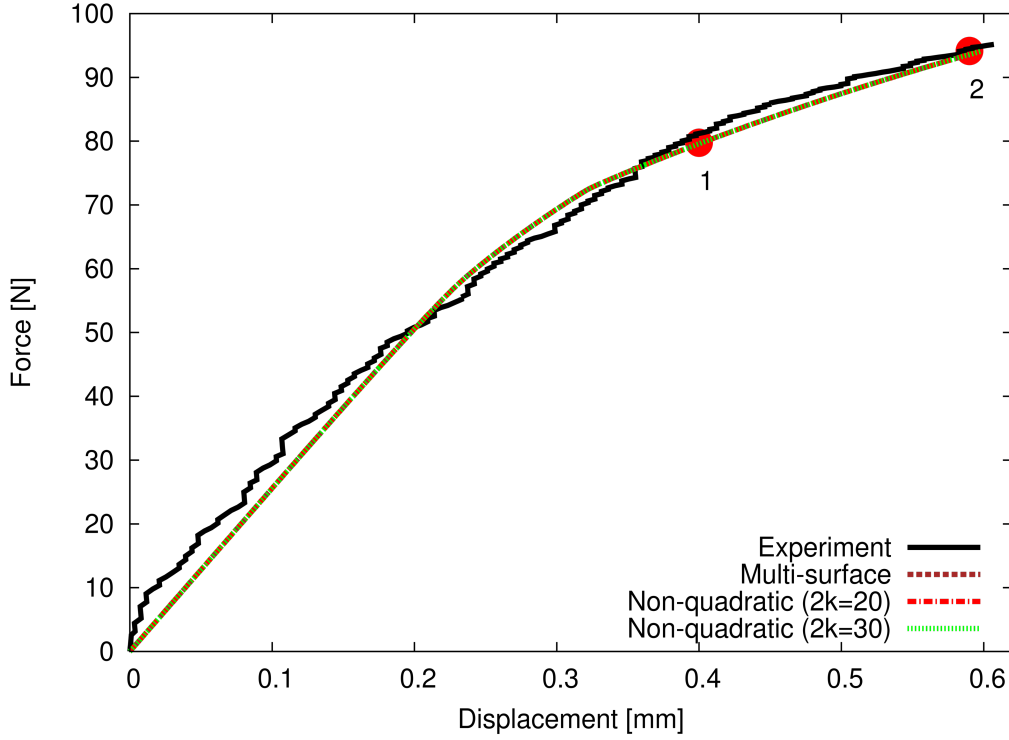


Figure 3.7.: Comparison of both models' predictions of the global force-displacement curve to experimental data.

Input : prescribed stress tensor $\Delta\sigma_{given}$

Output corresponding total strain ϵ

:

- 1 **Database**: strain ϵ_n , plastic strain ϵ_n^p , accumulated plastic strain κ_n , time at the beginning t_n , time at the end t_{end} , and number of steps n_{steps} .
- 2 Compute step size: $dt = (t_{end} - t_n) / n_{steps}$
- 3 Compute stress $\sigma_{given} = \Delta\sigma_{given} \times t_n$
- 4 Call UMAT subroutine to obtain ϵ_{n+1}^p , κ_{n+1} , σ and $\mathcal{C}_{cons}$ after convergence of the local Newton iteration i.e. $\|r_{loc}\| \leq loctol$.
- 5 Compute global residuum: $r_{glob} = \sigma_{given} - \sigma$
- 6 Check if the residuum is greater than the tolerance: $\|r_{glob}\| > globtol$
- 7 If this is the case, compute $\Delta\epsilon = \mathcal{C}_{cons}^{-1} [r_{glob}]$
- 8 Update $\epsilon_{n+1} = \epsilon_n + \Delta\epsilon$
- 9 Set: $\epsilon_n \leftarrow \epsilon_{n+1}$, $\epsilon_n^p \leftarrow \epsilon_{n+1}^p$, $\kappa_n \leftarrow \kappa_{n+1}$
- 10 Repeat step 4
- 11 Else set $t_n \leftarrow t_n + dt$ and repeat step 3 until $t_n = t_{end}$

Algorithm 1: Standalone algorithm which computes a total strain given a prescribed stress.

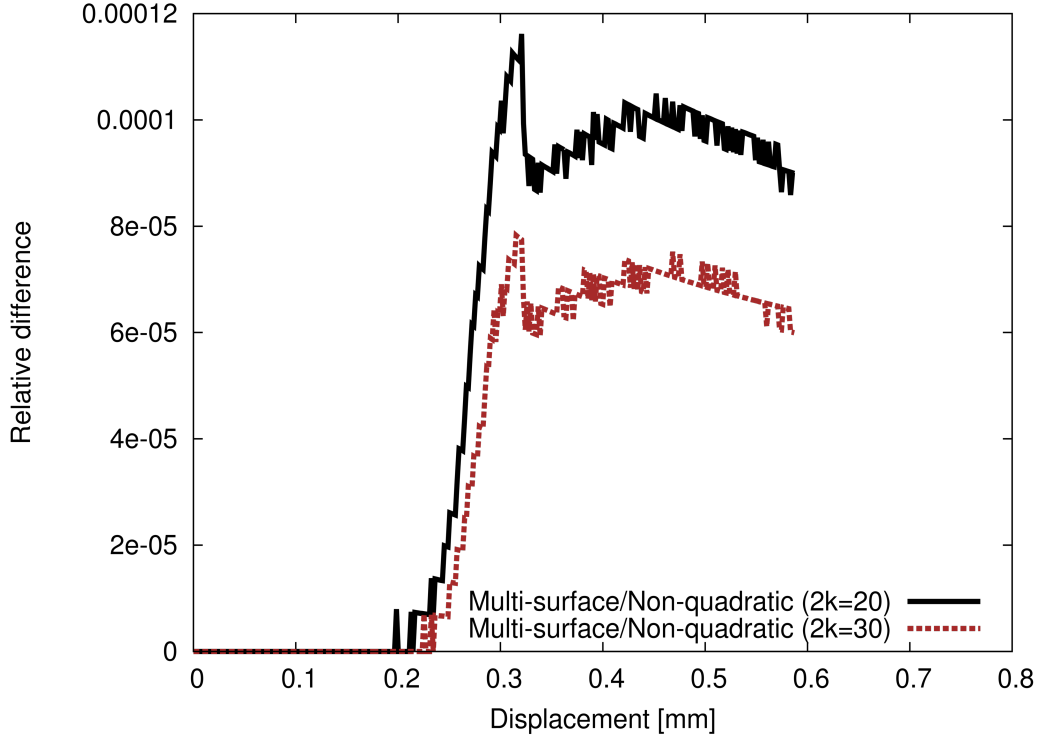


Figure 3.8.: Relative difference between multi-surface model and two variants of non-quadratic model for paperboard with a hole under uniform tension simulation.

Table 3.4.: Global convergence behaviour of multi-surface and non-quadratic plasticity model

glob. iter.	multi-surface $\ r_{glob}\ $	non-quad. $2k = 20$ $\ r_{glob}\ $	non-quad. $2k = 30$ $\ r_{glob}\ $
1	2.0	2.0	2.0
2	0.36448	0.36453	0.36454
3	2.55820E-002	2.55900E-002	2.56232E-002
4	1.57025E-004	1.81112E-004	1.63883E-004
5	8.83784E-011	4.21779E-008	1.68763E-007
6		2.13636E-013	3.70379E-013

3.5.5. Discussion

From the studies performed, both models are capable of yielding accurate results for the paperboard under consideration. In terms of implementation, the non-quadratic plasticity model is less laborious compared to the multi-surface plasticity model due to the active set search that has to be undertaken (refer to Bedzra et al. [2017a] for details). The difficulty resulting from the active set search can be circumvented by the Fischer-Baumeister complementary functions, although they are known to be numerically sensitive, see Gaser and Holzapfe [2002]; Schmidt-

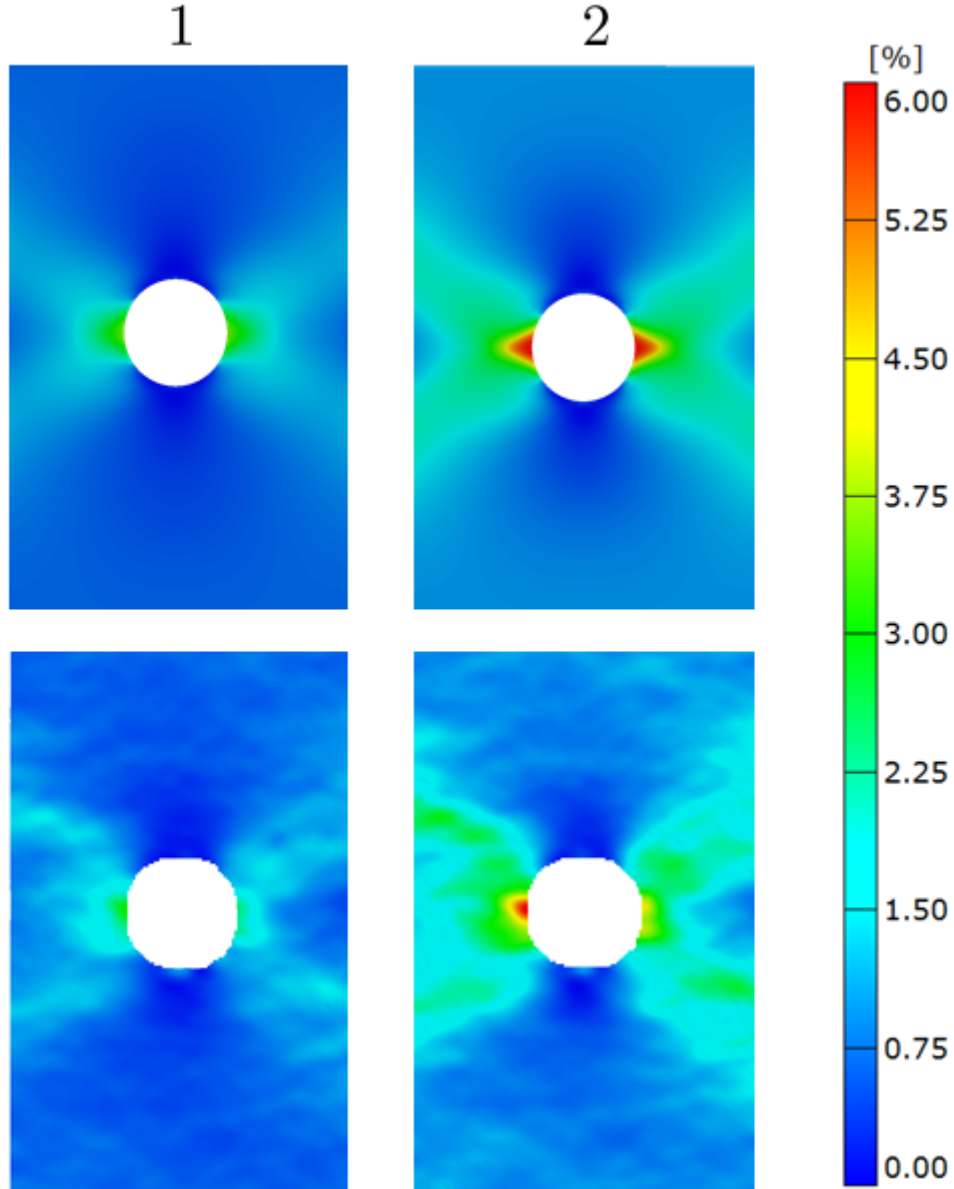


Figure 3.9.: Comparison of DIC image of the strain field corresponding to point 1 and 2 with top row as simulation results and bottom row as experimental results for CD direction.

Baldassari [2003]; Bartel and Hackl [2009]. For the computation of the consistent tangent operator, no regularization technique is employed for the non-quadratic plasticity model. On the contrary, in the case of the multi-surface plasticity model, the Jacobian matrix is regularized due to its ill-posedness (see Bedzra et al. [2017a]). Parameter identification, to the experience of the authors, is less complicated for the multi-surface plasticity model as compared to the non-quadratic plasticity model. Furthermore, the multi-surface model shows a superior rate of

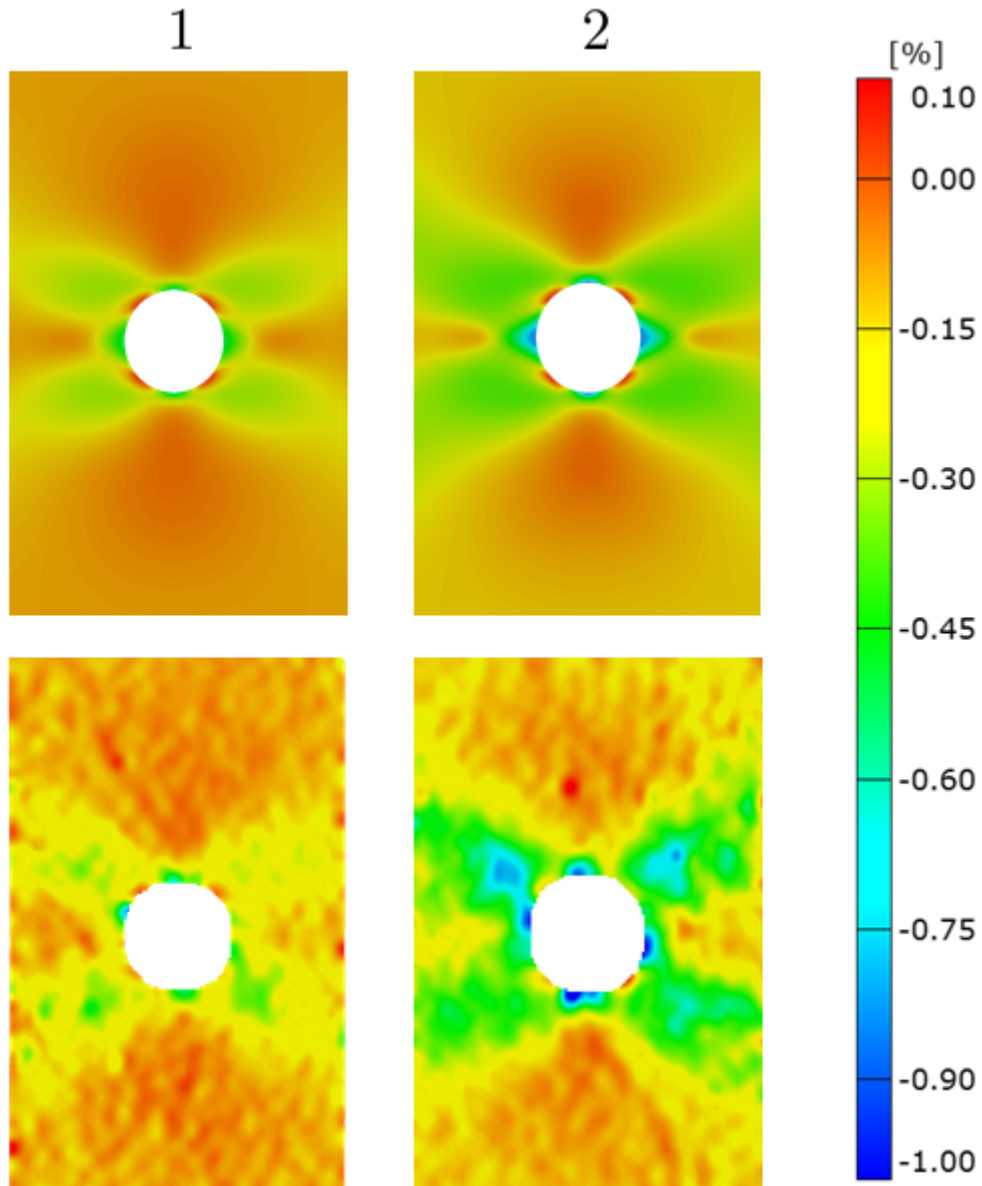


Figure 3.10.: Comparison of DIC image of the strain field corresponding to point 1 and 2 with top row as simulation results and bottom row as experimental results for MD direction.

convergence to the non-quadratic model.

3.6. Conclusion

The objective of this paper was to develop a multi-surface plasticity model for the in-plane modelling of the anisotropic elastoplastic behaviour of paper and paperboard and to compare

Table 3.5.: Corresponding local iteration after each global iteration for multi-surface and non-quadratic plasticity model

glob. iter.	multi-surface $\ \mathbf{r}_{loc}\ $	non-quad. $2k = 20$ $\ \mathbf{r}_{loc}\ $	non-quad. $2k = 30$ $\ \mathbf{r}_{loc}\ $
1	8.54265 0.37016 5.74400E-004 1.36947E-009	108.02903 39.47211 14.21453 4.94613 1.57314 0.39091 4.91965E-002 1.11004E-003 6.00839E-007 1.75493E-013	1137.41590 418.21456 153.39115 56.01894 20.26763 7.16324 2.37866 0.66535 0.11552 5.69684E-003 1.58552E-005 1.23729E-010
2	2.54409 2.54336E-002 2.36288E-006 2.13163E-014	3.28970 0.97953 0.20320 1.58521E-002 1.19801E-004 6.98372E-009	7.88295 2.63647 0.75380 0.13927 8.04348E-003 3.14399E-005 4.85418E-010
3	0.20712 1.55865E-004 8.77165E-011	0.12911 6.93265E-003 2.31730E-005 2.61251E-010	0.20022 1.55579E-002 1.16460E-004 6.65869E-009
4	1.28712E-003 5.98158E-009	8.73169E-004 3.70525E-007 7.11040E-014	1.18446E-003 6.87811E-007 2.26336E-013
5		2.03316E-007 2.00285E-014	1.22026E-006 7.25936E-013

it to an existing non-quadratic plasticity model. This was achieved by first developing a thermodynamically consistent multi-surface plasticity model for paper and paperboard where the elastic part of the model was described by an anisotropic strain energy function. The initial anisotropic yield surface was constructed by a set of planes in stress space which were characterized by structural tensors. The evolution of the yield surface during plastic strain was described by multiple hardening functions, thus providing anisotropic strain hardening of the yield surface. Next, the non-quadratic yield function originally proposed by Xia et al. [2002]

for the in-plane modelling of the anisotropic elastoplastic behaviour of paper and paperboard was formulated in a thermodynamically consistent manner.

The material parameters for both constitutive models were identified by fitting the models to uniaxial stress-strain curves obtained from loading in MD, CD, and 45° direction as well as lateral strain versus axial strain curves obtained from uniaxial tension in MD and CD directions. With the identified material parameters, the multi-surface constitutive model was validated by comparing it to experimentally obtained stress-strain curves for loading in 30° and 60° off-axis to MD direction as well as the non-quadratic plasticity model subjected to a similar load condition. It was observed that both plasticity models were in good agreement with the experimental results although the multi-surface model slightly over predicted the material response for loading in 60° off-axis to MD direction. Additionally, the constitutive models were employed in the finite element analysis of a paperboard with a circular hole under tension. The numerically predicted force-displacement curves and local strain fields were compared to experimental results. It was shown that both constitutive models were in good agreement with the experimental results.

Finally, the convergence behaviour of the multi-surface model was compared to the non-quadratic plasticity model using a stress-driven stand-alone algorithm. From the comparison, it was observed that an increase in the value of the parameter $2k$ led to an increase in the number of local iterations required for the non-quadratic plasticity model to reach local convergence as compared to the multi-surface plasticity model. Furthermore, It was also observed that the multi-surface model needed one less global iteration to reach global convergence.

4 | **Article 3:**

Micro-macro modelling of metallic composites

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Disclosure of the individual authors’ contributions to the article:

R. Bedzra formulated the actual concept, realized and implemented the model, and wrote the article. J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice. All authors drafted the work for intellectual content and approved the publication of the final version of the manuscript.

4.1. Abstract

This contribution describes a scale bridging approach for modelling unidirectional metallic composite materials by making use of an anisotropic elastoplastic constitutive model. The material under investigation is tungsten fibre reinforced copper (W/Cu) composite. To identify the yield surface of the composite, a finite element model of a unidirectional composite repeating unit cell (RUC) is set-up (micro-model). Through virtual experiments, the yield surface of the composite is identified. An anisotropic elastoplastic constitutive model based on the identified yield surface, which makes use of the concept of structural tensors, is developed. This material model serves as the material model for macro computations. To ensure a good agreement between constitutive model and the unidirectional composite RUC during plastic evolution, multiple hardening functions are employed. The parameters of the constitutive model are identified and validated against the response of the unidirectional composite RUC.

4.2. Introduction

Metal matrix composite (MMC) such as tungsten fibre reinforced copper (W/Cu) composites, are being considered for use in high temperature propulsion environments due to their ability to withstand high thermal loads and their relatively low density Doychak [1992]; Sanfeliz [1993].

To model such a material, different length scales have to be taken into account in order to capture the influence of the intrinsic microstructure of the composite material on the macro-scale. A method to accomplish this is to employ a computational homogenization scheme Miehe et al. [1999]; Kanouté et al. [2009a]; Geers et al. [2010]. This method is based on the construction of a micro-scale boundary value problem which is used to determine the governing behaviour of the material on the macro-scale. If the boundary value problem is solved simultaneously, a fully nested solution of two boundary value problems is obtained, often referred to as the FE^2 method. Although this method allows one to assess the macroscopic influence on the microscopic parameters, it is computationally expensive and time consuming. An alternative approach, which is less computationally expensive, is to develop a constitutive model which is able to predict the response of the micro-scale boundary value problem. This approach has been exploited in Reese [2003] for modelling the elastoplastic behaviour of pneumatic membranes and also in Stier et al. [2014] and Simon et al. [2015] for modelling layered fibre reinforced composites. In the current contribution, it is used to model the elastoplastic response of a unidirectional fibre reinforced metal matrix composite.

The developed anisotropic elastoplastic model employs the concept of structural tensors

to describe the initial yield surface of the composite. The structural tensors are second order tensors which are characterized by unit vectors pointing in privileged directions of the material. The structural tensors may be fixed Gaser and Holzapfe [2002]; Vladimirov et al. [2010]; Vogler et al. [2013] or may evolve with plastic flow Svendsen et al. [2006]; Noman et al. [2010]; Pietryga et al. [2012]. In the present case, they are considered to be fixed.

The paper is organized as follows: In Section 4.3, a finite element model of the unidirectional composite model is set-up, and the yield surface of the composite is identified by performing virtual experiments. In Section 4.4, the derivation of the anisotropic constitutive model is briefly described and validated.

4.3. Unidirectional composite (micro-scale)

To identify the yield surface of the composite as well as the material parameters of the continuum anisotropic constitutive model and for later validation, a repeating unit cell (RUC) of a unidirectional composite with random fibre distribution is generated.

4.3.1. Geometry generation

The fibre distribution in the RUC is generated through a uniform random point generator function in matlab. The length of the RUC in longitudinal fibre direction is $0.5 \mu m$ whereas the length in transverse fibre direction is $22.65 \mu m$. The diameter of the fibres is $7 \mu m$, the fibre volume ratio is 60% and the total number of fibres is 8. The RUC is assumed to be part of a much larger material specimen. Therefore, periodic boundary conditions are applied through equation constraints in the finite element package ABAQUS/standard Dessault systèmes [2014]. For details on the application of periodic boundary condition in ABAQUS/standard, see Barbero [2008].

For efficiency reasons, reduced integration eight node linear solid elements (C3D8R) are used to discretise the RUC. In total, the model is made up of 21110 number of elements. The meshed geometry of the unidirectional composite RUC is shown in Figure 4.1.

4.3.2. Fibre and matrix material

The fibres are modelled as General Electric 218CS (GE218CS) continuous tungsten wire and the matrix is modelled as a cold worked oxygen free high conductivity copper (OFHC) material. The constitutive model for both GE218CS and OFHC is summarized in Table 4.1 where σ^D represents the deviatoric part of the Cauchy stress tensor σ which in turn is related to

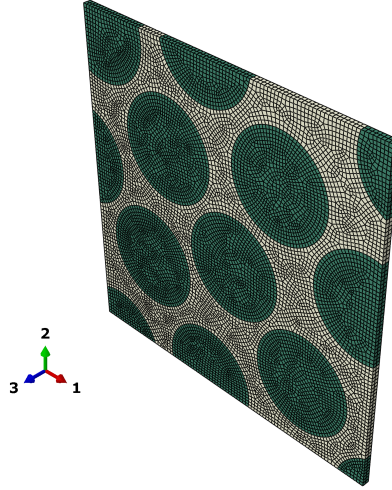


Figure 4.1.: Geometry of unidirectional composite RUC with random fibre distribution

Table 4.1.: Fibre and matrix material model

Elastic law	$\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\varepsilon}_e$
Strain	$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$
Yield function	$\Phi = \sqrt{\boldsymbol{\sigma}^D \cdot \boldsymbol{\sigma}^D} - \sqrt{\frac{2}{3}}(\sigma_Y + R)$
Hardening law	$R = Q_0(1 - e^{-\beta\kappa})$
Flowrule	$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}, \quad \dot{\kappa} = \dot{\lambda} \frac{\partial \Phi}{\partial R}$
K.T conditions	$\dot{\lambda} \geq 0, \quad \Phi \leq 0, \quad \dot{\lambda}\Phi = 0$

the elastic part of the strain tensor $\boldsymbol{\varepsilon}_e$ through the fourth-order isotropic elastic stiffness tensor $\mathbf{C}$, which is a function of the Poisson's ratio ν and the Young's modulus E , $\boldsymbol{\varepsilon}$ is the total strain which is additively decomposed into an elastic part $\boldsymbol{\varepsilon}_e$ and a plastic part $\boldsymbol{\varepsilon}_p$. The yield function Φ is assumed to be a standard von Mises yield function. The isotropic hardening stress R is chosen as a Voce's exponential hardening function, where κ is the isotropic hardening variable. Furthermore, β and Q_0 are material parameters which describe isotropic hardening. Also, the Kuhn-Tucker conditions for loading and unloading as well as the consistency condition are listed.

The fit of the constitutive model to experimental uniaxial stress-strain curves, obtained from Sanfeliz [1993] for GE218CS and OFHC, is shown in Figure 4.2a and 4.2b, respectively. Also, the material parameters identified through fitting the constitutive model to the experimental results is given in Table 4.2.

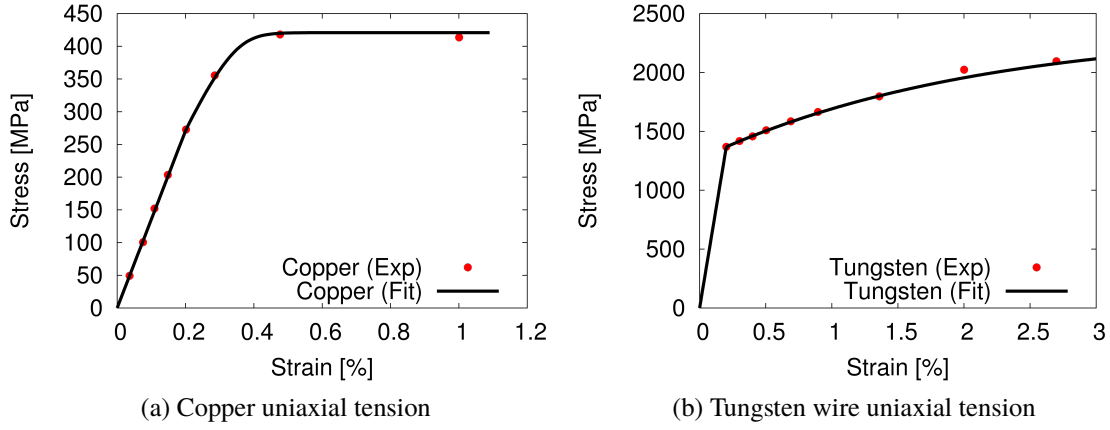


Figure 4.2.: Fit of fibre and matrix material model to experimentally obtained uniaxial stress-strain curves of copper and tungsten wire from Sanfeliz [1993]

Table 4.2.: Tow and matrix material constants

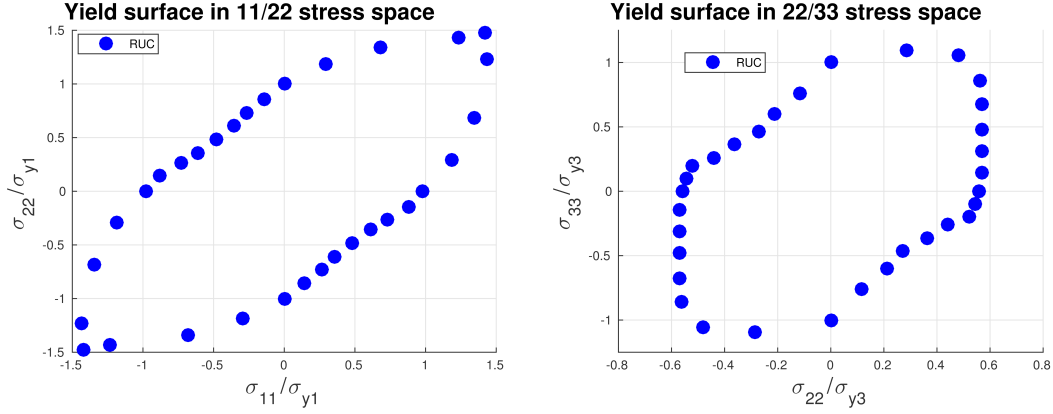
Fit	E[MPa]	ν [-]	σ_y [MPa]	Q_0 [MPa]	β [-]
Tungsten	677887	0.28	1368.87	987.20	52.60
Copper	135248	0.34	272.76	148.10	2994

4.3.3. Determination of unidirectional composite yield surface

To obtain a profile of the composite yield surface, the unidirectional fibre reinforced composite VE is subjected to a series of biaxial tensile tests as well as combined shear tension tests. The load ratios, σ_{xx}/σ_{yy} , σ_{xy}/σ_{xx} , σ_{xx}/σ_{zz} , σ_{xz}/σ_{xx} , σ_{xy}/σ_{yy} , and σ_{xz}/σ_{zz} , employed to identify the yield surface of the composite in 11/22- and 11/33-principal stress space, are summarized in Table 4.3. Due to geometrical and material symmetry, there is no need to identify the yield surface in 22/33-principal stress space since it will result in the same yield surface as identified in 11/33-principal stress space. The obtained yield surface in 11/22- and 22/33-principal stress space respectively, are displayed in Figures 4.3a and 4.3b.

Table 4.3.: Load ratios for biaxial and combined shear-tension virtual experiments

σ_{xx}/σ_{yy}	σ_{xx}/σ_{zz}	1/0	4/1	2/1	4/3	1/1
σ_{xx}/σ_{yy}	σ_{xx}/σ_{zz}	0/1	1/4	1/2	3/4	1/1
σ_{xy}/σ_{xx}	σ_{xz}/σ_{zz}	1/0	4/1	2/1	4/3	0/1
σ_{xy}/σ_{yy}	σ_{xz}/σ_{xx}	1/0	4/1	2/1	4/3	0/1



(a) Yield surface in 11/22-principal stress space (b) Yield surface in 22/33-principal stress space

Figure 4.3.: Yield surface characterization in principal stress-space; (a) 11/22-principal stress space normalized by uniaxial yield stress in 1-direction σ_{y1} ; (b) 22/33-principal stress space normalized by uniaxial yield stress in 3-direction σ_{y3}

4.4. Constitutive model of unidirectional composite (Macro-model)

To capture the identified yield surface of the unidirectional composite RUC, a constitutive model is developed.

4.4.1. Material model

The Helmholtz free energy per unit volume is given in the form

$$\psi = \psi_e(\boldsymbol{\varepsilon}_e, \mathbf{M}_1, \mathbf{M}_2) + \sum_{i=1}^6 \psi_i^{iso}(\kappa). \quad (4.1)$$

The first part ψ_e of the energy terms describes the macroscopic anisotropic elastic properties of the material. $\boldsymbol{\varepsilon}_e$ represents the elastic strain which is obtained from the additive decomposition of the total strain tensor $\boldsymbol{\varepsilon}$ into an elastic part and a plastic part $\boldsymbol{\varepsilon}_p$

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p, \quad (4.2)$$

and $\mathbf{M}_i$ ($i = 1, 2$) are structural tensors, more details to follow. The terms ψ_i^{iso} represent the additional amount of stored energy due to isotropic hardening and they are a function of the accumulated plastic strain κ .

Utilizing the Clausius-Duhem second law of thermodynamics, $-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0$, a relation for the Cauchy stress tensor $\boldsymbol{\sigma}$ and the isotropic hardening stresses R_i are obtained as:

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}, \quad R_i = -\frac{\partial \psi_i^{iso}}{\partial \kappa} = -Q_i(1 - e^{-\beta_i \kappa}). \quad (4.3)$$

The expression for the isotropic hardening stresses corresponds to Voce's exponential hardening function as given in Chaboche [2008], where Q_i and β_i are material parameters used to describe nonlinear isotropic hardening. Furthermore, to ensure thermodynamic consistency, the following evolution equations for associative plastic flow and accumulated plastic strain are specified.

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\mathbf{K}}{\|\mathbf{K}\|} \quad \text{where} \quad \mathbf{K} = \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}, \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}_p\| = \dot{\lambda}, \quad (4.4)$$

where Φ and $\dot{\lambda}$ are the yield function and the plastic multiplier, respectively.

To capture the yield surface obtained from the virtual experiments carried out on the unidirectional composite RUC, a yield surface corresponding to Hill [1948] is employed and is given here as:

$$\Phi = \frac{1}{2} \boldsymbol{\sigma}^D \cdot \mathcal{A} [\boldsymbol{\sigma}^D] - 1. \quad (4.5)$$

The superscript D denotes the deviator, which operates on a second order tensor to produce $\mathbf{B}^D = \mathbf{B} - \frac{1}{3} (\text{tr} \mathbf{B}) \mathbf{1}$. The fourth order anisotropy tensor $\mathcal{A}$ written in terms of structural tensors has the form:

$$\mathcal{A} = 3 (a_1 \mathcal{I} + a_2 \mathbf{M}_1 \otimes \mathbf{M}_1 + a_3 \mathbf{M}_2 \otimes \mathbf{M}_2 + a_4 (\mathbf{M}_1 \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{M}_1) + a_5 \mathcal{D}_1 + a_6 \mathcal{D}_2). \quad (4.6)$$

A second-order structural tensor as developed by Spencer [1971]; Boehler [1979] and Zhang and Rychlewski [1990], is defined as:

$$\mathbf{M}_i = \mathbf{n}_i \otimes \mathbf{n}_i, \quad i = 1, 2, 3, \quad (4.7)$$

where $\mathbf{n}_i$ are unit vectors pointing in privileged directions of the material. Additionally, these unit vectors $\mathbf{n}_i$ are orthogonal to each other, and hence the following relations hold

$$\sum_{i=1}^3 \mathbf{M}_i = \mathbf{n}_1 \otimes \mathbf{n}_1 + \mathbf{n}_2 \otimes \mathbf{n}_2 + \mathbf{n}_3 \otimes \mathbf{n}_3 = \mathbf{1}, \quad \mathbf{n}_i \cdot \mathbf{n}_j = \delta_{ij}, \quad i, j = 1, 2, 3 \quad (4.8)$$

δ_{ij} refers to the Kronecker symbol and $\mathbf{1}$ is the second order identity tensor. Furthermore, the

fourth order tensors $\mathcal{D}_1$ and $\mathcal{D}_2$ are defined as:

$$\mathcal{D}_{ijkl}^\alpha = \frac{1}{2} (M_{ik}^\alpha \delta_{jl} + M_{jl}^\alpha \delta_{ik} + M_{il}^\alpha \delta_{jk} + M_{jk}^\alpha \delta_{il}), \quad \alpha = 1, 2 \quad (4.9)$$

The tensor $\mathcal{I}$ represents the fourth order identity tensor.

The coefficients a_i ($i = 1, \dots, 6$), which describe the initial state of anisotropy, are obtained by setting them in relation to the classical Hill coefficients F, G, H, L, M , and N , see Vladimirov et al. [2011] for details:

$$\begin{aligned} a_1 &= \frac{2}{3} (L + M - N), \\ a_2 &= \frac{2}{3} (F + 4G + H - 2M), \\ a_3 &= \frac{2}{3} (4F + G + H - 2L), \\ a_4 &= \frac{2}{3} (2F + 2G - H - L - M + N), \\ a_5 &= \frac{2}{3} (N - L), \\ a_6 &= \frac{2}{3} (N - M). \end{aligned} \quad (4.10)$$

To take into account anisotropic plastic evolution, the classical Hill coefficients are redefined as:

$$\begin{aligned} F &= \frac{1}{2} \left[\frac{1}{(\sigma_{y2} - R_2)^2} + \frac{1}{(\sigma_{y3} - R_3)^2} - \frac{1}{(\sigma_{y1} - R_1)^2} \right], \\ G &= \frac{1}{2} \left[\frac{1}{(\sigma_{y3} - R_3)^2} + \frac{1}{(\sigma_{y1} - R_1)^2} - \frac{1}{(\sigma_{y2} - R_2)^2} \right], \\ H &= \frac{1}{2} \left[\frac{1}{(\sigma_{y1} - R_1)^2} + \frac{1}{(\sigma_{y2} - R_2)^2} - \frac{1}{(\sigma_{y3} - R_3)^2} \right], \\ L &= \frac{1}{2} \left[\frac{1}{(\sigma_{y23} - R_{23})^2} \right], \\ M &= \frac{1}{2} \left[\frac{1}{(\sigma_{y13} - R_{13})^2} \right], \\ N &= \frac{1}{2} \left[\frac{1}{(\sigma_{y12} - R_{12})^2} \right], \end{aligned} \quad (4.11)$$

where $\sigma_{y1}, \sigma_{y2}, \sigma_{y3}, \sigma_{y23}, \sigma_{y13}$ and σ_{y12} are the initial yield stresses. It should be noted that the

isotropic hardening stresses R_4 , R_5 , and R_6 correspond to R_{23} , R_{13} , and R_{12} , respectively.

The final form of the constitutive equations of the model is summarized below:

- Stress tensor

$$\boldsymbol{\sigma} = \frac{\partial \psi_e}{\partial \boldsymbol{\varepsilon}}.$$

- Yield function

$$\Phi = \frac{1}{2} \boldsymbol{\sigma}^D \cdot \mathcal{A}[\boldsymbol{\sigma}^D] - 1.$$

- Evolution equations

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\mathcal{P} : \mathcal{A}[\boldsymbol{\sigma}^D]}{\|\mathcal{P} : \mathcal{A}[\boldsymbol{\sigma}^D]\|} \quad \text{where} \quad \mathcal{P} = \mathcal{I} - \frac{1}{3}(\mathbf{1} \otimes \mathbf{1}), \quad \dot{\kappa} = \dot{\lambda}.$$

- Kuhn-Tucker conditions

$$\dot{\lambda} \geq 0, \quad \Phi \leq 0, \quad \dot{\lambda} \Phi = 0.$$

The energy term ψ_e is specified as a linearized version of the strain energy function proposed in Reese et al. [2001] for modelling bidirectional composite materials and is given as:

$$\begin{aligned} \psi_e(\boldsymbol{\varepsilon}_e, \mathbf{M}_1, \mathbf{M}_2) = & 4K_1^{iso} (I_1)^2 + 4K_2^{iso} (I_2 + I_1) + 4K_1^{ani1} (I_4)^2 + 4K_2^{ani1} (I_5 + I_4) \\ & + 4K_1^{ani2} (I_6)^2 + 4K_2^{ani2} (I_7 + I_6) + 4K^{kop1} (I_1) (I_4) + 4K^{kop2} (I_1) (I_6) \\ & + 4K^{kop12} (I_4) (I_6) \end{aligned} \quad (4.12)$$

where I_1 and I_2 represent the first and second invariant of the elastic strain tensor. Additionally, I_4 , I_5 , I_6 , and I_7 denote the first invariant of $\boldsymbol{\varepsilon}_e \mathbf{M}_1$, $\boldsymbol{\varepsilon}_e^2 \mathbf{M}_1$, $\boldsymbol{\varepsilon}_e \mathbf{M}_2$, and $\boldsymbol{\varepsilon}_e^2 \mathbf{M}_2$, respectively.

$$\begin{aligned} I_1 &:= \text{tr} \boldsymbol{\varepsilon}_e & I_2 &:= \frac{1}{2} [(\text{tr} \boldsymbol{\varepsilon}_e)^2 - \text{tr}(\boldsymbol{\varepsilon}_e^2)] & I_4 &:= \text{tr}(\boldsymbol{\varepsilon}_e \mathbf{M}_1) & I_5 &:= \text{tr}(\boldsymbol{\varepsilon}_e^2 \mathbf{M}_1) \\ I_6 &:= \text{tr}(\boldsymbol{\varepsilon}_e \mathbf{M}_2) & I_7 &:= \text{tr}(\boldsymbol{\varepsilon}_e^2 \mathbf{M}_2) \end{aligned} \quad (4.13)$$

Furthermore, the coefficients K_1^{iso} , K_2^{iso} , K_1^{ani1} , K_2^{ani1} , K_1^{ani2} , K_2^{ani2} , K^{kop1} , K^{kop2} , and K^{kop12} are related to the Young's moduli E_1, E_2, E_3 , the Poisson's ratios $\nu_{12}, \nu_{13}, \nu_{23}$, and the shear moduli G_{12}, G_{13}, G_{23} . Also, the energy terms ψ_i^{iso} are specified as:

$$\psi_i^{iso}(\kappa) = Q_i \left(\kappa + \frac{e^{-\beta_i \kappa}}{\beta_i} \right) \quad (4.14)$$

In total, the constitutive model has 27 material parameters which are $E_1, E_2, E_3, \nu_{12}, \nu_{13}, \nu_{23}, G_{12}, G_{13}, G_{23}, \sigma_{y1}, \sigma_{y2}, \sigma_{y3}, \sigma_{y23}, \sigma_{y13}, \sigma_{y12}, Q_i (i = 1, \dots, 6)$, and $\beta_i (i = 1, \dots, 6)$. The

material parameters can be obtained by performing virtual experiments on the unidirectional composite RUC.

The numerical integration of the evolution equations is performed by means of the backward Euler integration scheme at the Gauss point level. The integrated plastic flow rule and the yield function in a residuum format reads

$$\begin{aligned} \mathbf{r} &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda} \frac{\mathcal{P} : \mathcal{A}[\boldsymbol{\sigma}^D]}{\|\mathcal{P} : \mathcal{A}[\boldsymbol{\sigma}^D]\|}, \\ r &= \Phi, \end{aligned} \quad (4.15)$$

where $\bar{\lambda} := \dot{\lambda} \Delta t$. The system of equations consists of 7 nonlinear scalar equations which are solved iteratively by means of the Newton method. The integration of the evolution equation for isotropic hardening is also descritized by means of the backward Euler integration scheme as:

$$\kappa = \kappa_n + \bar{\lambda}. \quad (4.16)$$

The accumulated plastic strain κ is computed at the end of each local Newton iteration via the converged value of the plastic multiplier $\bar{\lambda}$.

4.4.2. Parameter identification and validation

To identify the parameters of the constitutive model, the fibers are assumed to coincide with the z-direction of the cartesian coordinate system. The unidirectional composite RUC is subjected to uniaxial tension in the direction of the fibers (3-direction) and in the transverse direction of the fibers (1- or 2-direction). Furthermore, the RUC is subjected to shear in the plane of the fibers (13- or 23-plane) and shear in the plane transverse to the direction of the fibers (12-plane). From the obtained stress-strain curves, the elasticity constants $E_1 = E_2$, E_3 , ν_{12} , $\nu_{13} = \nu_{23}$, G_{12} , $G_{13} = G_{23}$ are identified. Also the uniaxial yield stresses $\sigma_{y1} = \sigma_{y2}$, σ_{y3} , as well as the shear yield stresses $\sigma_{y23} = \sigma_{y13}$, σ_{y12} , are identified.

Next, the constants of the six exponential hardening functions are identified by manually fitting the isotropic hardening stresses R_i to the flow curves obtained from the six virtual experiments. From the fits, the constants Q_i ($i = 1, \dots, 6$) and β_i ($i = 1, \dots, 6$) are identified. To confirm the fit, simulations are performed using the identified material parameters and are compared to the stress-strain curves obtained from virtual experiment. The plot of the fit is shown in Figure 4.4a and 4.4b for uniaxial tensile test in the principal material directions and shear directions, respectively. Also summarized in Table 4.4 and 4.5 are the identified anisotropic elasticity constants and plasticity constants respectively.

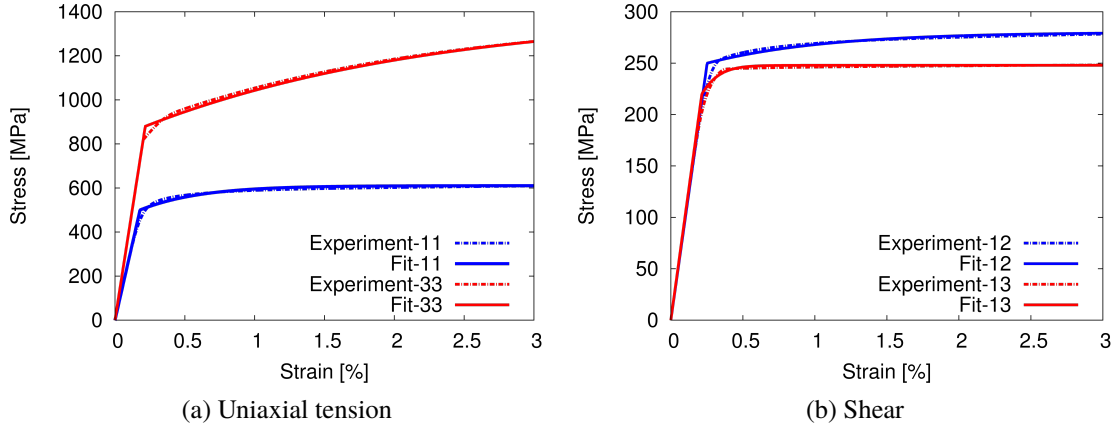


Figure 4.4.: Fit of constitutive model to uniaxial tension and shear; (a) uniaxial tension in 11- and 33-direction; (b) shear in 12- and 13-plane

Table 4.4.: Anisotropic elasticity constants

	Youngs modulus [MPa]		Shear modulus [MPa]		Poisson's ratio [-]
E_1	279211.11	G_{12}	99130.88	ν_{12}	0.36
E_3	405828.88	G_{13}	102206.22	ν_{13}	0.21

To validate the constitutive model, a geometry similar to the unidirectional composite RUC with the same mesh is generated. The geometry is assigned the constitutive model and it is subjected to periodic boundary conditions as well as the load ratios given in Table 4.3. The obtained yield surfaces resulting from the constitutive model are compared to the yield surfaces obtained from the unidirectional composite RUC. Displayed in Figures 4.6a and 4.6b are plots comparing the yield surfaces obtained from the constitutive model to those obtained from the unidirectional composite RUC in 11/22- and 22/33-principal stress space, respectively.

From Figures 4.6a and 4.6b, it can be observed that although the yield surface profile obtained from the constitutive model is in a good agreement with that obtained from the unidirectional composite RUC in the region corresponding to combined shear tensile test, some discrepancies

Table 4.5.: Plasticity constants

	σ_{yi} [MPa]	Q_i [MPa]	β_i [-]
1	500	110.4	191.6
3	880	515	41.78
13	220	27.92	1508
12	250	30.18	176.2

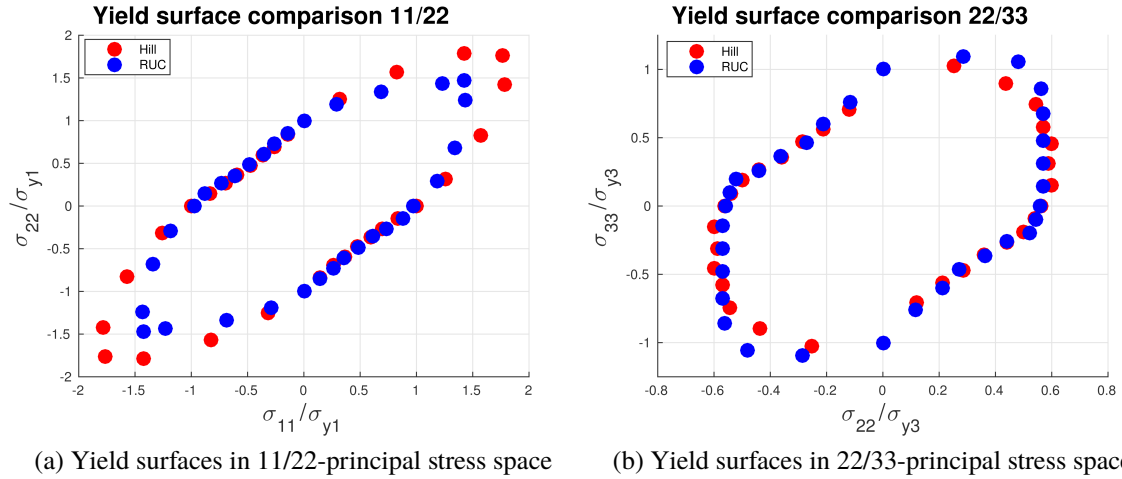


Figure 4.5.: Comparison between yield surface of constitutive model and unidirectional composite RUC in principal stress space; (a) 11/22-principal stress space normalized by uniaxial yield stress in 1-direction σ_{y1} ; (b) 22/33-principal stress space normalized by uniaxial yield stress in 3-direction σ_{y3}

are observed in the region corresponding to biaxial tensile test. This can be attributed to the fact that the yield function does not allow control of biaxial yielding. An extension of the yield function to take into account biaxial yielding could result in a better agreement between the constitutive model and the unidirectional composite RUC.

Furthermore to study the ability of the constitutive model to accurately predict lateral contraction during uniaxial tension in the principal material directions, the comparison between predicted lateral contraction versus axial strain to that generated from the unidirectional composite RUC is given in Figure 4.6.

From the plot, it can be observed that the constitutive model is able to predict the response of the unidirectional composite RUC for lateral contraction in 1-direction versus axial strain in 3-direction and also to some extent for lateral contraction in 2-direction versus axial strain in 1-direction. However, for lateral contraction in 3-direction versus axial strain in 1-direction, the curve obtained from the constitutive model differs from that obtained from the unidirectional composite RUC in the plastic flow regime. This discrepancy can be resolved by employing a non-associative flow rule which allows the plastic Poisson's ratios to be controlled.

4.5. Conclusion

The goal of this contribution was to develop a general anisotropic elastoplastic material model which is able to accurately describe the elastoplastic response of a unidirectional metallic

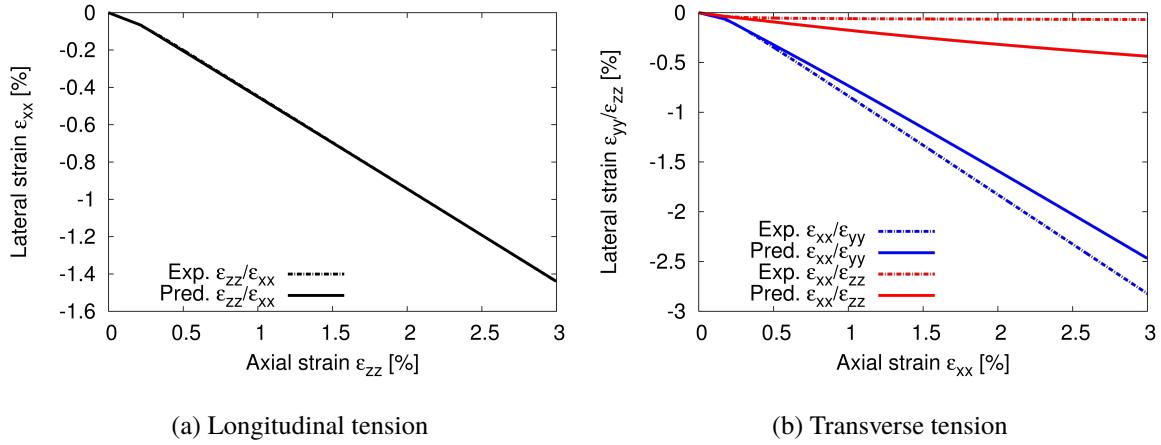


Figure 4.6.: Comparison between predicted lateral strain versus axial strain for uniaxial tension in 3- and 1-direction to that generated from the unidirectional composite RUC.

composite RUC.

For this purpose, a finite element model of the unidirectional composite was setup. It was subjected to various biaxial tensile test as well as combine shear tensile tests. From these virtual experiments, the initial yield surface of the unidirectional composite RUC was identified in principal stress-space. To capture the yield surface, a Hill type yield function was employed. Furthermore, to capture the anisotropic hardening behaviour of the yield surface, multiple isotropic hardening functions were employed. After parameter identification, through fitting the constitutive model to stress-strain curves generated from the unidirectional composite RUC, it was validated by comparing the predicted yield surface to that obtained from the RUC. Although the yield surface predicted by the constitutive model was in a good agreement with the yield surface of the RUC in regions corresponding to combined shear tensile tests, the same could not be said for regions corresponding to biaxial tensile tests. This is attributed to the fact that the yield function could not be controlled in biaxial yielding. An extension of the yield function to take into account biaxial yielding may rectify this problem. Also, the ability of the constitutive model to capture lateral strain versus axial strain response obtained from the RUC for uniaxial tension in 1- and 3-direction was investigated. Here, the response of the constitutive model was in an excellent agreement with the RUC response for lateral contraction in 1-direction versus axial strain in 3-direction and in a good agreement for lateral contraction in 2-direction versus axial strain in 1-direction. However, for lateral contraction in 3-direction versus axial strain in 1-direction, the response of the constitutive model differed from the RUC response in the plastic regime. This is attributed to lack of control of the plastic Poisson's ratios. By employing a non-associative flow rule, this problem may be rectified.

5 | Article 4:

Hierarchical modelling of flax fibre/epoxy composite by means of general anisotropic viscoelastic-viscoplastic constitutive models: Part I - Micromechanical model

This article was published as:

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Disclosure of the individual authors’ contributions to the article:

R. Bedzra formulated the actual concept, realized and implemented the model, and wrote the article. J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice. All authors drafted the work for intellectual content and approved the publication of the final version of the manuscript.

5.1. Abstract

A main problem for the development of comprehensive continuum mechanical models is the lack of experimental data. To overcome this problem, a non-associative viscoelastic-viscoplastic constitutive model which takes into account combined isotropic-kinematic hardening effects for epoxy matrix as well as a three dimensional non-associative anisotropic nonlinear elastic/plastic constitutive model for flax fibre is developed. The constitutive models are assigned to a representative volume element (RVE) of a unidirectional flax fibre/epoxy composite. Upon application of periodic boundary conditions (PBCs), different loading scenarios are subjected to the RVE and the mechanical response of the composite is studied. Based on the performed micromechanical analyses, a continuum model is developed for the unidirectional flax fibre/epoxy composite in Part II of this paper.

5.2. Introduction

Composite materials are commonly made from continuous unidirectional fibres, short fibres or textile fabrics which are embedded in a matrix material. They are extensively used in the aerospace and automotive industries due to their high stiffness-to-weight ratio, high strength, tailorability to application specific needs etc. For lightweight constructions, synthetic fibre based composites such as carbon and glass fibre in combination with thermoset or thermoplastic matrix are widely used. There are concerns however regarding the disposability of these composite materials at the end of their service life due to regulations Directive2000 [2000] concerning waste disposal. Furthermore, increasing cost of fossil resources and their depletion in the near future necessitates an investigation into the viability of natural fibre composites Saheb and Jog [1999]; Bogoeva-Gaceva et al. [2007]; Gibson [2010].

Cellulose based natural fibre composites (NFC) have been shown to display positive traits compared to synthetic fibre based composites. Primary of these traits are their low cost, lightweight, environmental friendliness (non-toxic recycling) Duigou et al. [2011] as well as their good specific mechanical properties Liang et al. [2012]; Garkhail et al. [2000]; Xie et al. [2015]. The performance of natural fibre composites such as flax fibre reinforced polymer composites (FFRP) have often been compared to glass fibre reinforced polymer composites (GFRP) Joshi et al. [2004]; Assarar et al. [2011]; Liang et al. [2012]. This is due to the performance of flax fibre which is reported to match or exceed E-glass fibre Joshi et al. [2004]. Although natural fibre composites show a lot of positive traits, there are still a lot of issues which needs to be addressed. Some of which are their limited range of operating temperatures

Dittenber and GangaRao [2012], their hydrophilic nature unless fibres are waterproofed Assarar et al. [2011]; Newman [2009], nonlinear fibre response Baley [2002]; Charlet et al. [2009]; Coroller et al. [2013], low fibre matrix bonding strength Hagstrand and Oksman [2001]; Sparnins et al. [2012]; Lu et al. [2014], limited availability of mechanical data etc. The successful application and innovation of high performance natural fibre composites depends on the understanding of their nonlinear deformation behaviour which is a first step towards the development of predictive numerical tools.

To understand the mechanical behaviour of natural fibre reinforced composites, elaborate experimental characterization of the material has to be undertaken (see e.g. Charlet et al. [2009, 2010]; Shah et al. [2012]; Charlet et al. [2007]; Mahboob, Sawi, Zdero, Fawaz and Bougherara [2017]). Semi-empirical analytical models have also been shown to reliably predict tensile modulus and strength of natural fibre composites (see e.g. Facca et al. [2006, 2007]; Shah et al. [2012]; Andersons et al. [2015]). However they are limited in scope due to their inability to capture residual inelastic effects. As a result more comprehensive constitutive models are required.

There are a number of constitutive models already available in the literature which describe various aspects of the mechanical behaviour of natural fibre reinforced composites. In Poilâne et al. [2014], a one dimensional thermodynamically consistent viscoelastic-viscoplastic constitutive model is developed for flax fibre/epoxy unidirectional plies and is validated against creep tests as well as uniaxial cyclic load unload tests carried out in the longitudinal fibre direction. The tests are undertaken at room temperature and at a particular strain rate. In a later publication Richard et al. [2018], the authors realized the model proposed in Poilâne et al. [2014] was unable to properly reproduce the experimental observation for a wide range of strain rates especially during unloading. To rectify this problem, they proposed a second model in which they introduced an internal variable which is analogous to a damage variable but results in stiffness increase as opposed to stiffness reduction. This modification led to an improved correlation between model and experiment. In Mahboob, Sawi, Zdero, Fawaz and Bougherara [2017] experimental observations are made regarding the stiffness degradation of flax/epoxy composites at room temperature. Based on this observation, the authors proposed and experimentally validated a rate-independent mesoscale (ply-level) in-plane continuum damage model in Mahboob, Chemisky, Meraghni and Bougherara [2017]. This model is based on the continuum damage framework described by Ladeveze and LeDantec [1992]; Ladeveze [1992] which has been shown to be robust in predicting damage response in composite structures under a variety of load conditions Abisset et al. [2011]; Feld et al. [2012]; Schueler et al. [2016]. The models described so far are in-plane models which do not account for out of plane

response. This requires the NFCs to be subjected to complex combined stress states which are difficult to perform experimentally and in some cases even impossible.

Micromechanical analysis however allows a detailed insight into the mechanical behaviour of the composite material by considering the influence of each constituent. This is achieved by developing proper constitutive models for each of the constituent materials in addition to homogenisation techniques which allows the possibility to perform a thorough study of the mechanical behaviour of a composite under any kind of load combinations. In Sliseris et al. [2016], a detailed micromechanical model for short flax fibre/polypropylene composite is developed. The fibres and the interface between the fibre bundles are modelled by means of a nonlocal isotropic continuum brittle damage model whereas the matrix is modelled by a standard Mises plasticity model with isotropic hardening. A mesomechanical model of flax textile/epoxy composites which takes into account tow topology is also developed in Sliseris et al. [2016]. Both models showed a good agreement with in-plane uniaxial monotonic loading experiments. Also in Panamoottil et al. [2016], an elaborate micromechanical model of a single flax/polypropylene and flax/epoxy resin impregnated yarn, composed of fibres with varying diameters, is generated. The fibres are modelled as anisotropic materials by means of a classical Hill yield function whereas the matrices are modelled as isotropic elastic-perfectly plastic materials.

The current study seeks to contribute to this development by generating a representative volume element (RVE) of a unidirectional flax fibre/epoxy composite with random fibre distribution. This is undertaken by developing a thermodynamically consistent anisotropic elastoplastic constitutive model for flax fibre which differentiates between tensile and compressive loading, accounts for lateral contraction during plastic evolution and is capable of capturing the characteristic s-shape observed in flax fibre uniaxial tensile stress-strain curves (see Charlet et al. [2009]). Furthermore, the paraboloidal yield function employed by Melro et al. [2013a] for modelling epoxy matrix is extended to account for kinematic hardening as well as viscoelastic and viscoplastic effects. The constitutive models are assigned to the generated RVE and micromechanical analyses are performed to study the deformation behaviour of the composite. A procedure for the identification of the yield surface of the composite by means of virtual experiments is also outlined. The results obtained from the micromechanical analysis will serve as a foundation for the later development of a continuum mechanical model of the composite.

5.3. Representative volume element

A continuous fibre unidirectional composite representative volume element (RVE) with random fibre distribution is generated by means of a Python script in the commercial finite element software package ABAQUS/standard Dassault systèmes [2014]. The Python script generates the RVE by randomly placing each fibre in a predefined area (determined from the fibre volume ratio, the number of fibres and the fibre diameter) subject to constraints which fulfil geometrical periodicity and the ability to mesh the generated RVE. The RVE contains a total of 12 fibres with a fibre volume ratio (total volume occupied by fibres as opposed to matrix) of 60% and a fibre diameter of $20\mu m$. The length of the RVE in transverse fibre direction (x- and y-direction) is $79.27\mu m$ whereas the length in longitudinal fibre direction (z-direction) is $0.8\mu m$. For efficiency reasons, the RVE is meshed with reduced integration eight node linear solid elements (C3D8R) with an average element size of $0.4\mu m$. Due to the fact that the RVE is considered to be part of a much larger material specimen, periodic boundary conditions (PBCs) are applied to the RVE by means of equation constraints in ABAQUS/standard Dassault systèmes [2014]. Also by applying PBCs to the RVE, it is much easier to subject the RVE to whatever stress state is desired. For details on the application of periodic boundary conditions in ABAQUS/standard Dassault systèmes [2014], see Barbero [2008]. The meshed geometry of the RVE is given in Figure 5.1.

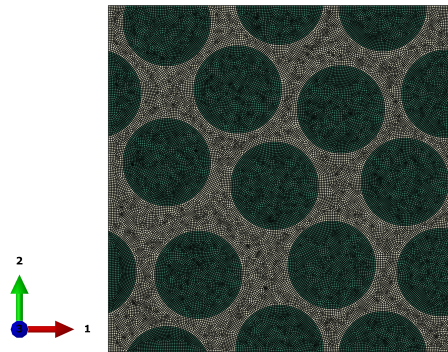


Figure 5.1.: Meshed geometry of the unidirectional composite representative volume element

5.4. Constitutive modelling

The three dimensional representative volume element of the composite considered contains two different materials which are the flax fibres and the epoxy matrix in which the fibres are embedded. Constitutive models have to be assigned to each of these materials. Furthermore,

an interface model which accounts for fibre/matrix debonding may have to be assigned to the fibre/matrix interface. However, it has been shown numerically and experimentally by Melro et al. [2013b] and Chevalier et al. [2019] to mainly lead to a reduction and underestimation of the RVE response in transverse tension and compression, respectively. Additionally for simplicity reasons, interface modelling is omitted since the initial focus is on the viscoelastic-viscoplastic response of the RVE. In what follows, constitutive models are developed for the flax fibre material and the epoxy matrix material. Both constitutive models are derived in the context of infinitesimal strain formulation.

5.4.1. Epoxy matrix

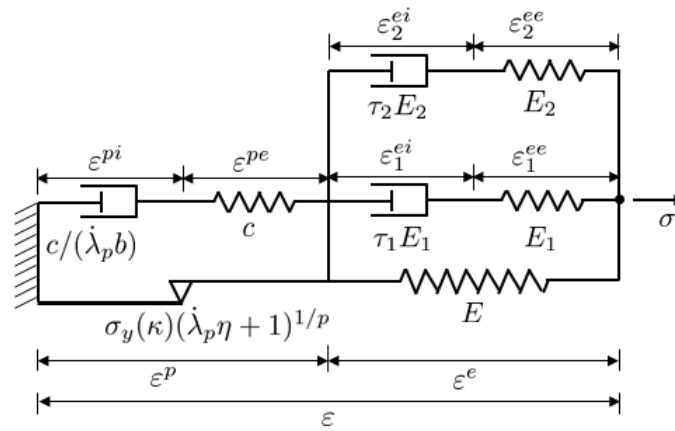


Figure 5.2.: Rheological model representation of matrix (composed of Armstrong-Frederick kinematic hardening coupled with a generalized Maxwell model).

To account for viscoelasticity, viscoplasticity as well as kinematic hardening effects, the constitutive response of epoxy matrix material is represented by the rheological model displayed in Figure 5.2. Based on this rheological model, the total strain ε is additively decomposed into an elastic part ε^e and a plastic part ε^p :

$$\varepsilon = \varepsilon^e + \varepsilon^p. \quad (5.1)$$

Additionally to account for viscoelastic effects, the elastic strain is additively split into

$$\varepsilon^e = \varepsilon_{1,2}^{ee} + \varepsilon_{1,2}^{ei}, \quad (5.2)$$

where $\varepsilon_{1,2}^{ee}$ are the strains in the two elastic springs and $\varepsilon_{1,2}^{ei}$ are the strains in the two dashpots of the generalized Maxwell model (see Figure 5.2). Furthermore to account for kinematic

hardening effects, the plastic strain is additively decomposed into

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\varepsilon}^{pe} + \boldsymbol{\varepsilon}^{pi}, \quad (5.3)$$

where $\boldsymbol{\varepsilon}^{pe}$ is the elastic part of the plastic strain and $\boldsymbol{\varepsilon}^{pi}$ is the inelastic part of the plastic strain.

The Helmholtz free energy for the epoxy matrix material ψ is then additively decomposed into six parts

$$\psi = \underbrace{\psi_e^m(\boldsymbol{\varepsilon}^e) + \psi_{ve1}^m(\boldsymbol{\varepsilon}_1^{ee}) + \psi_{ve2}^m(\boldsymbol{\varepsilon}_2^{ee})}_{\psi^e} + \underbrace{\psi_{kin}^m(\boldsymbol{\varepsilon}^{pe}) + \psi_{isot}^m(\kappa) + \psi_{isoc}^m(\kappa)}_{\psi^p}, \quad (5.4)$$

where the first part ψ_e^m represent macroscopic elastic behaviour. The second ψ_{ve1}^m and third term ψ_{ve2}^m represent the energy storage due to viscoelasticity. The fourth term ψ_{kin}^m represent the energy storage due to kinematic hardening. The fifth and sixth terms represent the additional amount of stored energy as a result of tensile and compressive isotropic hardening, respectively. The variable κ is called the isotropic hardening variable (accumulated plastic strain).

5.4.1.1. Derivation based on the Clausius-Duhem inequality

The constitutive model is derived based on the Clausius-Duhem form of the entropy inequality for isothermal processes which is given as

$$-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0, \quad (5.5)$$

where $\boldsymbol{\sigma}$ is the second order Cauchy stress tensor. A dot between two second order tensors denote their product. Differentiating (5.4) with respect to time and substituting the result into (5.5), yields

$$\begin{aligned} & \left(\boldsymbol{\sigma} - \left(\frac{\partial \psi_e^m}{\partial \boldsymbol{\varepsilon}^e} + \frac{\partial \psi_{ve1}^m}{\partial \boldsymbol{\varepsilon}_1^{ee}} + \frac{\partial \psi_{ve2}^m}{\partial \boldsymbol{\varepsilon}_2^{ee}} \right) \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\boldsymbol{\sigma} - \frac{\partial \psi_{kin}^m}{\partial \boldsymbol{\varepsilon}^{pe}} \right) \cdot \dot{\boldsymbol{\varepsilon}}^p + \frac{\partial \psi_{ve1}^m}{\partial \boldsymbol{\varepsilon}_1^{ee}} \cdot \dot{\boldsymbol{\varepsilon}}_1^{ei} + \frac{\partial \psi_{ve2}^m}{\partial \boldsymbol{\varepsilon}_2^{ee}} \cdot \dot{\boldsymbol{\varepsilon}}_2^{ei} \\ & + \frac{\partial \psi_{kin}^m}{\partial \boldsymbol{\varepsilon}^{pe}} \cdot \dot{\boldsymbol{\varepsilon}}^{pi} - \left(\frac{\partial \psi_{isot}^m}{\partial \kappa} + \frac{\partial \psi_{isoc}^m}{\partial \kappa} \right) \dot{\kappa} \geq 0. \end{aligned} \quad (5.6)$$

This inequality must be fulfilled for arbitrary thermodynamic processes, i.e. for arbitrary $\dot{\boldsymbol{\varepsilon}}$, $\dot{\boldsymbol{\varepsilon}}^p$, $\dot{\boldsymbol{\varepsilon}}_1^{ei}$, $\dot{\boldsymbol{\varepsilon}}_2^{ei}$, $\dot{\boldsymbol{\varepsilon}}^{pi}$ and $\dot{\kappa}$. This requirement leads to an expression for the Cauchy stress as

$$\boldsymbol{\sigma} = \left(\frac{\partial \psi_e^m}{\partial \boldsymbol{\varepsilon}^e} + \frac{\partial \psi_{ve1}^m}{\partial \boldsymbol{\varepsilon}_1^{ee}} + \frac{\partial \psi_{ve2}^m}{\partial \boldsymbol{\varepsilon}_2^{ee}} \right) \quad (5.7)$$

and the remaining inequality

$$\beta \cdot \dot{\epsilon}^p + \frac{\partial \psi_{ve1}^m}{\partial \epsilon_1^{ee}} \cdot \dot{\epsilon}_1^{ei} + \frac{\partial \psi_{ve2}^m}{\partial \epsilon_2^{ee}} \cdot \dot{\epsilon}_2^{ei} + \chi \cdot \dot{\epsilon}^{pi} + (R_m^t + R_m^c) \dot{\kappa} \geq 0, \quad (5.8)$$

where the following conjugate quantities to the internal variables are introduced

$$\beta = \sigma - \chi, \quad \chi = \frac{\partial \psi_{kin}^m}{\partial \epsilon^{pe}}, \quad R_m^t = -\frac{\partial \psi_{isot}^m}{\partial \kappa} \quad \text{and} \quad R_m^c = -\frac{\partial \psi_{isoc}^m}{\partial \kappa}. \quad (5.9)$$

The evolution equation for plasticity $\dot{\epsilon}^p$, kinematic hardening $\dot{\epsilon}^{pi}$ and accumulated plastic strain $\dot{\kappa}$ are specified as

$$\dot{\epsilon}^p = \dot{\lambda}_p \frac{\partial \sigma g_m}{\|\partial \sigma g_m\|}, \quad \dot{\epsilon}^{pi} = \dot{\lambda}_p \frac{b}{c} \chi \quad \text{and} \quad \dot{\kappa} = \|\dot{\epsilon}^p\| = \dot{\lambda}_p, \quad (5.10)$$

where g_m is a non-associative flow potential for plasticity (more details are given about g_m in a later section) and $\dot{\lambda}_p$ is the plastic multiplier. The form of the evolution equation for kinematic hardening (6.10)₂ corresponds to the nonlinear kinematic hardening rule of Armstrong and Frederick [n.d.], which can be derived from the rheological model given in Figure 5.2. Additionally, the constants b and c are nonlinear kinematic hardening material parameters which represent the initial kinematic hardening modulus and the rate of change of the kinematic hardening modulus, respectively.

The evolution equations for viscoelasticity $\dot{\epsilon}_1^{ei}$ and $\dot{\epsilon}_2^{ei}$ are derived from Figure 5.2 as

$$\dot{\epsilon}_1^{ei} = \frac{1}{\tau_1} (\epsilon^e - \epsilon_1^{ei}) \quad \text{and} \quad \dot{\epsilon}_2^{ei} = \frac{1}{\tau_2} (\epsilon^e - \epsilon_2^{ei}), \quad (5.11)$$

respectively, where τ_1 and τ_2 are viscoelastic material parameters. For ease of coupling viscoelasticity and plasticity, the viscoelastic evolution equations are often written in an integral form as

$$\epsilon_1^{ei}(t) = \epsilon^e(t) - \underbrace{\int_{-\infty}^t e^{\left(\frac{-(t-s)}{\tau_1}\right)} \dot{\epsilon}^e(s) ds}_{h_1} \quad \text{and} \quad \epsilon_2^{ei}(t) = \epsilon^e(t) - \underbrace{\int_{-\infty}^t e^{\left(\frac{-(t-s)}{\tau_2}\right)} \dot{\epsilon}^e(s) ds}_{h_2}, \quad (5.12)$$

(see Chung and Ryou [2009]; Miled et al. [2011]; Tjahjanto et al. [2015]) called Boltzmann hereditary integral form. In the current considerations, a similar approach is followed.

5.4.1.2. Viscoelasticity

To model the viscoelastic response of epoxy matrix, the elastic contributing part ψ^e of the free energy function which is a sum of a stationary macroscopic elastic contribution and viscoelastic contributions is specified as

$$\psi^e = \underbrace{\frac{1}{2} \boldsymbol{\varepsilon}^e \cdot \mathcal{C}_{el} [\boldsymbol{\varepsilon}^e]}_{\psi_e^m} + \underbrace{\frac{\gamma_1}{2} \boldsymbol{\varepsilon}_1^{ee} \cdot \mathcal{C}_{el} [\boldsymbol{\varepsilon}_1^{ee}]}_{\psi_{ve1}^m} + \underbrace{\frac{\gamma_2}{2} \boldsymbol{\varepsilon}_2^{ee} \cdot \mathcal{C}_{el} [\boldsymbol{\varepsilon}_2^{ee}]}_{\psi_{ve2}^m}, \quad \mathcal{C}_{el} = 2\mu \mathcal{I} + \Lambda (\mathbf{1} \otimes \mathbf{1}), \quad (5.13)$$

where $\mathcal{C}_{el}$ is the fourth order isotropic elasticity tensor which is a function of the Lamé parameters μ and Λ . The Lamé parameters are defined in terms of the standard elasticity parameters which are the Young's modulus E and the Poisson's ratio ν . Furthermore, γ_1 and γ_2 are viscoelastic material parameters. The tensors $\mathbf{1}$ and $\mathcal{I}$ denote the second and fourth order identity tensors, respectively.

By utilizing (6.7), the stress tensor is obtained as

$$\boldsymbol{\sigma} = \mathcal{C}_{el} [\boldsymbol{\varepsilon}_e + \gamma_1 (\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_1^{ei}) + \gamma_2 (\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_2^{ei})]. \quad (5.14)$$

5.4.1.3. Viscoplasticity

The epoxy matrix material is modelled based on the paraboloidal yield criterion proposed by Tschoegl [1971] which is implemented in Melro et al. [2013a] and employed in Melro et al. [2013b] for micromechanical analysis. The paraboloidal yield criterion has been shown to be the only criterion capable of capturing the multi-axial deformation behaviour of polymers, see Ghorbel [2008]. In the present contribution, it is extended to take into account kinematic hardening as well as viscoplastic effects.

To capture the hardening behaviour of the epoxy material, the plastic contributing part ψ^p of the free energy function which is a sum of kinematic hardening as well as tensile and compressive isotropic hardening energy terms is specified as

$$\psi^p = \underbrace{Q^t \left(\kappa + \frac{e^{-\beta^t \kappa} - 1}{\beta^t} \right)}_{\psi_{isot}^m} + \underbrace{Q^c \left(\kappa + \frac{e^{-\beta^c \kappa} - 1}{\beta^c} \right)}_{\psi_{isoc}^m} + \underbrace{\frac{c}{2} \boldsymbol{\varepsilon}^{pe} \cdot \boldsymbol{\varepsilon}^{pe}}_{\psi_{kin}^m}. \quad (5.15)$$

From (6.9), the thermodynamic driving forces associated with tensile and compressive

isotropic hardening behaviour are obtained as

$$R_m^t = -Q^t (1 - e^{-\beta^t \kappa}) \quad \text{and} \quad R_m^c = -Q^c (1 - e^{-\beta^c \kappa}), \quad (5.16)$$

respectively. The parameters Q^t , β^t , Q^c and β^c are responsible for describing isotropic hardening. The form of the isotropic hardening stresses are of a Vocé type exponential form, see for example Chaboche [1989]. More details of their physical meaning are discussed in Section 5.5.1. Also from (6.9)₂, the conjugate variable associated with kinematic hardening (back stress) χ is expressed as

$$\chi = c \epsilon^{pe} = c (\epsilon^p - \epsilon^{pi}), \quad (5.17)$$

where the second order strain like variable ϵ^{pe} is related to self equilibrating residual stresses that remain after elastic unloading.

Employing (5.15), (5.16) and (5.17), the extended yield function is defined as

$$\Phi^m = 3 (\beta^D \cdot \beta^D) + 2 (\beta \cdot \mathbf{1}) (\tilde{\sigma}_y^c - \tilde{\sigma}_y^t) - 2 \tilde{\sigma}_y^c \tilde{\sigma}_y^t, \quad \beta^D = \beta - \frac{1}{3} (\beta \cdot \mathbf{1}) \mathbf{1}, \quad (5.18)$$

where the material hardening functions $\tilde{\sigma}_y^c$ and $\tilde{\sigma}_y^t$ which control plastic evolution in compression and in tension are defined as

$$\tilde{\sigma}_y^c = (\sigma_y^c - R_m^c) (\dot{\kappa} \eta^c + 1)^{1/p^c} \quad \text{and} \quad \tilde{\sigma}_y^t = (\sigma_y^t - R_m^t) (\dot{\kappa} \eta^t + 1)^{1/p^t}, \quad (5.19)$$

respectively. The material parameters σ_y^t and σ_y^c represent the yield stress in tension and in compression, respectively. The factors $(\dot{\kappa} \eta^c + 1)^{1/p^c}$ and $(\dot{\kappa} \eta^t + 1)^{1/p^t}$ introduce the viscoplastic behaviour of the material. Furthermore, η^c , p^c , η^t and p^t are material parameters which control the viscoplastic response of the yield function. The definition of the hardening functions are analogous to a Peric type viscoplastic law, see Perić [1993]. The yield function converges to a rate independent plasticity model as $p^{c,t} \rightarrow \infty$ and $\eta^{c,t} \rightarrow 0$.

To account for the correct volumetric deformation during plastic flow, the following non-associative flow potential is specified

$$g_m = \frac{3}{2} (\beta^D \cdot \beta^D) + \frac{\alpha_m}{9} (\beta \cdot \mathbf{1})^2, \quad (5.20)$$

where α_m is a material parameter responsible for the correct definition of the volumetric plastic flow and can be identified by following the procedure outlined in Melro et al. [2013a] (for

$\chi = 0$). This leads to the following expression

$$\alpha_m = \frac{9(1 - 2\nu^p)}{2(1 + \nu^p)}. \quad (5.21)$$

The flow potential parameter α_m has to satisfy the following condition $\alpha_m \geq 0$ to ensure thermodynamic consistency, see C.1 for details.

The set of constitutive equations is completed by the Kuhn-Tucker conditions $\dot{\lambda}_p \geq 0$, $\Phi^m \leq 0$, and $\dot{\lambda}_p \Phi^m = 0$. The final form of the constitutive equations is summarized below:

- Stress tensors

$$\boldsymbol{\sigma} = \mathcal{C}_{\text{el}} \left[\boldsymbol{\varepsilon}^e + \gamma_1 (\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_1^{ei}) + \gamma_2 (\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_2^{ei}) \right], \quad \chi = c (\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}^{pi}).$$

- Yield function and flow potential

$$\Phi^m = 3 (\boldsymbol{\beta}^D \cdot \boldsymbol{\beta}^D) + 2 \text{tr}(\boldsymbol{\beta}) (\tilde{\sigma}_y^c - \tilde{\sigma}_y^t) - 2 \tilde{\sigma}_y^c \tilde{\sigma}_y^t, \quad g_m = \frac{3}{2} (\boldsymbol{\beta}^D \cdot \boldsymbol{\beta}^D) + \frac{\alpha_m}{9} (\boldsymbol{\beta} \cdot \mathbf{1})^2.$$

- Evolution equations

$$\boldsymbol{\varepsilon}_{1,2}^{ei}(t) = \boldsymbol{\varepsilon}^e(t) - \mathbf{h}_{1,2}, \quad \dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda}_p \frac{\partial_{\boldsymbol{\sigma}} g_m}{\|\partial_{\boldsymbol{\sigma}} g_m\|}, \quad \dot{\boldsymbol{\varepsilon}}^{pi} = \dot{\lambda}_p \frac{b}{c} \chi, \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}^p\| = \dot{\lambda}_p.$$

- Kuhn-Tucker conditions

$$\dot{\lambda}_p \geq 0, \quad \Phi^m \leq 0, \quad \dot{\lambda}_p \Phi^m = 0.$$

Remark 1. As opposed to the flow potential for the kinematic hardening constitutive model proposed in Vyas et al. [2011], the current flow potential is defined in terms of $\boldsymbol{\beta}$ instead of $\boldsymbol{\sigma}$. This is to ensure thermodynamic consistency.

For the numerical aspects of the derived matrix constitutive model, the reader is referred to C.2

5.4.2. Flax fibre

The flax fibre material is modelled as an anisotropic material with the total strain $\boldsymbol{\varepsilon}$ additively decomposed into an elastic part $\boldsymbol{\varepsilon}^e$ and a plastic part $\boldsymbol{\varepsilon}^p$ as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p. \quad (5.22)$$

The Helmholtz free energy is then specified as

$$\psi = \psi_e^f(\boldsymbol{\varepsilon}^e, \mathbf{M}_1) + \psi_{iso}^f(\kappa), \quad (5.23)$$

where the first part ψ_e^f represent anisotropic macroscopic elastic behaviour and is a function of a second order tensor $\mathbf{M}_1 = \mathbf{n}_1 \otimes \mathbf{n}_1$, which is often referred to as a structural tensor. The purpose of this tensor is to describe transverse isotropic material behaviour. For a detailed discussion on structural tensors, the reader is referred to Spencer [1971]; Boehler [1979]; Zhang and Rychlewski [1990]. Here, $\mathbf{n}_1$ denotes a unit vector which points in the longitudinal fibre direction. The last term ψ_{iso}^f represents the additional amount of stored energy due to isotropic hardening and is a function of the accumulated plastic strain κ .

5.4.2.1. Derivation based on the Clausius-Duhem inequality

Differentiating (5.23) with respect to time and substituting the result into (6.5), yields the Cauchy stress

$$\boldsymbol{\sigma} = \frac{\partial \psi_e^f}{\partial \boldsymbol{\varepsilon}} \quad (5.24)$$

and the remaining inequality

$$\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}^p + R_F \dot{\kappa} \geq 0, \quad (5.25)$$

where R_F is a conjugate to κ and is expressed as

$$R_F = -\frac{\partial \psi_{iso}^f}{\partial \kappa}. \quad (5.26)$$

The evolution equation for plasticity $\dot{\boldsymbol{\varepsilon}}^p$ and accumulated plastic strain $\dot{\kappa}$ are specified as

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda}_p \frac{\partial \boldsymbol{\sigma} g_f}{\|\partial \boldsymbol{\sigma} g_f\|} \quad \text{and} \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}^p\| = \dot{\lambda}_p, \quad (5.27)$$

where g_f is a non-associative flow potential (more details are given about g_f in a later section) and $\dot{\lambda}_p$ is the plastic multiplier.

5.4.2.2. Nonlinear anisotropic elasticity

The main load bearing S2-lamella of flax fibre has a unidirectional composite like microstructure (see Baley [2002] for a graphical depiction). As a result, the flax fibre material is modelled as a transverse isotropic material. The elastic part ψ_e^f of the free energy function is then represented by a modified version of the strain energy function proposed for modelling bidirectional

composite in Reese et al. [2001] as follows:

$$\psi_e^f = 4K_1^{\text{iso}} (I_1)^2 + 4K_2^{\text{iso}} (I_2) + 4K_1^{\text{ani1}} (I_4)^2 + 4K^{\text{kop1}} I_1 I_4 + 4K_2^{\text{ani1}} (I_5 - (I_4)^2), \quad (5.28)$$

where the invariants I_1, I_2, I_4 , and I_5 are defined as

$$I_1 := \text{tr } \boldsymbol{\epsilon}^e, \quad I_2 := \frac{1}{2} ((I_1)^2 - \text{tr } (\boldsymbol{\epsilon}^e)^2), \quad I_4 := \text{tr } (\boldsymbol{\epsilon}^e \mathbf{M}_1), \quad I_5 := \text{tr } ((\boldsymbol{\epsilon}^e)^2 \mathbf{M}_1), \quad (5.29)$$

and $K_1^{\text{iso}}, K_2^{\text{iso}}, K_1^{\text{ani1}}, K_2^{\text{ani1}}$ and K^{kop1} are material parameters which are defined in terms of the engineering material parameters $E_F, E_T, \nu_{FT}, \nu_{TT}$ and G_{FT} , see D.1. The physical meaning of the engineering parameters are discussed in Section 5.5.2.

To account for the experimentally observed nonlinear stress-strain response of flax fibre (see Charlet et al. [2009]), the engineering material parameter E_F (which can be imagined as the Young's modulus in the longitudinal fibre direction) is defined as

$$E_F = \underbrace{\mu_F^t \delta_F^t \left((I_4 + 1)^{\delta_F^t - 1} + \frac{1}{2} (I_4 + 1)^{-\left(\frac{\delta_F^t}{2} + 1\right)} \right)}_{E_F^t} \chi_e^t + E_F^c \chi_e^c, \quad (5.30)$$

where the first part E_F^t is a function of the material parameters μ_F^t and δ_F^t , which are responsible for modelling the nonlinear tensile elastic behaviour of the material whereas the second part E_F^c is responsible for modelling the linear elastic response of the material in compression. An analogous expression for E_F^t is employed in Reese [2003] for modelling polyester threads. χ_e^t and χ_e^c are switch controls which are defined as

$$\chi_e^t = \frac{1}{2} (1 + \text{sign } (I_4)) \quad \text{and} \quad \chi_e^c = \frac{1}{2} (1 - \text{sign } (I_4)), \quad (5.31)$$

respectively. The purpose of the switch controls is to differentiate between tension and compression response in the longitudinal fibre direction.

Using (5.24), the stress tensor is obtained as

$$\boldsymbol{\sigma} = \frac{\partial \psi_e^f}{\partial \boldsymbol{\epsilon}} = \mathcal{C}_{\text{ani}}^f [\boldsymbol{\epsilon}^e], \quad (5.32)$$

where the fourth order transverse isotropic nonlinear elastic stiffness tensor $\mathcal{C}_{\text{ani}}^f$ is expressed

as

$$\begin{aligned}
\mathcal{C}_{\text{ani}}^f = \partial_{\epsilon^e \epsilon^e}^2 \psi_e^f = & (8K_1^{\text{iso}} + 4K_2^{\text{iso}}) \mathbf{1} \otimes \mathbf{1} - 4K_2^{\text{iso}} \mathcal{I} + 4K^{\text{kop1}} (\mathbf{1} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \mathbf{1}) \\
& + 8K_1^{\text{ani1}} (\mathbf{M}_1 \otimes \mathbf{M}_1) + 4K_2^{\text{ani1}} (\mathcal{E}^1 - 2(\mathbf{M}_1 \otimes \mathbf{M}_1)) \\
& + 4\partial_{\epsilon^e \epsilon^e}^2 K_1^{\text{iso}} (I_1)^2 + 4\partial_{\epsilon^e \epsilon^e}^2 K_1^{\text{ani1}} (I_4)^2 + 4\partial_{\epsilon^e \epsilon^e}^2 K^{\text{kop1}} I_1 I_4 \\
& + 8I_1 (\partial_{\epsilon^e} K_1^{\text{iso}} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_{\epsilon^e} K_1^{\text{iso}}) + 8I_4 (\partial_{\epsilon^e} K_1^{\text{ani1}} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \partial_{\epsilon^e} K_1^{\text{ani1}}) \\
& + 4I_4 (\partial_{\epsilon^e} K^{\text{kop1}} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_{\epsilon^e} K^{\text{kop1}}) + 4I_1 (\partial_{\epsilon^e} K^{\text{kop1}} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \partial_{\epsilon^e} K^{\text{kop1}}).
\end{aligned} \tag{5.33}$$

$\partial_{\epsilon^e \epsilon^e}^2 K_1^{\text{iso}}$, $\partial_{\epsilon^e \epsilon^e}^2 K_1^{\text{ani1}}$, $\partial_{\epsilon^e \epsilon^e}^2 K_1^{\text{kop1}}$, $\partial_{\epsilon^e} K_1^{\text{iso}}$, $\partial_{\epsilon^e} K_1^{\text{ani1}}$ and $\partial_{\epsilon^e} K_1^{\text{kop1}}$ can be obtained from the definition of the material parameters K_1^{iso} , K_1^{ani1} and K^{kop1} given in D.1. The fourth-order tensor $\mathcal{E}^1$ is expressed as

$$\mathcal{E}_{ijkl}^1 = \frac{1}{2} (M_{ik}^1 \delta_{jl} + M_{jk}^1 \delta_{ik} + M_{il}^1 \delta_{jk} + M_{jl}^1 \delta_{il}). \tag{5.34}$$

5.4.2.3. Anisotropic plasticity

To capture the experimentally observed characteristic stress-strain response of flax fibre under uniaxial tension in the longitudinal fibre direction, the isotropic hardening contribution part ψ_{iso}^f of the free energy is specified as

$$\psi_{iso}^f = \frac{H_F^l}{2} \kappa^2 + \frac{H_F^{nl}}{c_F + 1} \kappa^{c_F + 1}, \tag{5.35}$$

where H_F^l , H_F^{nl} and c_F are material parameters which together with the nonlinear elastic parameters describe the experimentally observed stress-strain response. More details are given about the material parameters in Section 5.5.2. From (5.26), the thermodynamic force conjugate associated with the accumulated plastic strain is obtained as

$$R_F = - (H_F^l \kappa + H_F^{nl} \kappa^{c_F}). \tag{5.36}$$

Employing (6.20) and (5.36), the yield function is defined as

$$\Phi^f = \zeta (\langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle)^2 - 1, \tag{5.37}$$

where ζ is a material parameter which is expressed in terms of the uniaxial tensile yield stress

in the longitudinal fibre direction Y_F^t and the isotropic hardening stress R_F , as

$$\zeta = (Y_F^t + H_F^l \kappa + H_F^{nl} \kappa^{c_F})^{-2}. \quad (5.38)$$

The expression for ζ can be derived by setting $\Phi^f = 0$ for uniaxial tension in the longitudinal fibre direction at the onset of plastic yielding. To differentiate between the material response in tension and in compression, a Macauley bracket which operates as $\langle x \rangle = 1/2 (x + |x|)$ is defined.

Also to account for the correct volumetric deformation during plastic flow, the following non-associative flow potential is postulated

$$g_f = (\boldsymbol{\sigma}^D \cdot \mathbf{M}_1)^2 + \alpha_f (\boldsymbol{\sigma} \cdot \mathbf{M}_1)^2, \quad \boldsymbol{\sigma}^D = \boldsymbol{\sigma} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \mathbf{1}, \quad (5.39)$$

where the material parameter α_f is defined in terms of the plastic Poisson's ratio ν_{FT}^p as

$$\alpha_f = \frac{2}{9} \frac{(1 - 2\nu_{FT}^p)}{\nu_{FT}^p}. \quad (5.40)$$

The plastic Poisson's ratio controls lateral contraction during plastic evolution when the material is under a uniaxial tension in the longitudinal fibre direction. For details on the derivation of α_f , see C.4. Furthermore α_f has to satisfy the following condition $\alpha_f \geq 0$ to ensure thermodynamic consistency, see C.5 for details.

The set of constitutive equations is completed by the Kuhn-Tucker conditions $\dot{\lambda}_p \geq 0$, $\Phi^f \leq 0$, and $\dot{\lambda}_p \Phi^f = 0$. The final form of the constitutive equations is summarized below:

- Stress tensor

$$\boldsymbol{\sigma} = \frac{\partial \psi_e^f}{\partial \boldsymbol{\varepsilon}}.$$

- Yield function and flow potential

$$\Phi^f = \zeta (\langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle)^2 - 1, \quad g_f = (\boldsymbol{\sigma}^D \cdot \mathbf{M}_1)^2 + \alpha_f (\boldsymbol{\sigma} \cdot \mathbf{M}_1)^2.$$

- Evolution equations

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda}_p \frac{\partial \boldsymbol{\sigma} g_f}{\|\partial \boldsymbol{\sigma} g_f\|}, \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}^p\| = \dot{\lambda}_p.$$

- Kuhn-Tucker conditions

$$\dot{\lambda}_p \geq 0, \quad \Phi^f \leq 0, \quad \dot{\lambda}_p \Phi^f = 0.$$

For the numerical aspects of the derived flax fibre constitutive model, the reader is referred to C.6.

5.5. Parameter identification

This section deals with characterization of both the epoxy matrix and the flax fibre constitutive models. This is undertaken by fitting the constitutive model to experimental data which are taken from the literature.

5.5.1. Epoxy matrix calibration

The proposed constitutive model for epoxy has a total of 19 material parameters. These are 2 isotropic linear elastic Lamé parameters μ and Λ (which are functions of Young's modulus E and Poisson's ratio ν), 4 viscoelastic parameters $\gamma_{1,2}$ and $\tau_{1,2}$ (which describe the viscoelastic response of the material), 2 initial yield stresses σ_y^t and σ_c^t (which specify the onset of yielding in tension and in compression), 4 isotropic hardening parameters Q^t , β^t and Q^c , β^c (which represent the size of the elastic domain and the rate of change of the elastic domain for tension and compression, respectively), 4 viscoplastic parameters η^t , p^t and η^c , p^c (which describe rate dependent plastic response in tension and in compression), 2 kinematic hardening parameters c and b (which represent the initial kinematic hardening modulus and the rate of change of the kinematic hardening modulus, respectively) and 1 plastic Poisson's ratio ν^p (which is responsible for modeling the correct volumetric deformation during plastic flow).

To identify the aforementioned material parameters, rate dependent uniaxial tension and compression experiments as well as cyclic load unload tests are required. Furthermore, lateral versus axial strain data is also required. In the following, the epoxy matrix constitutive model is only fitted to rate dependent uniaxial tension and compression data for epoxy which are obtained from Littell et al. [2008]. This is due to the fact that the epoxy material considered by Littell et al. [2008] shows stiffness degradation in the cyclic tests which calls for a coupled viscoelastic-viscoplastic damage model. However damage modelling is out of the scope of the current contribution. Also without measuring from lateral versus axial strain data, the elastic Poisson's ratio and the plastic Poisson's ratio for the epoxy matrix material are taken from Littell et al. [2008] and Melro et al. [2013a], respectively.

5.5.1.1. Viscoelasticity

From the aforementioned rate dependent uniaxial stress-strain data, the Young's modulus evolution with time can be measured keeping the strain constant (relaxation data). The strain should be chosen in such a manner that it is in the elastic range and not the plastic range. By analytically solving the viscoelastic evolution equations in (6.11) keeping the elastic strain constant ($\epsilon^e = \epsilon_0^e$) and assuming initial boundary conditions ($\epsilon_{1,2}^{ei}(t=0) = 0$), analytical solutions are obtained for the viscoelastic evolution equations as

$$\epsilon_{1,2}^{ei} = \epsilon_0^e \left(1 + \gamma_{1,2} \exp \left(\frac{-t}{\tau_{1,2}} \right) \right). \quad (5.41)$$

By substituting the resulting viscoelastic evolution equations into (5.14), the stress tensor σ can be related to the constant elastic strain ϵ_0^e as

$$\sigma = \mathcal{C}_{el} \left(1 + \gamma_1 \exp \left(\frac{-t}{\tau_1} \right) + \gamma_2 \exp \left(\frac{-t}{\tau_2} \right) \right) [\epsilon_0^e]. \quad (5.42)$$

From the expression of the stress tensor in (5.42), the evolution of the viscoelastic stiffness can be approximated by the following function

$$E_{rel}(t) = E_m \left(1 + \gamma_1 \exp \left(\frac{-t}{\tau_1} \right) + \gamma_2 \exp \left(\frac{-t}{\tau_2} \right) \right). \quad (5.43)$$

By fitting (5.43) to the relaxation data, the viscoelastic parameters $\gamma_{1,2}$ and $\tau_{1,2}$ are identified. After identifying the parameters $\gamma_{1,2}$ and $\tau_{1,2}$, the stationary elastic Young's modulus E is identified making use of the relation

$$E = \frac{E_{rel}(t = 10 \text{ sec})}{\left(1 + \gamma_1 \exp \left(\frac{-10 \text{ sec}}{\tau_1} \right) + \gamma_2 \exp \left(\frac{-10 \text{ sec}}{\tau_2} \right) \right)}, \quad (5.44)$$

where $E_{rel}(t = 10 \text{ sec})$ is the instantaneous Young's modulus measured from the rate dependent uniaxial stress-strain experiment at time $t = 10 \text{ sec}$. The identified viscoelastic material parameters are listed in Table 5.1.

5.5.1.2. Viscoplasticity

By taking the time derivative of the backstress tensor χ (5.17), taking into account the plastic evolution equation $\dot{\epsilon}^p$ (6.10)₁, the kinematic hardening evolution equation $\dot{\epsilon}^{pi}$ (6.10)₂ and the accumulated plastic strain evolution equation $\dot{\kappa}$ (6.10)₃ together with the initial boundary

condition $\chi (\kappa = 0) = \mathbf{0}$, an analytical solution can be derived for the backstress tensor as

$$\chi = \frac{\partial_{\sigma} g_m}{\|\partial_{\sigma} g_m\|} \frac{c}{b} (1 - e^{-b\kappa}). \quad (5.45)$$

By substituting (6.40) into the matrix yield function Φ^m (5.18), the uniaxial tensile stress σ_t and the uniaxial compressive stress σ_c can be related to the plastic strain ε_{11}^p as

$$\begin{aligned} \sigma_t &= \frac{1}{2} (\tilde{\sigma}_y^t - \tilde{\sigma}_y^c) + an(1 + \nu^p) + \frac{1}{2} \sqrt{(\tilde{\sigma}_y^t + \tilde{\sigma}_y^c)^2 + 12an\nu^p (\tilde{\sigma}_y^t - \tilde{\sigma}_y^c)}, \\ \sigma_c &= \frac{1}{2} (\tilde{\sigma}_y^c - \tilde{\sigma}_y^t) - an(1 + \nu^p) + \frac{1}{2} \sqrt{(\tilde{\sigma}_y^c + \tilde{\sigma}_y^t)^2 - 12an\nu^p (\tilde{\sigma}_y^c - \tilde{\sigma}_y^t)}, \end{aligned} \quad (5.46)$$

where

$$an = \frac{(\partial_{\sigma} g_m)_{11}}{\|\partial_{\sigma} g_m\|} \frac{c}{b} (1 - e^{-b\kappa}) \quad \text{and} \quad \kappa = \frac{\|\partial_{\sigma} g_m\|}{(\partial_{\sigma} g_m)_{11}} \varepsilon_{11}^p. \quad (5.47)$$

The relation between the uniaxial plastic strain ε_{11}^p and the accumulated plastic strain κ is derived by substituting (6.10)₃ into (6.10)₁.

By simultaneously fitting (5.46)₁ and (5.46)₂ by means of e.g. least squares fit to tensile and compressive rate dependent stress-strain curves, respectively, the material parameters of the yield function can be identified. However to reduce the complexity of the fitting process, the equations are first fitted to the stress-strain curves at the lowest strain rate (in this case at $t = 10^5$ sec) without taking into account the effect of viscoplasticity. This is done by choosing the viscoplastic material parameters (η^t, p^t, η^c, p^c) in such a way that the constitutive model behaves like a rate independent model. After identifying the yield stresses, the parameters of the isotropic hardening functions as well as the kinematic hardening parameters, the viscoplastic material parameters are identified by fitting the equations in (5.46) to stress-strain curves at other strain rates. The identified material parameters are summarized in Table 5.1. Figures 5.3 and 5.4 shows the fit of the matrix constitutive model to rate dependent uniaxial tensile and compression stress-strain curves, respectively. The fit indicate a good agreement between the constitutive model and the experimental data.

Table 5.1.: Epoxy matrix material parameters

E [MPa]	ν	γ_1	γ_2	τ_1 [sec]	τ_2 [sec]	ν^p	σ_y^t [MPa]
2362.16	0.4	0.00005	0.09	0.19	13080	0.3	30
σ_y^c [MPa]	Q^t [MPa]	Q^c [MPa]	β^t	β^c	c [MPa]	b	$\eta^t = \eta^c$ [sec]
40	3.85	6.63	633.89	1181	2637.75	74.94	1.25E9
p^t	p^c						
20.88	21.09						

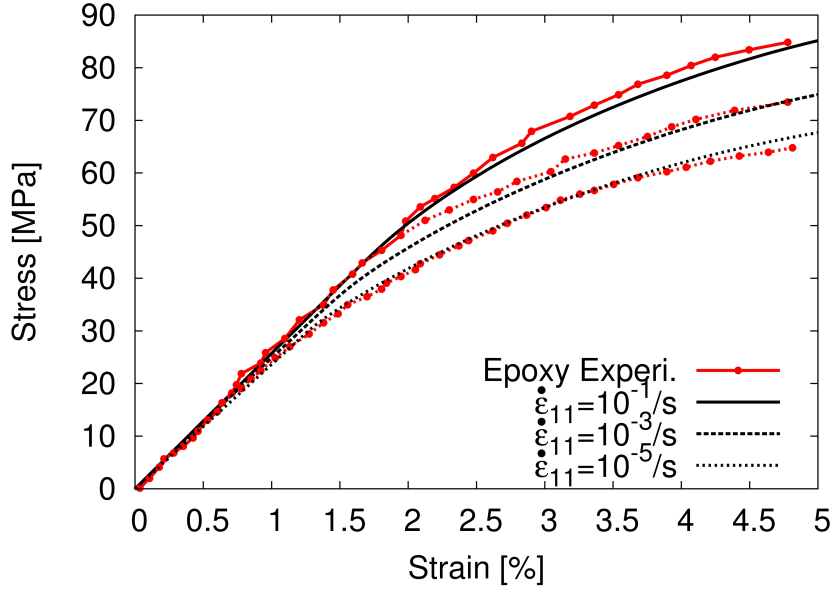


Figure 5.3.: Fit of constitutive model to rate-dependent tensile stress-strain curves obtained from Littell et al. [2008].

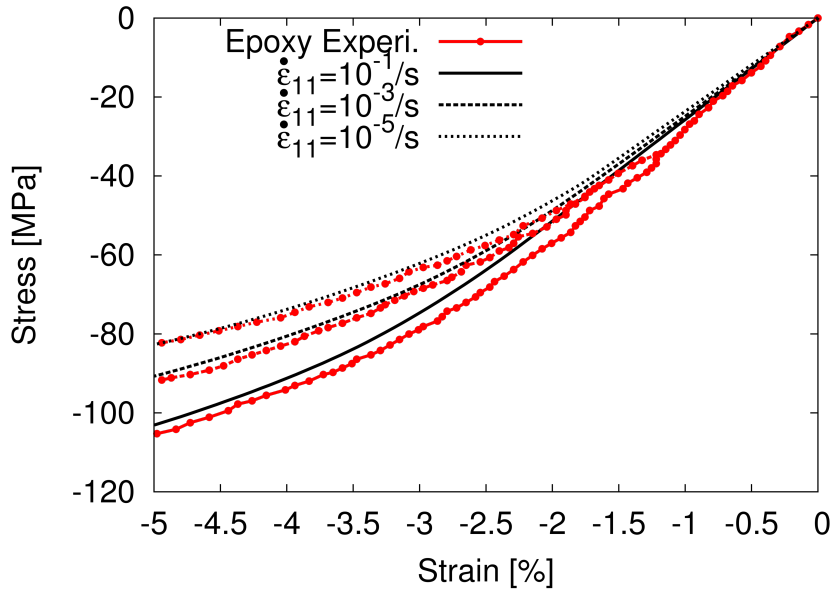


Figure 5.4.: Fit of constitutive model to rate-dependent compressive stress-strain curves obtained from Littell et al. [2008].

Remark 2. The effect of defining the flow potential in terms of β instead of only the Cauchy stress tensor σ is displayed in Figure 5.5. From the plot, it can be observed that with increasing plastic strain, the dependence of the flow potential g_m on the back stress tensor χ leads to

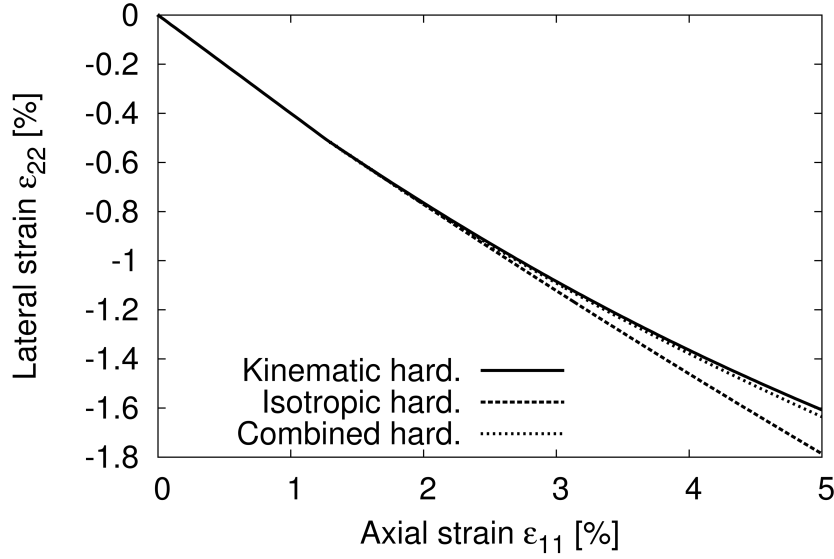


Figure 5.5.: Plot of axial versus lateral strain for isotropic hardening, kinematic hardening, and combined isotropic-kinematic hardening.

a nonlinear lateral/axial strain response (see kinematic hardening and combined hardening). This can be attributed to the fact that under uniaxial tension, the lateral components of the backstress tensor ($\chi_{22} \neq 0$, $\chi_{33} \neq 0$) are not zero, due to the dependence of the backstress tensor on the plastic strain ϵ^p (see (5.17)). This results in the nonlinear versus axial plastic strain response.

5.5.2. Flax fibre material calibration

The proposed constitutive model for flax fibre has a total of 12 material parameters. These are 7 elasticity parameters, μ_F^t and δ_F^t (which controls nonlinear elastic response for uniaxial tension in the longitudinal fibre direction), E_F^c (which controls linear elastic response during uniaxial compression in the longitudinal fibre direction), E_T (which controls linear elastic response during uniaxial tension or compression in transverse longitudinal fibre direction), ν_{FT} (which controls lateral elastic contraction in the plane of isotropy during uniaxial tension in the longitudinal fibre direction), ν_{TT} (which controls lateral elastic contraction in the plane of isotropy during uniaxial tension in transverse longitudinal fibre direction), G_{FT} (which controls linear elastic shear response in the planes defined by unit normal to the transverse longitudinal fibre direction), 1 initial yield stress Y_F^t (which controls the onset of plastic yielding in the longitudinal fibre direction), 3 isotropic hardening parameters H_F^l , H_F^{nl} , c_F and

1 plastic Poisson's ratio ν_{FT}^p (which controls lateral plastic contraction in the plane of isotropy during plastic loading in the longitudinal fibre direction). By assuming that the unit vector $\mathbf{n}_1 = [0, 0, 1]^T$ coincides with the longitudinal fibre direction, the material parameters can be expressed with respect to the Cartesian coordinate system by writing the subscripts of the material parameters making use of the convention ($F = 3, T = 1 = 2$).

Apart from μ_F^t and δ_F^t , the rest of the elasticity parameters are obtained from Panamoottil et al. [2016]. The Young's modulus for linear elastic compression in the longitudinal fibre direction E_F^c is assumed to be equal to the Young's modulus in the plane of isotropy E_T due to lack of experimental data. This assumption is reasonable since the fibre does not carry much load in compression.

Again due to the unavailability of experimental data, the plastic Poisson's ratio ν_{FT}^p is also assumed to be equal to its elastic counterpart ν_{FT} . The yield stress Y_F^t , the nonlinear elastic parameters μ_F^t , δ_F^t and the isotropic hardening parameters H_F^l , H_F^{nl} , c_F are identified by minimizing the error between uniaxial tensile experimental stress-strain data of flax fibre obtained from Charlet et al. [2009] and the stress-strain curve predicted by a one dimensional implementation of the constitutive model. The input of the constitutive model is the strain data from the uniaxial stress-strain experiment whereas the variables are the material parameters. The minimization is done by means of a nonlinear regression analysis performed in the commercial software Matlab MathWorks [2016]. Due to the fact that the fitting function is a one dimensional implementation, the accumulated plastic strain κ has to be converted to the uniaxial plastic strain using the following relation

$$\kappa = \frac{\|\partial_{\sigma} g_f\|}{(\partial_{\sigma} g_f)_{33}} \varepsilon_{33}^p. \quad (5.48)$$

The identified material parameters are summarized in Table 5.2. Figure 5.6 shows the fit of the constitutive model to the experimental data as well as an unloading and compression material response. The fit shows a good agreement between the model and the experimental data. Also from the unloading and compression part of the plot, it is clearly observed that the material shows a nonlinear elastic response during unloading and a linear elastic response during compression. Figure 5.7 shows lateral versus axial strain which depicts the effect of the plastic Poisson's ratio on the material response. As opposed to the matrix material (see Figure 5.5), the response is linear. This is due to the fact that kinematic hardening effect is not taken into account. As a result, the flow potential g_f does not depend on the components of a back stress tensor.

Table 5.2.: Flax fibre material parameters

μ_F^t [MPa]	δ_F^t	E_T [MPa]	G_{FT} [MPa]	ν_{FT}	ν_{TT}
2612	11.16	12314	3408	0.2	0.18
ν_{FT}^p	Y_F^t [MPa]	H_F^l [MPa]	H_F^{nl} [MPa]	c_F	
0.2	116.58	41174.7	3.278×10^{10}	3.648	

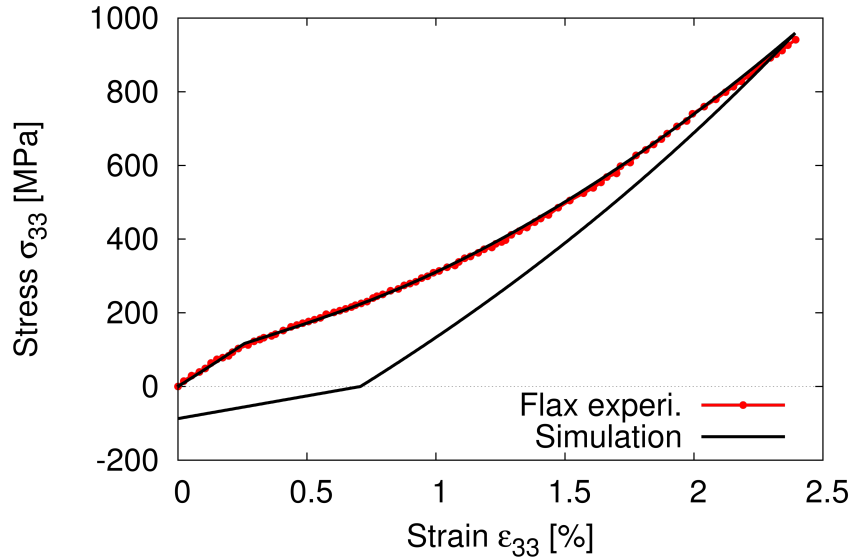


Figure 5.6.: Fit of constitutive model to flax fibre uniaxial stress-strain data obtained from Charlet et al. [2009].

5.6. Micromechanical analyses

This section deals with the study of the deformation behaviour of the composite as well as the determination of the composite yield surface. The data derived in this section will form the basis of a continuum model of the composite in Part II of this paper.

5.6.1. Composite deformation behaviour

To study the deformation behaviour of the unidirectional composite, the RVE is subjected to rate dependent transverse tension, transverse compression, longitudinal tension, longitudinal compression, transverse biaxial tension, transverse biaxial compression, transverse shear and longitudinal shear. The applied far field strain tensors for the tensile load cases are defined in Table 6.2. A change of sign in Table 6.2 will result in the compression load cases. Furthermore cyclic tests are conducted for longitudinal shear and transverse shear as well as load-unload-

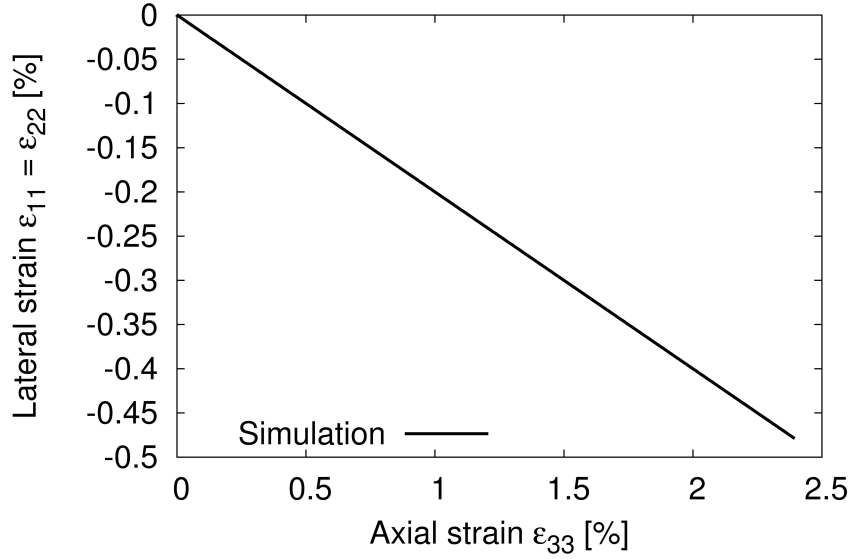


Figure 5.7.: Lateral strain evolution depicting a constant plastic Poisson's ratio.

compression-reload tests for transverse uniaxial tension and longitudinal tension. For each of the load cases, homogenized stress-strain plots are provided. Also for some of the load cases, a shot of the field distribution of accumulated plastic strain in the RVE is provided. The provided accumulated plastic strain shot corresponds to the red marking on the stress-strain curves.

Displayed in Figure 5.8 are the rate dependent stress-strain plots for transverse tension and transverse compression as well as their corresponding accumulated plastic strain distribution. The material shows a different response in tension and in compression. The rate dependent response of the material in this load regime can be seen from the linear viscoelastic effects as well as viscoplastic effects displayed in the obtained stress-strain curves. From the transverse tension accumulated plastic strain distribution in the RVE (see 5.8a), the highest plastic strains which occur in the matrix are located between fibres which are in close proximity and are in the direction of loading. For compression, shear bands are formed at an angle to the direction of loading (see 5.8b). This phenomenon has been observed by other authors (Puck and Schürmann [2002]; Melro et al. [2013b]; González and Llorca [2007]). According to these authors, the shear bands are at an angle of 53° to the direction of loading. The cyclic response of the material in transverse tension is also shown in Figure 6.12a. From the load-unload-compression-reload curve, the role of kinematic hardening can clearly be seen as a result of the early onset of plastic yielding in compression. The volumetric deformation of the composite due to transverse tension is also shown in Figure 6.13a. The plot clearly shows a more pronounced lateral contraction in the transverse fibre direction ($\epsilon_{22}/\epsilon_{11}$) as compared to

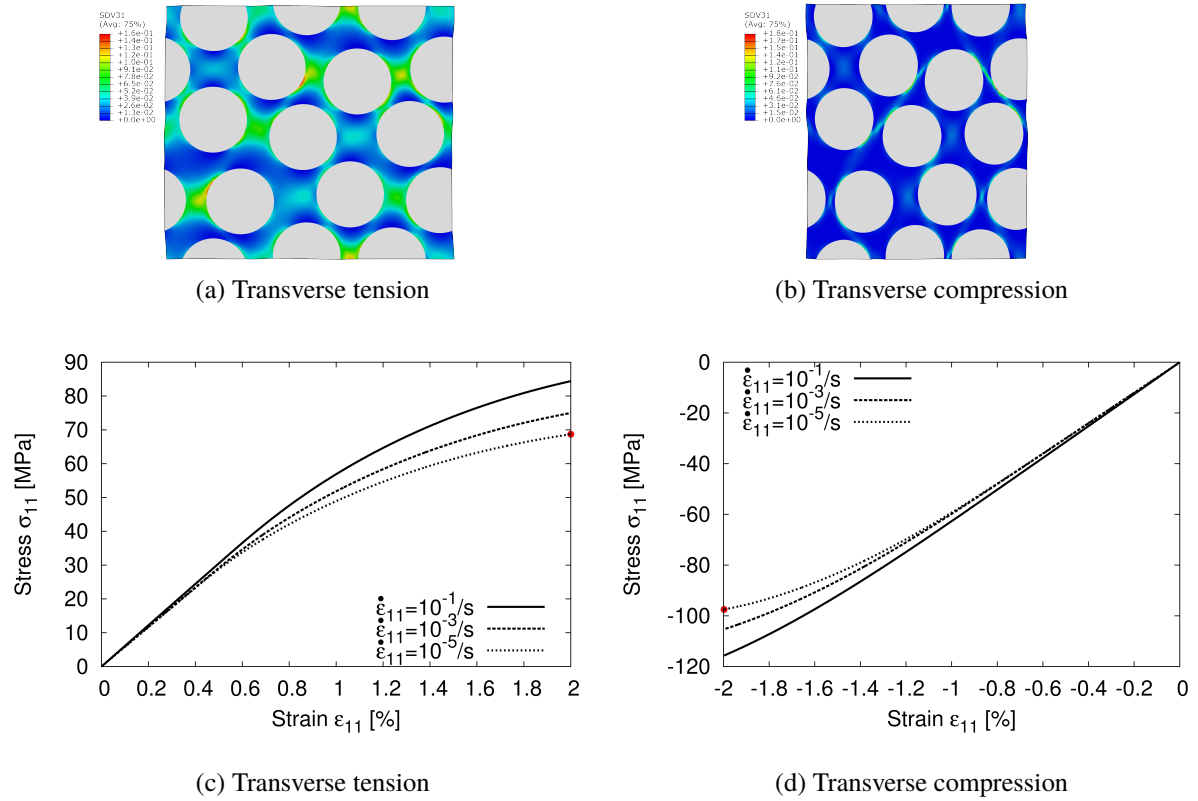


Figure 5.8.: Accumulated plastic strain plots and homogenized stress-strain curves for transverse tension and transverse compression.

Table 5.3.: Far field tensor applied for each load case

Load case	Far field strain tensor $[10^{-2}]$	Diagram
Transverse tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1$	
Longitudinal tension	$\epsilon^0 = \mathbf{e}_3 \otimes \mathbf{e}_3$	
Transverse biaxial tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2$	
Longitudinal biaxial tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_3 \otimes \mathbf{e}_3$	
Transverse shear	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1$	
Longitudinal shear	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_3$	
Transverse combined shear tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1)$	
Longitudinal combined shear tension	$\epsilon^0 = \mathbf{e}_3 \otimes \mathbf{e}_3 + (\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1)$	
Longitudinal off-axis tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_3 \otimes \mathbf{e}_3 + (\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1)$	

the lateral contraction in the longitudinal fibre direction ($\epsilon_{33}/\epsilon_{11}$).

Figure 5.9 shows rate dependent stress-strain response of the composite under longitudinal tension and compression. The material shows a difference in response for tension and compression. Furthermore, the response does not change with increasing strain rate for both longitudinal tension and compression. Also the cyclic response of the composite shows no effect of kinematic hardening (see Figure 6.12b). However from experimental observations, flax/fibre epoxy composites exhibit rate dependent response under uniaxial tension in the longitudinal fibre direction as well as kinematic-hardening effects (see Poilâne et al. [2014]; Mahboob, Chemisky, Meraghni and Bougherara [2017]). It is however not clear whether this phenomenon is as a result of fibre breakage leading to the load being carried by the polymer, which exhibits a viscoelastic-viscoplastic stiffness reduction kinematic hardening behaviour as evident from experiments (see Littell et al. [2008]; Bednarczyk et al. [2015]), or if it is as a result of a viscoelastic-viscoplastic deformation behaviour of the flax fibre. Also from experimental

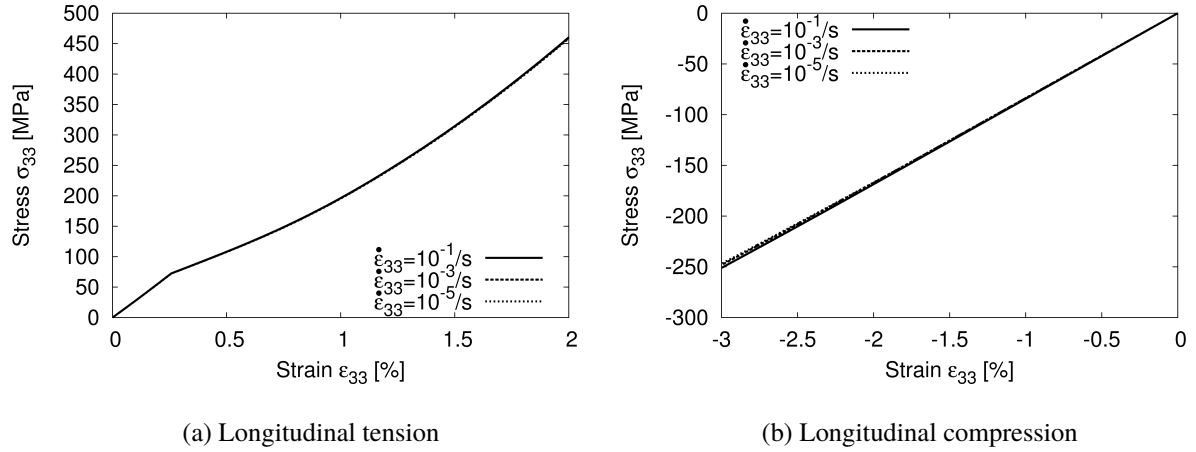


Figure 5.9.: Homogenized stress-strain curves for longitudinal tension and longitudinal compression.

observation as well as numerical studies (see Kyriakides et al. [1995]; Wind et al. [2014]; Zhou et al. [2018]), compression of unidirectional composites with initial imperfections (fibre misalignment or waviness) leads to kink band formation which results in a kink stress and a snap back. However, such an observation is not made in Figure 6.11d since flax fibre waviness or misalignment is not taken into account in the generated RVE. These effects should be investigated in future studies by first coupling the matrix material model with an isotropic non-local damage model and the fibre model with an anisotropic non-local damage model as well as taking into account fibre waviness in the generated RVE. The volumetric deformation of the composite due to longitudinal tension is shown in Figure 6.13b.

Figure 5.10 shows rate dependent biaxial tension and biaxial compression response as well as their corresponding accumulated plastic strain distribution in the RVE. The material shows high nonlinearity in biaxial tension but an almost linear response in biaxial compression. Furthermore, the rate dependence of the material in biaxial compression is very minimal and can almost be ignored. The zones in the RVE which experience the highest plastic deformation when the material is subjected to biaxial tension are the zones around the fibres. This will lead to decohesion and possible damage if an interface damage model had been employed to describe the interface between the matrix material and the fibre material as well as a coupled viscoelastic-viscoplastic nonlocal damage model for the matrix material (see for example Melro et al. [2013b]). For the case of biaxial compression, the accumulated plastic strains are minimal leading to an almost linear viscoelastic material response in compression.

Figure 6.11 shows rate dependent transverse shear and rate dependent longitudinal shear material response as well as their corresponding accumulated plastic strain distributions in the

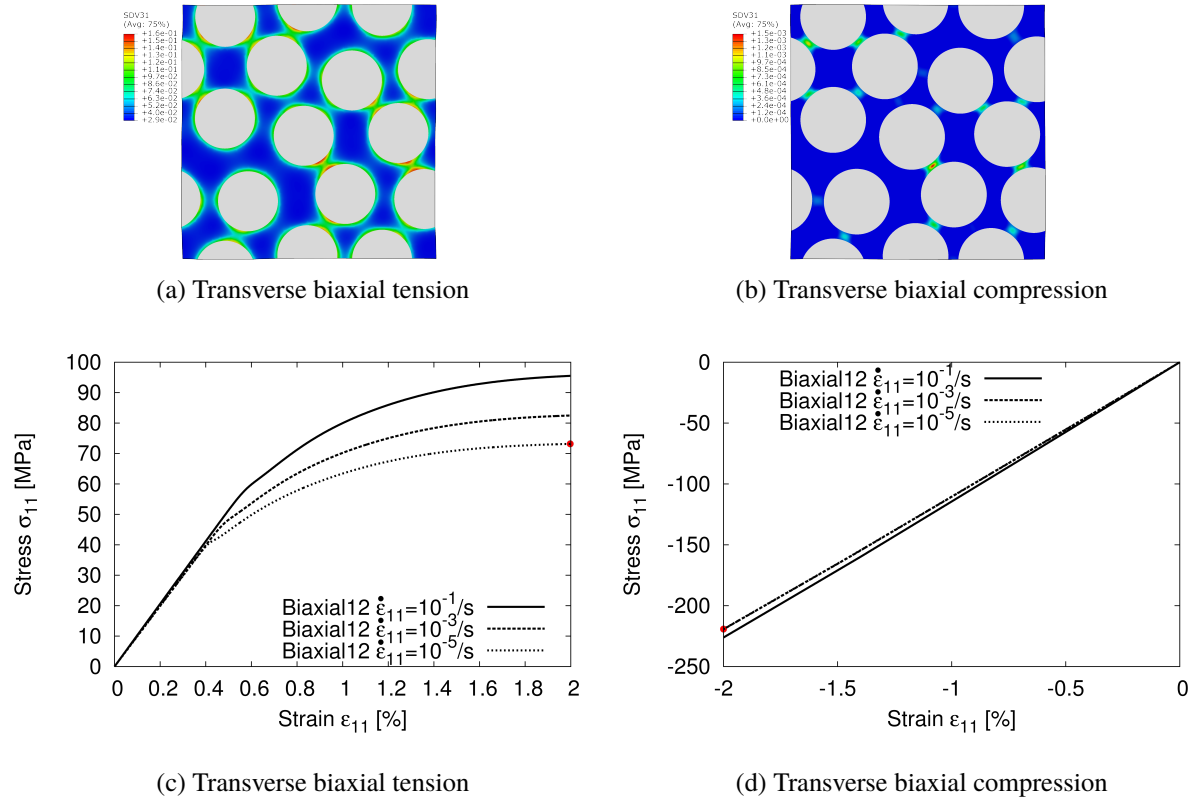


Figure 5.10.: Accumulated plastic strain plots and homogenized stress-strain curves for transverse biaxial tension and transverse biaxial compression.

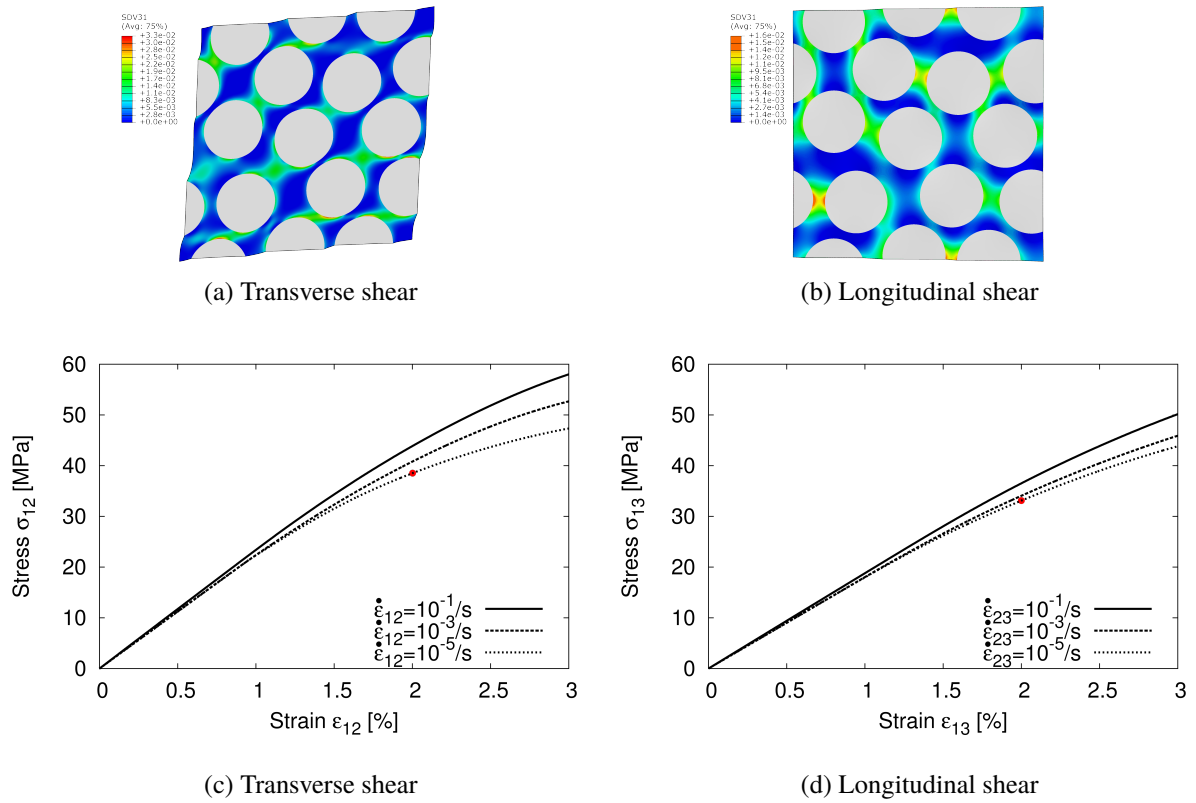


Figure 5.11.: Accumulated plastic strain plots and homogenized stress-strain curves for transverse shear and longitudinal shear.

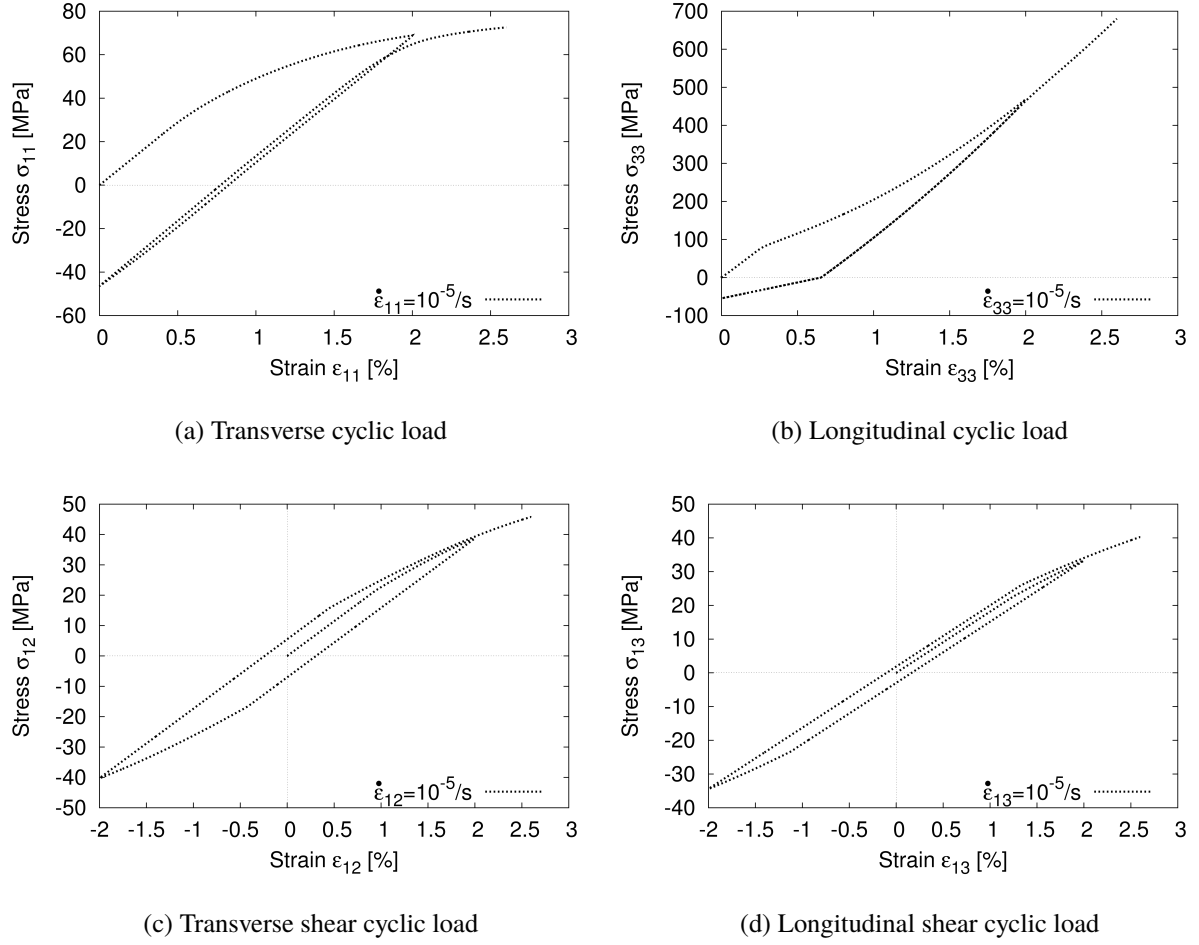


Figure 5.12.: Homogenized stress-strain curves for transverse tension cyclic load, longitudinal tension cyclic load, transverse shear cyclic load and longitudinal shear cyclic load.

RVE. The material exhibits viscoelastic response and viscoplastic response in shear loading. Furthermore, the cyclic response of the material in shear clearly shows combined isotropic-kinematic hardening effects (see Figure 6.12c and 6.12d). This is due to the fact that the matrix material bears most of the load in shear. Also from the accumulated plastic strain distribution, the highest plastic deformations occur in the direction of loading for both transverse shear and longitudinal shear.

5.6.2. Composite yield surface identification

For the purpose of the continuum mechanical model which is developed in Part II of this paper, the yield surface of the composite has to be identified. This is done by subjecting the

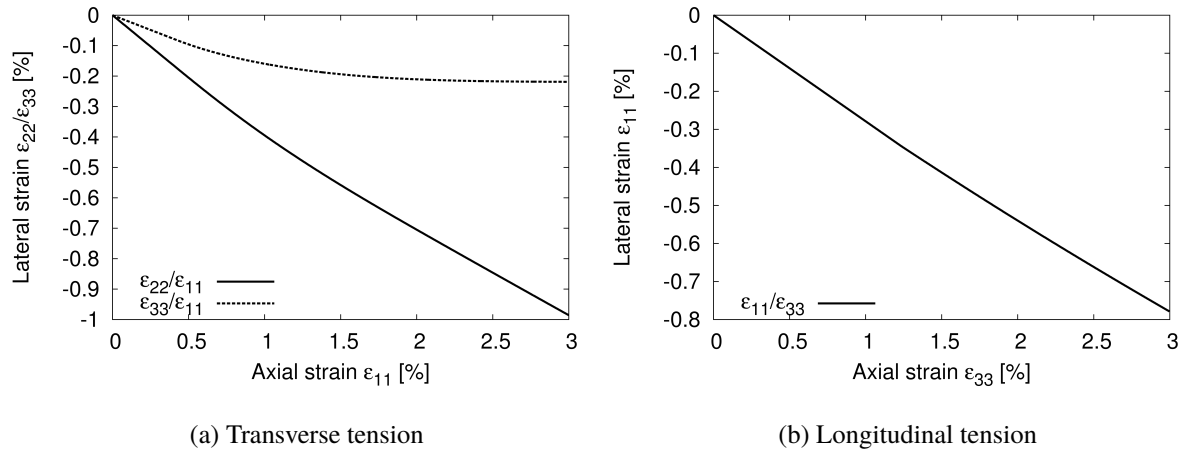


Figure 5.13.: Homogenized lateral strain versus axial strain plots for transverse tension and longitudinal tension.

unidirectional flax fibre/epoxy RVE to various biaxial tensile and compressive tests as well as combined shear tension and combined shear compression tests (see Table 6.2 for the applied far field strains). To determine the correct far field strain ϵ^0 to achieve a required stress state σ , the RVE is first subjected to a series of uniaxial tension and compression tests based on which an appropriate elastic stiffness tensor $\mathcal{C}_{\text{ani}}$ (see Part II of this paper for the form of the elastic stiffness tensor) which is able to describe the elastic response of the composite in tension and in compression is fitted. Once the fitted elastic stiffness tensor is obtained, the following formula

$$\epsilon^0 = \mathcal{C}_{\text{ani}}^{-1} [\sigma] \quad (5.49)$$

can be used to compute the required far field strain.

The yield stress which is required to plot the yield surface is determined by fitting a straight line to the linear part of the homogenized stress-strain curve obtained from a specified far field strain. The distance between the points on the straight line and the points on the stress-strain curve are measured. If the distance exceeds a specified tolerance, the discrete value of the stress corresponding to the point which exceeds the specified tolerance is considered the yield stress. The combination of applied stresses subjected to the RVE to determine the yield surface of the composite in 11/22, 12/22, 11/33, and 13/33 stress space are summarized in Table 5.4. It should be noted that to fully characterize the composite yield surfaces, the RVE has to further be subjected to the compression counterpart of the stress combinations given in Table 5.4. Due to material symmetry, it is not necessary to identify the yield surface in 22/33 and 23/33 stress space. The obtained yield surfaces in 11/22 and 12/22 stress space are displayed in Figure 6.6a,

whereas the yield surface obtained in 22/33 and 13/33 stress space are displayed in Figure 6.6b. For comparison purposes, the yield surface in 11/22 and 12/22 stress-space is compared to the paraboloidal yield function of the matrix material.

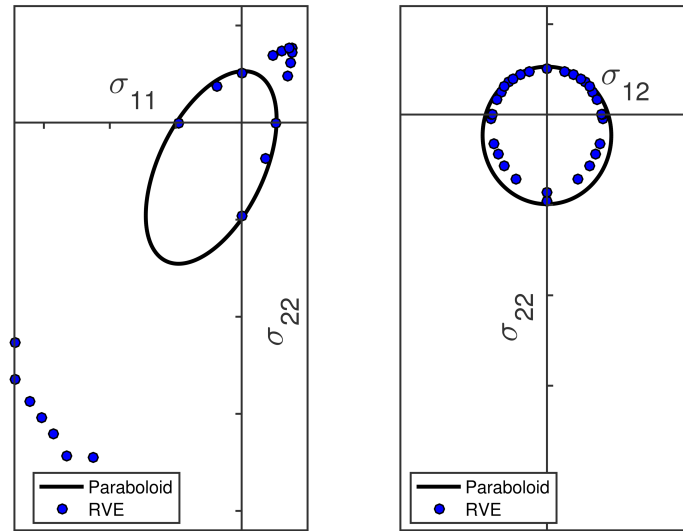
Table 5.4.: Load combinations for biaxial tensile and compressive virtual experiments as well as combined shear-tensile virtual experiments.

σ_{xx}/σ_{yy}	σ_{xx}/σ_{zz}	1/0	4/1	2/1	4/3	1/1
σ_{xx}/σ_{yy}	σ_{xx}/σ_{zz}	0/1	1/4	1/2	3/4	
σ_{xy}/σ_{yy}	σ_{xz}/σ_{zz}	1/0	4/1	2/1	4/3	1/1
σ_{xy}/σ_{yy}	σ_{xz}/σ_{zz}	0/1	1/4	1/2	3/4	
$-\sigma_{xy}/\sigma_{yy}$	$-\sigma_{xz}/\sigma_{zz}$	4/1	2/1	4/3	1/1	
$-\sigma_{xy}/\sigma_{yy}$	$-\sigma_{xz}/\sigma_{zz}$	1/4	1/2	3/4		

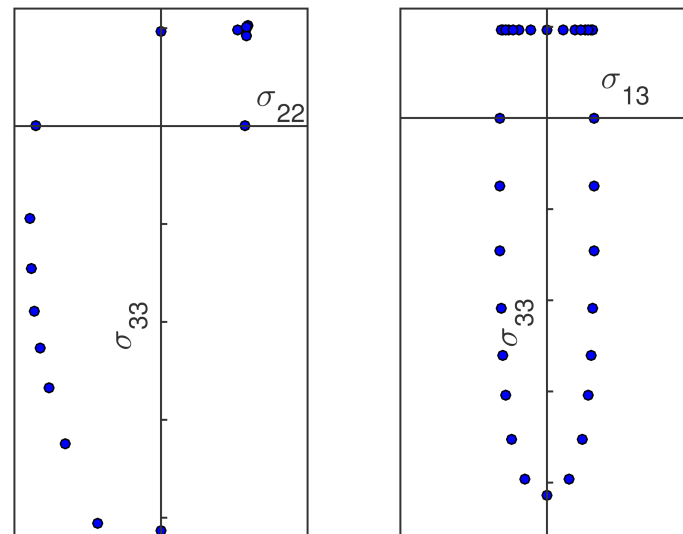
From Figure 6.6a, it is clear that the transverse biaxial yield stress in 11/22 stress space far exceeds the biaxial yield stress obtained from the paraboloidal yield function. This places the requirement of controllability on biaxial yielding in the composite plane of isotropy for any yield function of the continuum mechanical model of the composite.

5.6.3. Discussions

The current micromechanical model developed for the unidirectional flax fibre/epoxy matrix composite has not been validated against actual experiments. However before this is undertaken, a few extensions to the model may have to be carried out. The matrix material model may have to be coupled with a non-local damage model as evident in the stiffness degradation behaviour of polymer matrices (see Littell et al. [2008]; Bednarczyk et al. [2015]). Also an extension of the flax fibre constitutive model to take into account anisotropic non-local damage may have to be undertaken due to a suspected matrix dominated response as a result of fibre breakage as well as fibre waviness in the generated unidirectional composite RVE (see ??). If this does not result in the characteristic viscoelastic-viscoplastic kinematic hardening behaviour exhibited by the unidirectional flax fibre/epoxy composite specimens tested in Poilâne et al. [2014], a further extension of the flax fibre constitutive model to account for viscoelastic-viscoplastic kinematic hardening effect may have to be undertaken. The interface between the matrix material and the fibre material may have to be described by a cohesive zone model or a non-local brittle damage model as done in Sliseris et al. [2016], since this is shown to lead to a significant decrease in the obtained stress-strain response (see Melro et al. [2013b]). It is also known that flax fibres are hydrophilic (see Assarar et al. [2011]; Newman [2009]). This phenomenon if required can be taken into account by following the approach outlined in Pan



(a) Yield surface in 11/22 and 12/22 stress space



(b) Yield surface in 22/33 and 13/33 stress space

Figure 5.14.: Identified composite yield surface in stress space and comparison with a paraboloidal yield function in 11/22 and 12/22 stress space.

and Zhong [2014]. However, these are all issues to be addressed in the future.

Although the aforementioned extensions may have to be undertaken before the micromechanical model can be experimentally validated, the current model is enough to form the basis of a three dimensional viscoelastic-viscoplastic continuum mechanical model of the unidirectional flax/fibre epoxy composite.

5.7. Conclusion

The aim of the current contribution was to develop a finite element model of a unidirectional flax fibre/epoxy composite for micromechanical analyses. As part of this aim, a non-associative plasticity model which accounts for linear viscoelasticity as well as combined isotropic-kinematic hardening effects was developed for the epoxy matrix material. Additionally a three dimensional non-associative plasticity model which takes into account yielding in the longitudinal fibre direction as well as nonlinear elasticity was developed for the flax fibre material. Both constitutive models were assigned to a computer model of the unidirectional composite and micromechanical analyses were carried out. From the obtained results, the following conclusions are made regarding the development of a constitutive model for the unidirectional composite: A proper constitutive model of the composite should take into account the anisotropic viscoelastic behaviour of the composite including its nonlinear elastic response for uniaxial tension in longitudinal fibre direction. The anisotropic kinematic hardening response of the composite as well as the anisotropic viscoplastic hardening behaviour of the composite has to also be taken into account. Furthermore, the proper description of the volumetric deformation of the composite has to be undertaken. Any yield function employed to describe the onset of plastic yielding should have the ability to control biaxial yielding in the composite plane of isotropy.

6 | Article 5:

Hierarchical modelling of flax fibre/epoxy composite by means of general anisotropic viscoelastic-viscoplastic constitutive models: Part II - Mesomechanical model

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R. Bedzra formulated the actual concept, realized and implemented the model, and wrote the article. J.-W. Simon and S. Reese provided intellectual content and gave conceptual advice. All authors drafted the work for intellectual content and approved the publication of the final version of the manuscript.

6.1. Abstract

A new approach for the systematic development of constitutive models for composites is proposed. The approach relies on the generation of a representative volume element of the composite microstructure, which in this case is a flax fibre/epoxy matrix unidirectional composite. The microstructure is subjected to different deformation states based on which the deformation profile as well as the yield surface of the composite is identified. A non-associative anisotropic viscoelastic-viscoplastic continuum model is developed for the microstructure and is validated by subjecting the microstructure to other load states. The continuum model is assigned to the tows of a plain weave flax fibre/epoxy composite and the deformation behaviour of the composite is studied as well as the yield surface is identified through virtual experiments.

6.2. Introduction

Textile fabric reinforced polymer composites provide enhanced characteristics compared to unidirectional laminate composites. Some of these advantages are better drape properties and improved resistance to delamination. There are a variety of fabric architecture which depends on the undulation of the yarns, yarn crimps (bending as a result of undulations), yarn density etc. The crimps reduce stiffness and strength in the in-plane direction. In this paper, attention is restricted to the simplest of these fabrics called a plain weave. Application of woven composites in the design of parts by means of simulation tools requires detailed continuum mechanical models of the composite. As a result, a fundamental understanding of the inelastic deformation behaviour of the composite is essential. Modelling of these composites requires the consideration of different length scales. The tows or yarns are composed of fibre filaments which are embedded in a matrix material making them essentially unidirectional composites. The scale of the tow is considered as the micro-scale whereas the scale of the weave is considered as the meso-scale. There are numerous methods available in the literature for modelling and analysing plain weave composites. These can be categorized into analytical and numerical methods.

Analytical methods use mathematical relations to predict the effective mechanical response of the fabric. Some authors model the woven composite by means of classical lamination theory where a representative volume of the woven composite is idealized as a series of cross-ply laminates stacked in a sequence which mimic the woven fabric architecture. For pioneering works see Ishikawa and Chou [1982] and for various extensions to this work see Hahn and

Pandey [1994]; Vandeurzen et al. [1996*b,a*]; Ito and Chou [1997, 1998]; Scida et al. [1999]. Due to the fact that these models do not account for the crimp regions of the fabric, they are unable to accurately predict out of plane elastic response. In Barbero et al. [2005] an approach which accounts for the crimp regions of plain weave architecture is developed based on the micromechanical method introduced by Nemat-Nasser et al. [1993]. This approach yields better predictions of the elastic properties of the composite compared to the classical lamination theory approach. For a detail overview of other analytical methods, the reader is referred to Dexit and Mali [2013]. Although analytical methods are fast and are able to determine the elastic properties of the woven composite, they are limited in scope and usually do not take into account inelastic deformation effects.

Numerical methods on the other hand rely on the use of the finite element method for example to construct a full field discretization of the composite. This results in models which are able to account for the geometrical details of the fabric. To achieve greater computational efficiency, some authors employ a mix of solid elements and truss elements or only truss elements in the modelling process (see Cherouat and Billoët [2001]; Reese [2003]; McGlockton et al. [2003]; King et al. [2005]). Other authors however construct a repeating unit cell of the mesostructure of the fabric, see Dasgupta and Bhandarkar [1994]; Ng et al. [1998]; Kollegal and Sridharan [1998] for pioneering works. The level of detail taken into account in the latter approach is higher than the mixed element approach. However a major drawback is the computational effort. The repeating unit cell modelling approach is widely used in the literature. In B.Stier et al. [2015] it is used to model the elastoplastic deformation of a twill weave composite. Also in Daggumati et al. [2010]; Melro et al. [2012] it is used to study the damage behaviour of a satin weave. Furthermore it is used in Barbero et al. [2006] to model the damage behaviour of a plain weave composite. Most of the models described so far are for carbon fibre reinforced plastics. One of the few models which takes into account the in-plane deformation behaviour of a plain weave flax fibre reinforced epoxy composite is described in Sliseris et al. [2016]. Another model which takes into account the deformation behaviour of a plain weave tungsten/copper composite is developed in Bedzra et al. [2017*a*]. The difference between the latter models and the carbon fibre reinforced plastic models is the fact that the tows exhibit elastoplastic deformation. Also available are other numerical approaches e.g. the digital element method where the tow filaments are treated as beam elements with contact constraints specified between the filaments. This method is employed in Döbrich et al. [2016] for the determination of the linear elastic mechanical properties of a plain weave textile composite.

In the current contribution, the plain weave composite is modelled by means of the finite element method. The main difficulty in using this approach is the correct modelling of the

constituent materials. Most of the models described so far simplify the tow material as a coupled transverse isotropic linear elastic damage material (see e.g. Barbero et al. [2006]; Daggumati et al. [2010]; Melro et al. [2012]). This however is not the case in reality since the embedding polymer matrix usually exhibits a coupled viscoelastic-viscoplastic damage behaviour (see e.g. Littell et al. [2008]). However for carbon fibre filaments, this omission should not significantly alter the mesomechanical results due to the high stiffness of the carbon fibre material. For natural fibres such as flax fibre, it is imperative to take the viscoelastic-viscoplastic deformation behaviour of the tows into account since the fibres exhibit elastoplastic deformation (see Charlet et al. [2009]). An approach to incorporate this effect will be to simultaneously solve a two scale boundary value problem where the representative volume element (RVE) developed in Bedzra et al. [2020] determines the governing behaviour of the tow material based on far field strains from a second boundary value problem (in this case a finite element model of the woven composite). Although this approach is viable and eliminates the need for deriving a continuum mechanical model of the tow material, it is computationally expensive. For details on the aforementioned modelling approach, the reader is referred to Miehe et al. [1999]; Kanouté et al. [2009a]; Geers et al. [2010]. In this paper, the non-associative anisotropic viscoelastic-viscoplastic deformation behaviour of the unidirectional flax fibre/epoxy composite RVE observed in Bedzra et al. [2020] (which represents the tow material response) is incorporated into the tow by developing a continuum mechanical model of the RVE based on the concept of structural tensors. Structural tensors are second order tensors which are characterized by unit vectors which point in particular directions of the material. The unit vectors represent material directions which in the context of crystal plasticity may be seen as slip lines. This allows an elegant coordinate system free description of anisotropy based on the representation of the material anisotropy as a material property. The tensors may be fixed (Gaser and Holzapfe [2002]; Vladimirov et al. [2010]; Vogler et al. [2013]; Dean et al. [2016]; Bedzra et al. [2017a,b]) or may evolve with plastic flow (Reese [2003]; Svendsen et al. [2006]; Noman et al. [2010]; Pietryga et al. [2012]). The developed constitutive model is assigned to the tows of the generated plain weave composite repeating unit cell (RUC). Next, mesomechanical analyses are carried out on the plain weave RUC to study the deformation behaviour of the composite and to identify the yield surface of the composite. The derived knowledge should serve as a basis for the future development of a continuum mechanical model of the plain weave composite.

6.3. Textile composite model

A thorough description of the textile composite geometry is described in Bednarczyk et al. [2015]. However for completeness, the essential parts of the modelling approach is summarized. The geometry of the internal architecture of the RUC is represented by an idealized repeating unit cell. An alternative procedure is to construct the geometry based on computer tomography scans (CT-scan) of an actual plain weave composite which result in a geometry which is much closer to reality. The idealized plain weave repeating unit cell (RUC) geometry has a length of 3.8 mm in both x - and y -directions and a thickness of 0.4 mm (see Figure 6.1). In idealized geometry, the tows are often assumed to be elliptic which leads to a relatively low tow-to-total-volume fraction as a result of maintaining proper aspect ratios of the matrix elements between the tows due to the undulation of the tows. To overcome this problem, the cross sections of the undulating tows are varied along the length of the tows. This leads to a tow-to-total volume fraction of 0.746 as opposed to the typical values of ca 0.5 – 0.55 usually obtained for elliptic tows. With a high tow-to-total volume fraction, realistic tow fibre volumes can be assigned to the tows eliminating the need to assign high fibre volume ratios due to a reduced tow-to-total volume ratio.

Since the repeating unit cell of the plain weave is assumed to be part of a much larger material specimen, periodic boundary conditions are applied through equation constraints in the commercial finite element analysis software package ABAQUS/standard Dessault syst mes [2014]. To apply periodic boundary conditions, the mesh needs to coincide on the opposite outer faces of the RUC. This is readily achieved for the tows by sweeping the mesh along the path of the tows. For the matrix region however, only a free mesh generation is possible in Abaqus. In order to constraint the mesh in such a manner that they coincide on the outer face of the RUC, the faces of the RUC are partitioned. Once the faces are subdivided into patches, the nodal positions along the edges of the patches can be controlled. This way, a coinciding mesh is generated using the free mesh generator for the inter tow matrix. For more details on the application of periodic boundary conditions via equation constraints in ABAQUS, the reader is referred to Barbero [2008].

For efficiency reasons, reduced integration eight node linear solid elements (C3D8R) are used to discretize the tow geometry. The surrounding matrix regions are discretized with linear tetrahedral elements. In total the model is made up of 30,969 elements. A detailed representation of both the meshed tows and the RUC is displayed in Figures 6.1a and 6.1b, respectively.

The constitutive model of the unidirectional composite flax fibre/epoxy RVE which is to be

developed is assigned by a discrete definition of the fibre direction using the sweep path as the local 1-direction, the transverse direction as the local 2-direction and allowing the 3-direction to change along the path of the tow. Figure 6.1c shows the tow material directions.

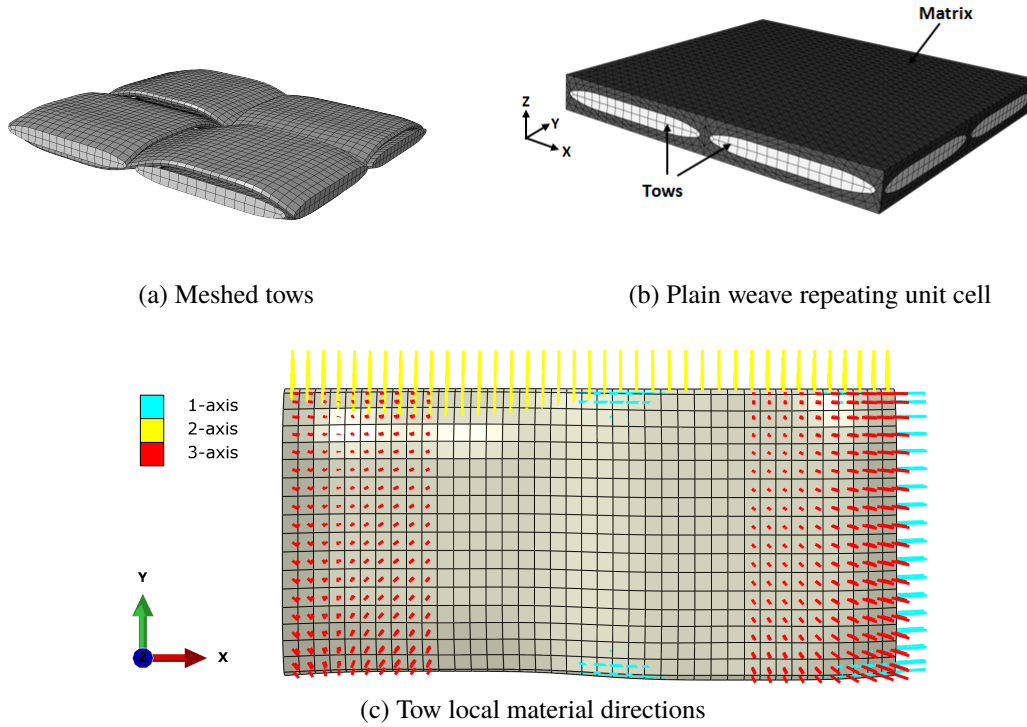


Figure 6.1.: Finite element mesh of the tows and the plain weave composite repeating unit cell

6.4. Constitutive modelling

The textile composite finite element model contains two different materials. These are the tows which are made of unidirectional flax fibre/epoxy composite as well as the epoxy matrix in which the tows are embedded. Constitutive models have to be assigned to each of these materials. A thorough description of the epoxy matrix constitutive model including its material calibration procedure is outlined in Bedzra et al. [2020]. In what follows, a constitutive model is developed for the unidirectional flax fibre/epoxy composite tows.

6.4.1. Tow

The tow material behaviour is defined by the response of the flax fibre/epoxy unidirectional composite RVE generated in Bedzra et al. [2020]. As a result, a continuum mechanical model is developed for the RVE. To account for the anisotropic viscoelastic-viscoplastic and anisotropic hardening behaviour of the RVE as well as the different response of the RVE in tension and in compression, the continuum description of the RVE is represented by an extended version of the rheological model utilized for the epoxy matrix material model in Bedzra et al. [2020] by adding extra Maxwell arms as well as extra dashpot/spring series connections to the Armstrong-Frederick kinematic hardening part of the rheological model. This leads to the additive decomposition of the total strain $\boldsymbol{\varepsilon}$ into an elastic apart $\boldsymbol{\varepsilon}^e$ and a plastic part $\boldsymbol{\varepsilon}^p$ as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad (6.1)$$

where for anisotropic viscoelastic effects, the elastic strain is additively decomposed into

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}_i^{ee} + \boldsymbol{\varepsilon}_i^{ei} \quad \forall \quad i = 1, \dots, 6. \quad (6.2)$$

$\boldsymbol{\varepsilon}_i^{ee}$ are the strains in the elastic springs and $\boldsymbol{\varepsilon}_i^{ei}$ are the strains in the dashpots of the generalized Maxwell model (see Bedzra et al. [2020] for a graphical illustration). Furthermore to account for anisotropic kinematic hardening effects, the plastic strain is additively decomposed into

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\varepsilon}_i^{pe} + \boldsymbol{\varepsilon}_i^{pi} \quad \forall \quad i = 1, 2, 3, \quad (6.3)$$

where $\boldsymbol{\varepsilon}_i^{pe}$ are the strains in the elastic springs and $\boldsymbol{\varepsilon}_i^{pi}$ are the inelastic strains in the dashpots of the generalized Armstrong-Frederick kinematic hardening rheological model.

The Helmholtz free energy ψ is then additively decomposed into eighteen parts as

$$\psi = \underbrace{\psi_{tow}^e(\boldsymbol{\varepsilon}^e, \mathbf{M}_1, \mathbf{M}_2) + \sum_{i=1}^6 \psi_i^{ve}(\boldsymbol{\varepsilon}_i^{ee}, \mathbf{M}_1)}_{\psi^e} + \underbrace{\sum_{i=1}^3 \psi_i^{kin}(\boldsymbol{\varepsilon}_i^{pe}, \mathbf{M}_1) + \sum_{i=1}^8 \psi_i^{iso}(\kappa)}_{\psi^p}, \quad (6.4)$$

where the first part ψ_{tow}^e is responsible for macroscopic anisotropic elastic deformation of the RVE and is a function of two second order tensors $\mathbf{M}_i = \mathbf{n}_i \otimes \mathbf{n}_i$ ($i = 1, 2$) called structural tensors. The structural tensors are characterized by unit vectors $\mathbf{n}_i$ which account for the directional dependence of the material and are an isotropic function of the strain energy ψ_{tow}^e . For details on structural tensors, the reader is referred to Spencer [1971]; Boehler

[1979]; Zhang and Rychlewski [1990]. The energy terms ψ_i^{ve} and ψ_i^{kin} model the transverse isotropic viscoelastic response of the RVE and the transverse anisotropic kinematic hardening deformation behaviour of the RVE, respectively, and are a function of the structural tensor $\mathbf{M}_1$. Additionally, the energy terms ψ_i^{iso} are responsible for the tension and compression anisotropic hardening deformation behaviour of the RVE. The variable κ is called the accumulated plastic strain.

6.4.1.1. Derivation based on the Clausius-Duhem inequality

The constitutive model is derived based on the Clausius-Duhem form of the entropy inequality for isothermal processes which is given as

$$-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} \geq 0, \quad (6.5)$$

where $\boldsymbol{\sigma}$ is the second order Cauchy stress tensor. A dot between two second order tensors denote their product. Differentiating (6.4) with respect to time and substituting the result into (6.5), yields

$$\begin{aligned} & \left(\boldsymbol{\sigma} - \left(\frac{\partial \psi_{tow}^e}{\partial \boldsymbol{\varepsilon}^e} + \sum_{i=1}^6 \frac{\partial \psi_i^{ve}}{\partial \boldsymbol{\varepsilon}_i^{ee}} \right) \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\boldsymbol{\sigma} - \sum_{i=1}^3 \frac{\partial \psi_i^{kin}}{\partial \boldsymbol{\varepsilon}_i^{pe}} \right) \cdot \dot{\boldsymbol{\varepsilon}}^p + \sum_{i=1}^6 \frac{\partial \psi_i^{ve}}{\partial \boldsymbol{\varepsilon}_i^{ee}} \cdot \dot{\boldsymbol{\varepsilon}}_i^{ei} \\ & + \sum_{i=1}^3 \frac{\partial \psi_i^{kin}}{\partial \boldsymbol{\varepsilon}_i^{pe}} \cdot \dot{\boldsymbol{\varepsilon}}_i^{pi} - \sum_{i=1}^8 \frac{\partial \psi_i^{iso}}{\partial \kappa} \dot{\kappa} \geq 0. \end{aligned} \quad (6.6)$$

This inequality must be fulfilled for arbitrary thermodynamic processes, i.e. for arbitrary $\dot{\boldsymbol{\varepsilon}}$, $\dot{\boldsymbol{\varepsilon}}^p$, $\dot{\boldsymbol{\varepsilon}}_i^{ei}$, $\dot{\boldsymbol{\varepsilon}}_i^{pi}$ and $\dot{\kappa}$. This requirement leads to an expression for the Cauchy stress

$$\boldsymbol{\sigma} = \frac{\partial \psi_{tow}^e}{\partial \boldsymbol{\varepsilon}^e} + \sum_{i=1}^6 \frac{\partial \psi_i^{ve}}{\partial \boldsymbol{\varepsilon}_i^{ee}} \quad (6.7)$$

and the following remaining inequality

$$\boldsymbol{\beta} \cdot \dot{\boldsymbol{\varepsilon}}^p + \sum_{i=1}^6 \frac{\partial \psi_i^{ve}}{\partial \boldsymbol{\varepsilon}_i^{ee}} \cdot \dot{\boldsymbol{\varepsilon}}_i^{ei} + \sum_{i=1}^3 \boldsymbol{\chi}_i \cdot \dot{\boldsymbol{\varepsilon}}_i^{pi} + \sum_{i=1}^8 R_i \dot{\kappa} \geq 0, \quad (6.8)$$

where the following conjugate quantities to the internal variables are introduced

$$\boldsymbol{\beta} = \boldsymbol{\sigma} - \sum_{i=1}^3 \boldsymbol{\chi}_i, \quad \boldsymbol{\chi}_i = \frac{\partial \psi_i^{kin}}{\partial \boldsymbol{\varepsilon}_i^{pe}} \quad \text{and} \quad R_i = -\frac{\partial \psi_i^{iso}}{\partial \kappa}. \quad (6.9)$$

The evolution equation for plasticity $\dot{\epsilon}^p$, kinematic hardening $\dot{\epsilon}_i^{pi}$ and accumulated plastic strain $\dot{\kappa}$ are specified as

$$\dot{\epsilon}^p = \dot{\lambda}_p \frac{\partial \sigma g_t}{\|\partial \sigma g_t\|}, \quad \dot{\epsilon}_i^{pi} = \dot{\lambda}_p \frac{b_i}{c_i} \chi_i \quad \text{and} \quad \dot{\kappa} = \|\dot{\epsilon}^p\| = \dot{\lambda}_p, \quad (6.10)$$

where g_{UD} is a non-associative flow potential which accounts for the anisotropic volumetric plastic deformation of the RVE (more details are given about g_{UD} in Section 6.4.1.4) whereas $\dot{\lambda}_p$ is the plastic multiplier. The form of the evolution equation for kinematic hardening (6.10)₂ corresponds to the nonlinear kinematic hardening rule of Armstrong and Frederick [n.d.]. Additionally, the constants b_i and c_i are nonlinear kinematic hardening material parameters which represent the initial kinematic hardening modulus and the rate of change of the kinematic hardening modulus, respectively. The evolution equations for viscoelasticity $\dot{\epsilon}_i^{ei}$ which can be derived from the generalized Maxwell model are specified as

$$\dot{\epsilon}_i^{ei} = \frac{1}{\tau_i} (\epsilon^e - \epsilon_i^{ei}), \quad (6.11)$$

where τ_i are viscoelastic material parameters, see Bedzra et al. [2020] for a graphical illustration. For ease of coupling viscoelasticity and plasticity, the viscoelastic evolution equations are often written in an integral form as

$$\epsilon_i^{ei}(t) = \epsilon^e(t) - \underbrace{\int_{-\infty}^t e^{\left(\frac{-(t-s)}{\tau_i}\right)} \dot{\epsilon}_e(s) ds}_{h_i}, \quad (6.12)$$

called Boltzmann hereditary integral form (see Chung and Ryou [2009]; Miled et al. [2011]; Tjahjanto et al. [2015]). In the current consideration, a similar approach is followed.

6.4.1.2. Nonlinear anisotropic elasticity

The elastic response of the RVE in Bedzra et al. [2020] deviates slightly from a transversely isotropic elastic material due to the obtained elastic stress-strain response of the RVE under transverse shear. To capture this deviation, an extra invariant I_{10} is introduced which leads to the following definition of ψ_{tow}^e (compare to the elastic strain energy function for flax fibre in

Bedzra et al. [2020]) as

$$\begin{aligned} \psi_{tow}^e = & 4K_1^{\text{iso}} (I_1)^2 + 4K_2^{\text{iso}} (I_2) + 4K_1^{\text{ani1}} (I_4)^2 + 4K^{\text{kop1}} I_1 I_4 + 4K_2^{\text{ani1}} (I_5 - (I_4)^2) \\ & + 4K^{\text{ani2}} \underbrace{(I_1 I_4 + I_1 I_6 - I_4 I_6 - I_2 - (I_5 + (I_6)^2))}_{I_{10}}, \end{aligned} \quad (6.13)$$

where the invariants I_1, I_2, I_4, I_5 and I_6 are defined as

$$\begin{aligned} I_1 &:= \text{tr } \boldsymbol{\varepsilon}^e, \quad I_2 := \frac{1}{2} ((I_1)^2 - \text{tr } (\boldsymbol{\varepsilon}^e)^2), \quad I_4 := \text{tr } (\boldsymbol{\varepsilon}^e \mathbf{M}_1), \quad I_5 := \text{tr } ((\boldsymbol{\varepsilon}^e)^2 \mathbf{M}_1), \\ I_6 &:= \text{tr } (\boldsymbol{\varepsilon}^e \mathbf{M}_2). \end{aligned} \quad (6.14)$$

The derived form of ψ_{tow}^e is based on the elastic strain energy function proposed in Reese [2003]. To gain a deeper insight into the purpose of invariant I_{10} , consider the situation where the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ points in the longitudinal fibre direction and $\mathbf{n}_2 = [0, 1, 0]^T$ points in the transverse fibre direction. This leads to the following definition of

$$I_{10} = \varepsilon_{23}^e \varepsilon_{32}^e. \quad (6.15)$$

From (6.15), it is clear that the purpose of I_{10} is to control elastic shear in the plane of isotropy. The material parameters $K_1^{\text{iso}}, K_2^{\text{iso}}, K_1^{\text{ani1}}, K_2^{\text{ani1}}, K^{\text{kop1}}$ and K^{ani2} are defined in terms of the engineering material parameters $E_F, E_T, \nu_{FT}, \nu_{TT}, G_{TT}$ and G_{FT} , see D.1. The physical meaning of the engineering parameters are discussed in Section 6.5.

To capture the different elastic response of the RVE in longitudinal tension and compression, the material parameter E_F is decomposed into two parts as

$$E_F = \underbrace{\mu_F^t \delta_F^t \left((I_4 + 1)^{\delta^t - 1} + \frac{1}{2} (I_4 + 1)^{-\left(\frac{\delta^t}{2} + 1\right)} \right)}_{E_F^t} \chi_e^{1t} + E_F^c \chi_{1e}^c, \quad (6.16)$$

where the first part E_F^t , which is a function of the parameters μ_F^t and δ_F^t , is responsible for the observed nonlinear elastic response of the RVE in longitudinal tension whereas the second part E_F^c is responsible for the observed linear elastic response in compression. This differentiation is enforced by the functions

$$\chi_e^{1t} = \frac{1}{2} (1 + \text{sign } (I_4)) \quad \text{and} \quad \chi_e^{1c} = \frac{1}{2} (1 - \text{sign } (I_4)). \quad (6.17)$$

Furthermore to capture the different response of the RVE in transverse tension, transverse biax-

ial tension, transverse compression and transverse biaxial compression, the material parameters E_T and ν_{TT} are also decomposed as follows

$$E_T = E_T^t \chi_e^{2t} + E_T^c \chi_e^{2c} \quad \text{and} \quad \nu_{TT} = \nu_{TT}^t \chi_e^{2t} + \nu_{TT}^c \chi_e^{2c}, \quad (6.18)$$

where E_T^t and ν_{TT}^t are responsible for the observed linear elastic response in transverse tension and transverse biaxial tension whereas E_T^c and ν_{TT}^c are responsible for the observed linear elastic response in transverse compression and transverse biaxial compression. This differentiation is enforced by the functions

$$\chi_e^{2t} = \frac{1}{2} (1 + \text{sign}(I_1 - I_4)) \quad \text{and} \quad \chi_e^{2c} = \frac{1}{2} (1 - \text{sign}(I_1 - I_4)). \quad (6.19)$$

By utilizing equation (6.7), the stationary part of the stress tensor is obtained as

$$\frac{\partial \psi_{tow}^e}{\partial \boldsymbol{\varepsilon}^e} = \mathcal{C}_{\text{ani}} [\boldsymbol{\varepsilon}^e], \quad (6.20)$$

where the fourth-order anisotropic nonlinear elastic stiffness tensor $\mathcal{C}_{\text{ani}}$ is expressed as

$$\begin{aligned} \mathcal{C}_{\text{ani}} = \partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 \psi_{tow}^e = & (8K_1^{\text{iso}} + 4K_2^{\text{iso}} - 4K^{\text{ani}2}) \mathbf{1} \otimes \mathbf{1} + (4K^{\text{ani}2} - 4K_2^{\text{iso}}) \mathcal{I} \\ & + (4K^{\text{kop1}} + 4K^{\text{ani}2}) (\mathbf{1} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \mathbf{1}) + 8K_1^{\text{ani1}} (\mathbf{M}_1 \otimes \mathbf{M}_1) \\ & + 4K_2^{\text{ani1}} (\boldsymbol{\mathcal{E}}^1 - 2(\mathbf{M}_1 \otimes \mathbf{M}_1)) \\ & - 4K^{\text{ani}2} ((\mathbf{M}_1 \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{M}_1) - (\mathbf{1} \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{1}) + (\boldsymbol{\mathcal{E}}^1 + 2(\mathbf{M}_2 \otimes \mathbf{M}_2))) \\ & + 4\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K_1^{\text{iso}} (I_1)^2 + 4\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K_1^{\text{ani1}} (I_4)^2 + 4\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K^{\text{kop1}} I_1 I_4 \\ & + 8I_1 (\partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{iso}} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{iso}}) + 8I_4 (\partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{ani1}} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{ani1}}) \\ & + 4I_4 (\partial_{\boldsymbol{\varepsilon}^e} K^{\text{kop1}} \otimes \mathbf{1} + \mathbf{1} \otimes \partial_{\boldsymbol{\varepsilon}^e} K^{\text{kop1}}) + 4I_1 (\partial_{\boldsymbol{\varepsilon}^e} K^{\text{kop1}} \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \partial_{\boldsymbol{\varepsilon}^e} K^{\text{kop1}}). \end{aligned} \quad (6.21)$$

$\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K_1^{\text{iso}}$, $\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K_1^{\text{ani1}}$, $\partial_{\boldsymbol{\varepsilon}^e \boldsymbol{\varepsilon}^e}^2 K_1^{\text{kop1}}$, $\partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{iso}}$, $\partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{ani1}}$ and $\partial_{\boldsymbol{\varepsilon}^e} K_1^{\text{kop1}}$ can be obtained from the definition of the material parameters K_1^{iso} , K_1^{ani1} and K^{kop1} given in D.1. The fourth-order tensor $\boldsymbol{\mathcal{E}}^1$ is expressed as

$$\mathcal{E}_{ijkl}^1 = \frac{1}{2} (M_{ik}^1 \delta_{jl} + M_{jk}^1 \delta_{il} + M_{il}^1 \delta_{jk} + M_{jk}^1 \delta_{il}). \quad (6.22)$$

The tensors $\mathbf{1}$ and $\mathcal{I}$ denote the second and fourth order identity tensors, respectively.

6.4.1.3. Anisotropic viscoelasticity

To model the anisotropic viscoelastic response of the RVE, the elastic contributing part ψ^e of the free energy function which is a sum of a stationary macroscopic anisotropic elastic contribution and anisotropic viscoelastic contributions is specified as

$$\begin{aligned} \psi^e = & \psi_{tow}^e + \sum_{i=1}^2 \underbrace{\frac{\gamma_i}{2} \boldsymbol{\varepsilon}_i^{ee} \cdot (\mathbf{C}_{ani} : \mathcal{H}_1) [\boldsymbol{\varepsilon}_i^{ee}]}_{\psi_i^{ve}} + \sum_{i=3}^4 \underbrace{\frac{\gamma_i}{2} \boldsymbol{\varepsilon}_i^{ee} \cdot (\mathbf{C}_{ani} : \mathcal{H}_2) [\boldsymbol{\varepsilon}_i^{ee}]}_{\psi_i^{ve}} \\ & + \sum_{i=5}^6 \underbrace{\frac{\gamma_i}{2} \boldsymbol{\varepsilon}_i^{ee} \cdot (\mathbf{C}_{ani} : \mathcal{H}_3) [\boldsymbol{\varepsilon}_i^{ee}]}_{\psi_i^{ve}}, \end{aligned} \quad (6.23)$$

where γ_i are viscoelastic material parameters which model the observed anisotropic viscoelastic response of the RVE. The fourth-order tensors $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ are projection tensors which allow the material anisotropic viscoelastic response to be taken into account and are defined as

$$\mathcal{H}_1 = (\mathbf{M}_1 \otimes \mathbf{M}_1), \quad \mathcal{H}_2 = (\mathcal{I} + (\mathbf{M}_1 \otimes \mathbf{M}_1) - \boldsymbol{\varepsilon}^1), \quad \mathcal{H}_3 = (\boldsymbol{\varepsilon}^1 - 2(\mathbf{M}_1 \otimes \mathbf{M}_1)). \quad (6.24)$$

More details are given about the projection tensors in Section 6.4.1.4.

By utilizing (6.7), the stress tensor is obtained as

$$\begin{aligned} \boldsymbol{\sigma} = & \mathbf{C}_{ani} [\boldsymbol{\varepsilon}^e] + \sum_{i=1}^2 \underbrace{\gamma_i \frac{1}{2} (\mathbf{C}_{ani} : \mathcal{H}_1 + \mathcal{H}_1 : \mathbf{C}_{ani}) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}]}_{\text{sym}(\mathbf{C}_{ani} : \mathcal{H}_1)} \\ & + \sum_{i=3}^4 \underbrace{\gamma_i \frac{1}{2} (\mathbf{C}_{ani} : \mathcal{H}_2 + \mathcal{H}_2 : \mathbf{C}_{ani}) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}]}_{\text{sym}(\mathbf{C}_{ani} : \mathcal{H}_2)} + \sum_{i=5}^6 \underbrace{\gamma_i \frac{1}{2} (\mathbf{C}_{ani} : \mathcal{H}_3 + \mathcal{H}_3 : \mathbf{C}_{ani}) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}]}_{\text{sym}(\mathbf{C}_{ani} : \mathcal{H}_3)}. \end{aligned} \quad (6.25)$$

6.4.1.4. Anisotropic viscoplasticity

To capture the yield surface obtained from the characterization of the RVE carried out in Bedzra et al. [2020], the invariant based yield function proposed by Vogler et al. [2013] is modified and extended to take into account yielding in longitudinal tension and compression, anisotropic kinematic hardening effects as well as anisotropic viscoplastic effects.

For this purpose, the plastic contributing part ψ^p of the free energy function, which is a sum of kinematic hardening energy terms as well as isotropic hardening energy terms, is specified

as

$$\psi^p = \underbrace{\frac{H_F^l}{2}\kappa^2 + \frac{H_F^{nl}}{c_F + 1}\kappa^{c_F+1}}_{\psi_1^{iso}} + \sum_{i=2}^7 \underbrace{Q_i \left(\kappa + \frac{e^{-\beta_i \kappa} - 1}{\beta_i} \right)}_{\psi_i^{iso}} + \sum_{i=1}^3 \underbrace{\frac{c_i}{2} \boldsymbol{\varepsilon}_i^{pe} \cdot \boldsymbol{\mathcal{H}}_i [\boldsymbol{\varepsilon}_i^{pe}]}_{\psi_i^{kin}}, \quad (6.26)$$

where H_F^l , H_F^{nl} , c_F , Q_i and β_i are material parameters which are responsible for describing anisotropic hardening. More details are given concerning the physical meaning of the variables in the hardening calibration procedure. The kinematic hardening parts ψ_i^{kin} of the plastic contributing part of the strain energy function can be explicitly written, assuming the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ points in the longitudinal tow direction, as

$$\begin{aligned} \psi_1^{kin} &= \frac{c_1}{2} (\varepsilon_{1,11}^{pe})^2, \quad \psi_2^{kin} = \frac{c_2}{2} \left((\varepsilon_{2,22}^{pe})^2 + (\varepsilon_{2,33}^{pe})^2 + 2\varepsilon_{2,23}^{pe}\varepsilon_{2,32}^{pe} \right) \\ \psi_3^{kin} &= c_3 (\varepsilon_{3,12}^{pe}\varepsilon_{3,21}^{pe} + \varepsilon_{3,13}^{pe}\varepsilon_{3,31}^{pe}). \end{aligned} \quad (6.27)$$

The purpose of the fourth order tensors $\boldsymbol{\mathcal{H}}_1$, $\boldsymbol{\mathcal{H}}_2$ and $\boldsymbol{\mathcal{H}}_3$ as can be seen from (6.27) is to differentiate between the observed kinematic hardening response of the RVE in longitudinal tension-unload-compression-reload, in cyclic deformation in the plane of isotropy and in cyclic longitudinal shear deformation (see Bedzra et al. [2020]).

From (6.9)₃, the thermodynamic driving forces associated with isotropic hardening are obtained as

$$R_1 = - (H_F^l \kappa + H_F^{nl} \kappa^{c_F}) \quad \text{and} \quad R_i = -Q_i (1 - e^{-\beta_i \kappa}). \quad (6.28)$$

Also from (6.9)₂, the conjugate variables associated with kinematic hardening (back stresses) $\boldsymbol{\chi}_i$ are obtained as

$$\boldsymbol{\chi}_i = c_i \boldsymbol{\mathcal{H}}_i [\boldsymbol{\varepsilon}_i^{pe}] = c_i \boldsymbol{\mathcal{H}}_i [\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_i^{pi}], \quad (6.29)$$

where the second order strain like variables $\boldsymbol{\varepsilon}_i^{pe}$ are related to self equilibrating residual stresses which remain after elastic unloading.

By employing (6.28) and (6.29), the extended yield function is defined as

$$\Phi^{\text{UD}} = \zeta_1 I_8^* + \zeta_2 I_5^* + \zeta_3^t \langle I_9^* \rangle_+ + \zeta_3^c \langle I_9^* \rangle_- + \zeta_4^t (\langle I_9^* \rangle_+)^2 + \zeta_4^c (\langle I_9^* \rangle_-)^2 + \zeta_5^t (\langle I_4^* \rangle_+)^2 + \zeta_5^c (\langle I_4^* \rangle_-)^2 - 1, \quad (6.30)$$

where ζ_1 , ζ_2 , ζ_3^t , ζ_3^c , ζ_4^t , ζ_4^c , ζ_5^t and ζ_5^c are material parameters which are expressed in terms of

the following hardening functions

$$\begin{aligned}\tilde{Y}_F^t &= (Y_F^t - R_1) (\dot{\kappa}\eta_1^t + 1)^{1/p_1^t}, & \tilde{Y}_F^c &= (Y_F^c - R_2) (\dot{\kappa}\eta_1^c + 1)^{1/p_1^c}, \\ \tilde{Y}_T^t &= (Y_T^t - R_3) (\dot{\kappa}\eta_2^t + 1)^{1/p_2^t}, & \tilde{Y}_T^c &= (Y_T^c - R_4) (\dot{\kappa}\eta_2^c + 1)^{1/p_2^c}, \\ \tilde{Y}_{BTT}^t &= (Y_{BTT}^t - R_5) (\dot{\kappa}\eta_3^t + 1)^{1/p_3^t}, & \tilde{Y}_{BTT}^c &= (Y_{BTT}^c - R_6) (\dot{\kappa}\eta_3^c + 1)^{1/p_3^c}, \\ \tilde{Y}_{STT} &= (Y_{STT} - R_7) (\dot{\kappa}\eta_4 + 1)^{1/p_4}, & \tilde{Y}_{SFT} &= (Y_{SFT} - R_8) (\dot{\kappa}\eta_5 + 1)^{1/p_5},\end{aligned}\quad (6.31)$$

The parameters Y_F^t , Y_F^c , Y_T^t , Y_T^c , Y_{BTT}^t , Y_{BTT}^c , Y_{STT} and Y_{SFT} are the initial yield stresses obtained by subjecting the RVE to longitudinal tension, longitudinal compression, transverse tension, transverse compression, transverse biaxial tension, transverse biaxial compression, transverse shear and longitudinal shear, respectively. For a graphical illustration of the load cases, see Bedzra et al. [2020]. Furthermore the parameters $\eta_1^{t,c}$, $p_1^{t,c}$, $\eta_2^{t,c}$, $p_2^{t,c}$, $\eta_3^{t,c}$, $p_3^{t,c}$, η_4 , p_4 , η_5 , and p_5 control the viscoplastic response of the RVE. The definition of the hardening functions correspond to a Peric type (Perić [1993]) viscoplastic law where the rate-independent response of the RVE is recovered as $p_1^{t,c} \rightarrow \infty$, $p_2^{t,c} \rightarrow \infty$, $p_3^{t,c} \rightarrow \infty$, $p_4 \rightarrow \infty$, $p_5 \rightarrow \infty$, $\eta_1^{t,c} \rightarrow 0$, $\eta_2^{t,c} \rightarrow 0$, $\eta_3^{t,c} \rightarrow 0$, $\eta_4 \rightarrow 0$ and $\eta_5 \rightarrow 0$. For the relation between the yield surface parameters and the hardening functions, see D.2. To ensure thermodynamic consistency, the hardening functions have to satisfy the following conditions $\tilde{Y}_F^{t,c} \geq 0$, $\tilde{Y}_T^{t,c} \geq 0$, $\tilde{Y}_{BTT}^{t,c} \geq 0$, $\tilde{Y}_{STT} \geq 0$ and $\tilde{Y}_{SFT} \geq 0$, see D.4 for details.

The invariants I_4^* , I_5^* , I_8^* and I_9^* are defined as

$$\begin{aligned}I_4^* &:= \text{tr}(\beta \mathbf{M}_1), & I_5^* &:= \text{tr}(\beta_p^2 \mathbf{M}_1), & I_8^* &:= \frac{1}{2} \text{tr}(\beta_p^2) - I_5^*, & I_9^* &:= \text{tr}\beta - I_4^*, \\ \beta_p &= \beta - \frac{1}{2} (\text{tr}\beta - I_4^*) \mathbf{1} + \frac{1}{2} (\text{tr}\beta - 3I_4^*) \mathbf{M}_1.\end{aligned}\quad (6.32)$$

Assuming the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ points in the longitudinal fibre direction, the invariants can explicitly be written as

$$I_4^* = \beta_{11}, \quad I_5^* = \beta_{12}\beta_{21} + \beta_{13}\beta_{31}, \quad I_8^* = \frac{(\beta_{22} - \beta_{33})^2}{4} + \beta_{23}\beta_{32}, \quad I_9^* = \beta_{22} + \beta_{33}. \quad (6.33)$$

From the definition of the invariants, it is obvious that I_4^* controls yielding in longitudinal fibre direction, I_5^* controls longitudinal shear yielding whereas I_8^* and I_9^* control transverse shear, transverse biaxial yielding and transverse uniaxial yielding. This differentiation allows the possibility to account for the anisotropic viscoplastic deformation behaviour of the RVE. Furthermore to differentiate between the anisotropic viscoplastic response of the RVE in tension

and in compression, the following Macaulay brackets are defined

$$\langle x \rangle_+ = \frac{1}{2} (x + |x|) \quad \text{and} \quad \langle x \rangle_- = \frac{1}{2} (-x + |x|). \quad (6.34)$$

To account for the correct anisotropic plastic volumetric deformation of the RVE, the following non-associative flow potential is proposed

$$g_{\text{UD}} = (\boldsymbol{\beta}^D \cdot \mathbf{M}_1)^2 + \alpha_1 I_8^* + \alpha_2 I_5^* + \alpha_3 I_9^{*2} + \alpha_4 I_4^{*2}, \quad \boldsymbol{\beta}^D = \boldsymbol{\beta} - \frac{1}{3} (\text{tr} \boldsymbol{\beta}) \mathbf{1}, \quad (6.35)$$

where α_1 , α_2 , α_3 and α_4 are material parameters which are defined in terms of the plastic Poisson's ratios ν_{FT}^p (which controls lateral contraction in transverse direction during longitudinal tension), ν_{TF}^p and ν_{TT}^p (which controls lateral contraction in transverse and longitudinal directions during transverse tension) and $\nu_{FT}^{p45^\circ}$ (which controls lateral contraction in a plane defined by a unit normal to a uniaxial tensile load at an angle 45° in a plane parallel to the longitudinal fibre direction). For details on the derivation of the relation between the flow potential parameters and the plastic Poisson's ratios, see D.3. To ensure thermodynamic consistency, the flow potential parameters have to satisfy the following conditions $\alpha_i \geq 0$, see D.4 for details.

The set of constitutive equations is completed by the Kuhn-Tucker conditions $\dot{\lambda}_p \geq 0$, $\Phi^{\text{UD}} \leq 0$, and $\dot{\lambda}_p \Phi^{\text{UD}} = 0$. The final form of the constitutive equations is summarized below:

- Stress tensors

$$\begin{aligned} \boldsymbol{\sigma} &= \mathbf{C}_{\text{ani}} [\boldsymbol{\varepsilon}^e] + \sum_{i=1}^2 \gamma_{i\text{sym}} (\mathbf{C}_{\text{ani}} : \mathcal{H}_1) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}] + \sum_{i=3}^4 \gamma_{i\text{sym}} (\mathbf{C}_{\text{ani}} : \mathcal{H}_2) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}] \\ &\quad + \sum_{i=5}^6 \gamma_{i\text{sym}} (\mathbf{C}_{\text{ani}} : \mathcal{H}_3) [\boldsymbol{\varepsilon}^e - \boldsymbol{\varepsilon}_i^{ei}], \\ \boldsymbol{\chi}_i &= c_i \mathcal{H}_i [\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_i^{pi}]. \end{aligned}$$

- Yield function and flow potential

$$\begin{aligned} \Phi^{\text{UD}} &= \zeta_1 I_8^* + \zeta_2 I_5^* + \zeta_3^t \langle I_9^* \rangle_+ + \zeta_3^c \langle I_9^* \rangle_- + \zeta_4^t (\langle I_9^* \rangle_+)^2 + \zeta_4^c (\langle I_9^* \rangle_-)^2 + \zeta_5^t (\langle I_4^* \rangle_+)^2 \\ &\quad + \zeta_5^c (\langle I_4^* \rangle_-)^2 - 1, \\ g_{\text{UD}} &= (\boldsymbol{\beta}^D \cdot \mathbf{M}_1)^2 + \alpha_1 I_8^* + \alpha_2 I_5^* + \alpha_3 I_9^{*2} + \alpha_4 I_4^{*2}. \end{aligned}$$

- Evolution equations

$$\boldsymbol{\varepsilon}_i^{ei}(t) = \boldsymbol{\varepsilon}^e(t) - \mathbf{h}_i, \quad \dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda}_p \frac{\partial \boldsymbol{\sigma} g_{UD}}{\|\partial \boldsymbol{\sigma} g_{UD}\|}, \quad \dot{\boldsymbol{\varepsilon}}_i^{pi} = \dot{\lambda}_p \frac{b_i}{c_i} \boldsymbol{\chi}_i, \quad \dot{\kappa} = \|\dot{\boldsymbol{\varepsilon}}^p\| = \dot{\lambda}_p.$$

- Kuhn-Tucker conditions

$$\dot{\lambda}_p \geq 0, \quad \Phi^{UD} \leq 0, \quad \dot{\lambda}_p \Phi^{UD} = 0.$$

For the numerical aspects of the derived unidirectional flax fibre/epoxy composite tow constitutive model, the reader is referred to D.5.

6.5. Parameter identification and validation

This section deals with calibration and validation of the tow constitutive model. This is done by fitting the constitutive model to rate dependent stress-strain curves generated from the unidirectional flax fibre/epoxy composite RVE as well as the yield surface of the composite identified in Bedzra et al. [2020]. Furthermore the derived constitutive model for the tow is validated against off-axis stress-strain curves generated from the RVE. For a detail description of the calibration procedure for the matrix material, the reader is referred to Bedzra et al. [2020].

6.5.1. Tow parameter identification

The proposed constitutive model for the tow has a total of 73 material parameters. These parameters include: 10 elasticity parameters, i.e. μ_F^t and δ_F^t (which control nonlinear elastic response in longitudinal tension), E_F^c (which controls linear elastic response in longitudinal compression), ν_{FT} (which controls transverse elastic contraction during longitudinal tension), E_T^t (which controls linear elastic response in transverse tension), E_T^c (which controls linear elastic response in transverse compression), ν_{TT}^t (which controls transverse elastic contraction during transverse tension), ν_{TT}^c (which controls transverse elastic expansion during transverse compression), G_{FT} (which controls elastic longitudinal shear response) and G_{TT} (which controls elastic transverse shear response), 12 viscoelastic parameters, i.e. γ_i ($i = 1, \dots, 6$) and τ_i ($i = 1, \dots, 6$) (which describe anisotropic viscoelastic response), 8 initial yield stresses, i.e. $Y_F^{t,c}$, $Y_T^{t,c}$, $Y_{FTT}^{t,c}$, Y_{STT} and Y_{SFT} (which specify the onset of anisotropic plastic yielding in tension and compression), 17 isotropic hardening parameters H_F^l , H_F^{nl} , c_F , Q_i ($i = 2, \dots, 8$)

and β_i ($i = 2, \dots, 8$) (which describe the size of the elastic domain and the rate of change of the elastic domain), 16 viscoplastic parameters $\eta_1^{t,c}, p_1^{t,c}, \eta_2^{t,c}, p_2^{t,c}, \eta_3^{t,c}, p_3^{t,c}, \eta_4, p_4, \eta_5$ and p_5 (which describe rate dependent plastic response in tension and in compression), 6 kinematic hardening parameters, i.e. c_i ($i = 1, 2, 3$) and b_i ($i = 1, 2, 3$) (which describe anisotropic kinematic hardening) and 4 plastic Poisson's ratios, i.e. $\nu_{FT}^p, \nu_{TF}^p, \nu_{TT}^p$ and $\nu_{FT}^{p45^\circ}$ (which describe anisotropic plastic volumetric deformation). Although the number of material parameters may seem to be quite alot, each of the material parameters plays a significant role in the description of the deformation behaviour of the RVE. By assuming the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ points in the longitudinal fibre direction and $\mathbf{n}_2 = [0, 1, 0]^T$ points in the transverse fibre direction, the material parameters can be expressed with respect to the Cartesian coordinate system by writing the subscripts of the parameters making use of the convention ($F = 1, T = 2 = 3$).

To identify the material parameters, rate dependent stress-strain curves for transverse tension, transverse compression, biaxial tension, biaxial compression, longitudinal tension, longitudinal compression, transverse shear and longitudinal shear, are generated from the RVE (see Bedzra et al. [2020] for details). Additionally cyclic stress-strain curves are generated for longitudinal shear and transverse shear as well as load-unload-compression-reload curves for transverse tension and longitudinal tension.

6.5.2. Anisotropic viscoelasticity

From the generated rate dependent stress-strain data, the evolution of the RVE elastic stiffness in transverse tension, transverse compression, transverse shear and longitudinal shear with time are measured keeping the strain constant (stiffness relaxation data). The strain should be chosen in the elastic range to ensure a good fit. By analytically solving the viscoelastic evolution equations in (6.11) for ϵ_i^{ei} ($i = 1, \dots, 6$), assuming a constant elastic strain ($\epsilon^e = \epsilon_0^e$) and assuming initial boundary conditions ($\epsilon_i^{ei}(t = 0) = 0$), the following relations for the viscoelastic evolution equations are obtained

$$\epsilon_i^{ei} = \epsilon_0^e \left(1 + \gamma_i \exp \left(\frac{-t}{\tau_i} \right) \right). \quad (6.36)$$

From (6.36), a relation can be established between the stress tensor σ and the constant elastic strain ϵ_0^e making use of (6.25) as

$$\begin{aligned} \sigma = & \mathcal{C}_{\text{ani}} [\epsilon_0^e] + \sum_{i=1}^2 \gamma_i \exp\left(\frac{-t}{\tau_i}\right) \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_1) [\epsilon_0^e] + \sum_{i=3}^4 \gamma_i \exp\left(\frac{-t}{\tau_i}\right) \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_2) [\epsilon_0^e] \\ & + \sum_{i=5}^6 \gamma_i \exp\left(\frac{-t}{\tau_i}\right) \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_3) [\epsilon_0^e]. \end{aligned} \quad (6.37)$$

By employing the expression in (6.37), the evolution of the RVE stiffness in longitudinal tension, in transverse tension and in longitudinal shear can be approximated by the functions

$$\begin{aligned} E_{F,rel}^t(t) &= E_{F,int}^t \left(1 + \gamma_1 \exp\left(\frac{-t}{\tau_1}\right) + \gamma_2 \exp\left(\frac{-t}{\tau_2}\right) \right), \\ E_{T,rel}^t(t) &= E_{T,int}^t \left(1 + \gamma_3 \exp\left(\frac{-t}{\tau_3}\right) + \gamma_4 \exp\left(\frac{-t}{\tau_4}\right) \right), \\ G_{FT,rel}(t) &= G_{FT,int} \left(1 + \gamma_5 \exp\left(\frac{-t}{\tau_5}\right) + \gamma_6 \exp\left(\frac{-t}{\tau_6}\right) \right). \end{aligned} \quad (6.38)$$

By fitting the resulting expressions in (6.38) to their respective relaxation data, the viscoelastic parameters γ_i ($i = 1, \dots, 6$) and τ_i ($i = 1, \dots, 6$) are obtained. However due to the fact that the stress-strain curves generated from loading the RVE in the longitudinal fibre direction does not show any influence of viscoelasticity, the influence of viscoelasticity for longitudinal fibre direction in the tow constitutive model is cancelled by setting $\gamma_{1,2} = 0$ and choosing $\tau_{1,2}$ to be any small value. After identifying the viscoelasticity parameters, the stationary elastic parameters are identified by making use of the following relations

$$\begin{aligned} E_T^{t,c} &= \frac{E_{T,rel}^{t,c}(t = 10 \text{ sec})}{\left(1 + \gamma_3 \exp\left(\frac{-10 \text{ sec}}{\tau_3}\right) + \gamma_4 \exp\left(\frac{-10 \text{ sec}}{\tau_4}\right) \right)}, \\ G_{TT} &= \frac{G_{TT,rel}(t = 10 \text{ sec})}{\left(1 + \gamma_3 \exp\left(\frac{-10 \text{ sec}}{\tau_3}\right) + \gamma_4 \exp\left(\frac{-10 \text{ sec}}{\tau_4}\right) \right)}, \\ G_{FT} &= \frac{G_{FT,rel}(t = 10 \text{ sec})}{\left(1 + \gamma_5 \exp\left(\frac{-10 \text{ sec}}{\tau_5}\right) + \gamma_6 \exp\left(\frac{-10 \text{ sec}}{\tau_6}\right) \right)}, \end{aligned} \quad (6.39)$$

where $E_{T,rel}^{t,c}(t = 10 \text{ sec})$, $G_{TT,rel}(t = 10 \text{ sec})$ and $G_{FT,rel}(t = 10 \text{ sec})$ are the instantaneous stiffnesses measured from their corresponding relaxation data at time ($t = 10 \text{ sec}$). The elastic stiffness in longitudinal compression E_F^c is measured directly from its corresponding stress-strain curve. The elastic Poisson's ratios ν_{FT} and ν_{TT}^t are also obtained by directly measuring

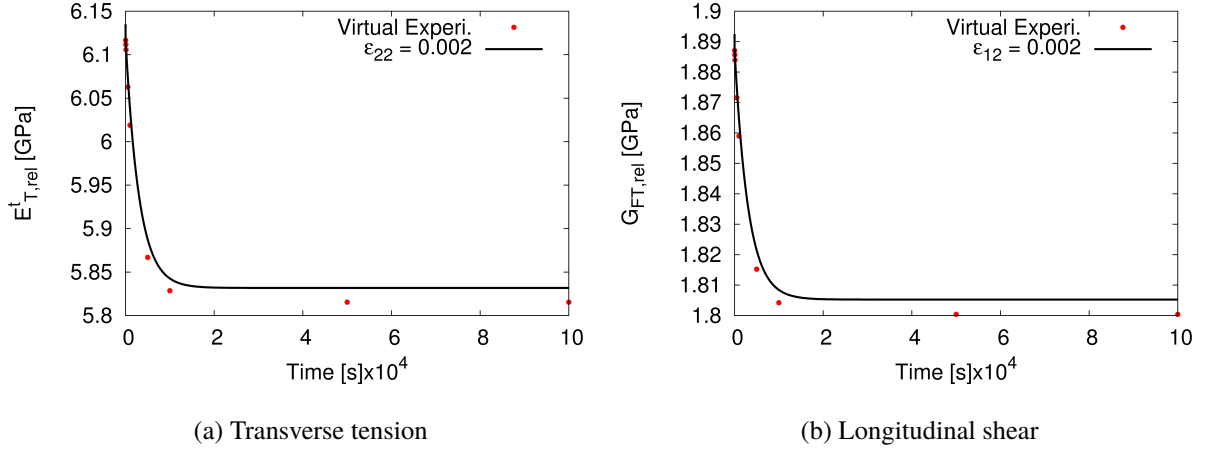


Figure 6.2.: Fit of constitutive model to; (a) transverse tension relaxation modulus evolution; (b) longitudinal shear relaxation modulus evolution.

from their corresponding axial/lateral strain plots at time ($t = 10^5$ sec). The compressive elastic Poisson's ratio in transverse fibre direction ν_{TT}^c is obtained from the fit of the constitutive model to transverse biaxial compression data. The fit of the nonlinear elasticity parameters μ_F^t and δ_F^t are discussed in the following section. The identified viscoelastic material parameters are listed in Table 6.1. Also displayed in Figure 6.2 are the fit of the constitutive model to the evolution of the relaxation modulus for transverse tension and longitudinal shear. The fit indicate a relatively good agreement between the constitutive model and the RVE. The obtained fit can further be improved if the number of viscoelastic parameters is increased. However for simplicity reasons, the current fit is maintained.

6.5.3. Anisotropic viscoplasticity

By taking the time derivative of the back stress tensors χ_i (6.29), taking into account the plastic evolution equation $\dot{\epsilon}^p$ (6.10)₁, the kinematic hardening evolution equations $\dot{\epsilon}_i^{pi}$ (6.10)₂ and the accumulated plastic strain evolution equation $\dot{\kappa}$ (6.10)₃ as well as the initial boundary conditions ($\chi_i(\kappa = 0) = 0$), analytical solutions for the back stress tensors can be derived as

$$\chi_i = \frac{\partial_{\sigma} g_{UD}}{\|\partial_{\sigma} g_{UD}\|} \frac{c_i}{b_i} (1 - e^{-b_i \kappa}). \quad (6.40)$$

By substituting (6.40) into the yield function Φ^{UD} , assuming the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ points in the longitudinal fibre direction, the longitudinal tensile stress σ_{11}^t , the longitudinal compressive stress σ_{11}^c , the transverse tensile stress σ_{22}^t , the transverse compressive stress σ_{22}^c ,

the biaxial tensile stress σ_{b22}^t , the biaxial compressive stress σ_{b22}^c , the longitudinal shear stress σ_{12} as well as the transverse shear stress σ_{23} can be related to their corresponding plastic strains as

$$\begin{aligned}\sigma_{11}^{t,c} &= a_{11}^1 + \sqrt{\frac{1}{\zeta_5^{t,c}} \left(1 - 2\zeta_3^{t,c} (\nu_{FT}^p a_{11}^2) - 4\zeta_3^{t,c} (\nu_{FT}^p a_{11}^2)^2 \right)}, \\ \sigma_{22}^{t,c} &= \frac{1}{2A_{22}^{t,c}} \left(-B_{22}^{t,c} + \sqrt{(B_{22}^{t,c})^2 - 4A_{22}^{t,c} C_{22}^{t,c}} \right), \\ \sigma_{b22}^{t,c} &= \frac{1}{2A_{b22}^{t,c}} \left(-B_{b22}^{t,c} + \sqrt{(B_{b22}^{t,c})^2 - 4A_{b22}^{t,c} C_{b22}^{t,c}} \right), \\ \sigma_{12} &= a_{12}^3 + \sqrt{\frac{1}{\zeta_2}}, \\ \sigma_{23} &= a_{23}^2 + \sqrt{\frac{1}{\zeta_1}},\end{aligned}\tag{6.41}$$

where

$$\begin{aligned}A_{22}^{t,c} &= \zeta_4^{t,c} + \frac{1}{4}\zeta_1, \quad B_{22}^{t,c} = \zeta_3^{t,c} + 2\zeta_4^{t,c} (\nu_{TT}^p - 1) a_{22}^2 - \frac{1}{2}\zeta_1 a_{22}^2, \\ C_{22}^{t,c} &= \zeta_5^{t,c} (\nu_{TF}^p a_{22}^1)^2 + \zeta_3^{t,c} (\nu_{TT}^p - 1) a_{22}^2 + \zeta_4^{t,c} ((\nu_{TT}^p - 1) a_{22}^2)^2 + \frac{1}{4}\zeta_1 (a_{22}^2)^2 - 1, \\ A_{b22}^{t,c} &= 4\zeta_4^{t,c}, \quad B_{b22}^{t,c} = 2\zeta_3^{t,c} + 8\zeta_4^{t,c} (\nu_{TT}^p - 1) a_{b22}^2, \\ C_{b22}^{t,c} &= 4\zeta_5^{t,c} (\nu_{TF}^p a_{b22}^1)^2 + 2\zeta_3^{t,c} (\nu_{TT}^p - 1) a_{b22}^2 + 4\zeta_4^{t,c} ((\nu_{TT}^p - 1) a_{b22}^2)^2 - 1, \\ a_{11}^{1,2} &= \frac{1}{\sqrt{1 + 2(\nu_{FT}^p)^2}} \frac{c_{1,2}}{b_{1,2}} (1 - e^{-b_{1,2}\kappa_{11}}), \quad \kappa_{11} = \frac{\|\partial_{\sigma} g_{UD}\|}{(\partial_{\sigma} g_{UD})_{11}} \varepsilon_{11}^p, \\ a_{22}^{1,2} &= \frac{1}{\sqrt{1 + (\nu_{TF}^p)^2 + (\nu_{TT}^p)^2}} \frac{c_{1,2}}{b_{1,2}} (1 - e^{-b_{1,2}\kappa_{22}}), \quad \kappa_{22} = \frac{\|\partial_{\sigma} g_{UD}\|}{(\partial_{\sigma} g_{UD})_{22}} \varepsilon_{22}^p, \\ a_{b22}^{1,2} &= \frac{1}{\sqrt{2(\nu_{TT}^p - 1)^2 + 4(\nu_{TF}^p)^2}} \frac{c_{1,2}}{b_{1,2}} (1 - e^{-b_{1,2}\kappa_{b22}}), \quad \kappa_{b22} = \frac{\|\partial_{\sigma} g_{UD}\|}{(\partial_{\sigma} g_{UD})_{b22}} \varepsilon_{b22}^p, \\ a_{12}^3 &= \frac{1}{\sqrt{2}} \frac{c_3}{b_3} (1 - e^{-b_3\kappa_{12}}), \quad \kappa_{12} = \frac{\|\partial_{\sigma} g_{UD}\|}{(\partial_{\sigma} g_{UD})_{12}} \frac{\varepsilon_{12}^p}{2}, \\ a_{23}^2 &= \frac{1}{\sqrt{2}} \frac{c_2}{b_2} (1 - e^{-b_2\kappa_{23}}), \quad \kappa_{23} = \frac{\|\partial_{\sigma} g_{UD}\|}{(\partial_{\sigma} g_{UD})_{23}} \frac{\varepsilon_{23}^p}{2},\end{aligned}\tag{6.42}$$

The relation between the plastic strains ε_{11}^p , ε_{22}^p , ε_{b22}^p , ε_{12}^p , ε_{23}^p and the accumulated plastic strains κ are obtained by substituting (6.10)₃ into (6.10)₁. For the definition of ζ_1 , ζ_2 , $\zeta_3^{t,c}$, $\zeta_4^{t,c}$ and $\zeta_5^{t,c}$, the reader is referred to D.2.

By fitting $(6.41)_4$ and $(6.41)_5$ by means of e.g. least squares fit to the plastic part of the rate dependent cyclic longitudinal shear and cyclic transverse shear stress-strain curves, respectively, the material parameters responsible for controlling the material response in transverse shear and longitudinal shear, i.e. $Y_{SFT}, Y_{STT}, Q_{7,8}, \beta_{7,8}, \eta_{4,5}, p_{4,5}, c_{2,3}, b_{2,3}$, are identified.

The material parameters responsible for longitudinal tension and compression, i.e. $Y_F^{t,c}, H_F^l, H_F^{nl}, c_F, Q_2, \beta_2, \eta_1^{t,c}, p_1^{t,c}, c_1, b_1$, are identified by simultaneously fitting $(6.41)_1^t$ and $(6.41)_1^c$ to their corresponding stress-strain curves. However due to the difficulty entailed in the decomposition of the elastic and plastic parts of the nonlinear longitudinal tension stress-strain data, the parameters Y_F^c, Q_2, β_2, c_1 and b_1 are first identified by fitting $(6.41)_1^c$ to the obtained stress-strain data for longitudinal compression. The rest of the plastic parameters, i.e. $Y_F^t, H_F^l, H_F^{nl}, c_F$, including the nonlinear elasticity parameters μ_F^t, δ_F^t , are identified by minimizing the error between the obtained stress-strain data for longitudinal tension and the obtained stress-strain curve from a one dimensional implementation of a yield function constructed from $(6.41)_1^t$ through a nonlinear regression analysis performed in the commercial software Matlab MathWorks [2016]. The input of the one-dimensional constitutive model is the strain part of the stress-strain data whereas the variables are the material parameters to be identified. Due to the fact that the RVE does not show rate dependent plastic deformation in longitudinal fibre direction, the viscoplastic parameters are chosen to ensure rate-independent response, i.e. $p_1^{t,c} \rightarrow \infty$.

The material parameters responsible for transverse tension, transverse compression, biaxial tension and biaxial compression, are identified by fitting equations $(6.41)_2^{t,c}$ and $(6.41)_3^{t,c}$ to their respective rate dependent stress-strain curves. The RVE does not show any significant viscoplastic effect in transverse biaxial compression, as a result, the responsible viscoplastic parameters are chosen in a manner that ensures rate-independent transverse biaxial compression response, i.e. $p_3^c \rightarrow \infty$.

The plastic Poisson's ratios $\nu_{FT}^p, \nu_{TF}^p, \nu_{TT}^p$ and $\nu_{FT}^{p45^\circ}$ are identified by fitting the constitutive model to their corresponding axial/lateral plastic strain curves at a strain rate of $\dot{\epsilon} = 10^5/\text{sec}$. The identified anisotropic viscoplastic parameters are listed in Table 6.1.

Figures 6.3a and 6.3b shows the fit of the constitutive model to the volumetric deformation of the RVE for transverse tension, longitudinal tension and off-axis tension in the plane parallel to the longitudinal fibre direction (12-plane). The constitutive model agrees relatively well with the RVE response except for lateral contraction in the longitudinal fibre direction during transverse tension ($\varepsilon_{11}/\varepsilon_{22}$). The reason for this discrepancy is the limit in the value of the plastic Poisson's ratio ν_{TF}^p which can be assigned to the constitutive model as a result of the coupling between ν_{TF}^p and ν_{FT}^p due to the dependence of the flow potential g_{UD} on the back

stress tensor β . A value of $\nu_{TF}^p < 0.1$ will result in the inability to control the lateral/axial strain ($\varepsilon_{22}/\varepsilon_{11}$) obtained from the constitutive model (see Figure 6.3b).

Figures 6.3c and 6.3d shows the fit of the constitutive model to rate dependent transverse and longitudinal shear RVE response. Displayed in Figure 6.4 are also the fit of the constitutive model to transverse tension and compression, longitudinal tension and compression as well as biaxial tension and compression rate dependent stress-strain curves. Furthermore, Figure 6.5 shows the fit of the constitutive model to transverse and longitudinal load-unload-compression-reload stress-strain curves as well as transverse and longitudinal shear cyclic stress-strain curves. The fits indicate a good agreement between the constitutive model and the RVE response.

Depicted in Figure 6.6 is a comparison between the yield surface obtained from the virtual experiments conducted on the unidirectional flax fibre/epoxy composite RVE (see Bedzra et al. [2020]) and the tow constitutive model. In general, the tow constitutive model shows a good agreement with the yield surfaces generated from the RVE although some discrepancies remain in the compression and tensile parts of the yield surfaces in 22/33 (Figure 6.6a) and 11/22 stress space (Figure 6.6b), respectively. However from the validation of the tow constitutive model in the subsequent section based on the off-axis load cases carried out in the plane of isotropy (23-plane) and in the plane of the fibre (12-plane), these discrepancies do not have a significant effect on the predictive capability of the tow constitutive model (see Figure 6.7).

Remark 1. From the identified unidirectional flax fibre/epoxy composite yield surface in the plane of isotropy (see Figure 6.6a), rate dependent biaxial tension may lead to a singular point depending on the value of the responsible material parameters. This will result in an ill conditioned consistent tangent operator due to the discontinuity of the yield function and will cause the simulation to break. To circumvent this problem, the viscoplastic transverse shear hardening function is recalibrated by setting the isotropic hardening material parameter $Q_7 = 0.0001$. This leads to a reduction in the size of the transverse shear elastic domain.

6.5.4. Tow constitutive model validation

To check the validity of the derived tow constitutive model, the constitutive model is compared to off-axis stress-strain curves generated by loading the RVE in the plane of isotropy and in the plane parallel to the longitudinal fibre direction. The procedure to determine the correct far field strain tensor ε^0 to effect the desired off-axis stress state σ relies on the compliance tensor $\mathcal{C}_{\text{ani}}^{-1}$ (see Bedzra et al. [2020]). Due to the fact that the stiffness tensor $\mathcal{C}_{\text{ani}}$ depends on the invariant I_4 , it is imperative to determine I_4 before the far field strain tensor can be computed especially for off-axis loading in the plane parallel to the longitudinal fibre direction. This

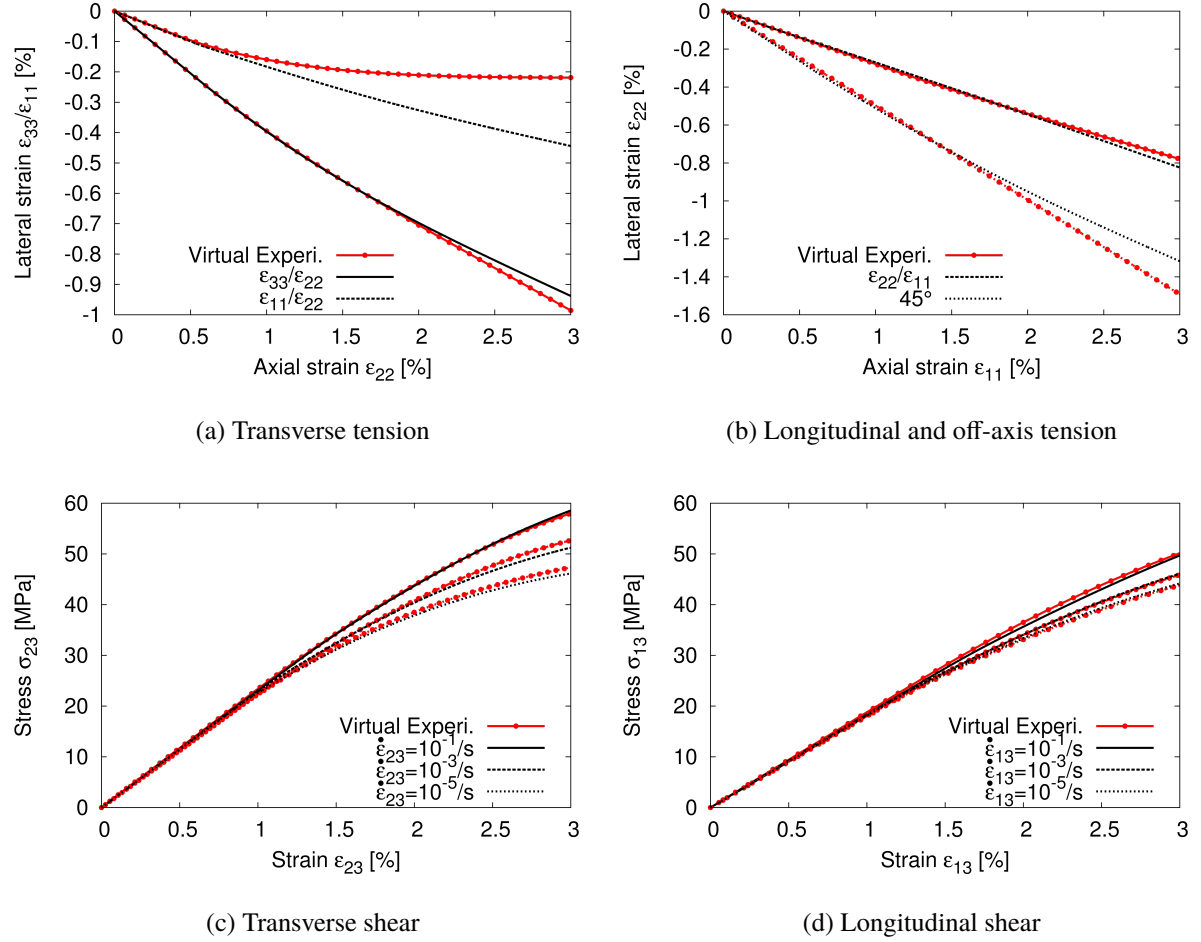


Figure 6.3.: Fit of constitutive model to virtual experiments; (a) lateral strain evolution during uniaxial tension in the transverse fibre direction at $\dot{\epsilon}_{22} = 10^{-5}/s$; (b) lateral strain evolution during uniaxial tension in the longitudinal fibre direction as well as uniaxial tension at an angle 45° to the longitudinal fibre direction at $\dot{\epsilon}_{11} = 10^{-5}/s$; (c) shear in the plane transverse to fibre direction; (d) shear in the plane of the fibre.

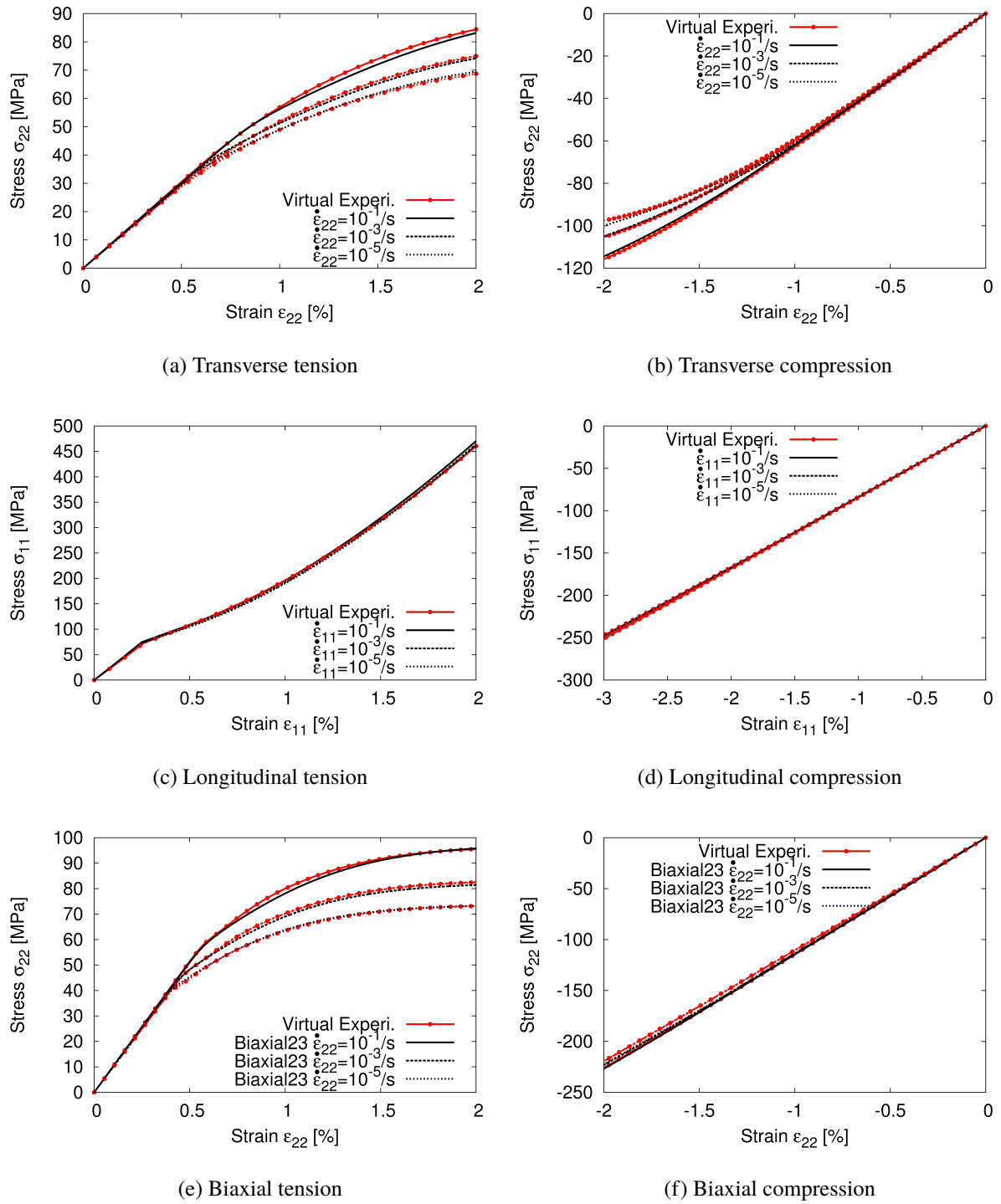
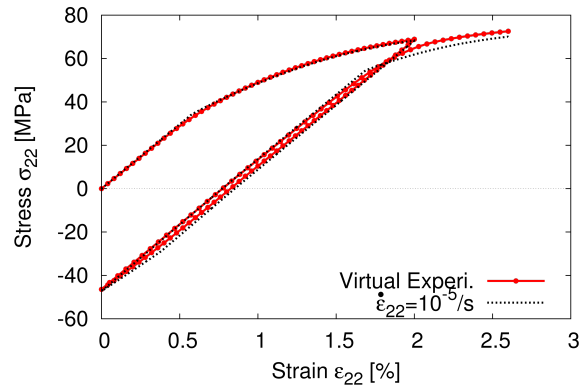
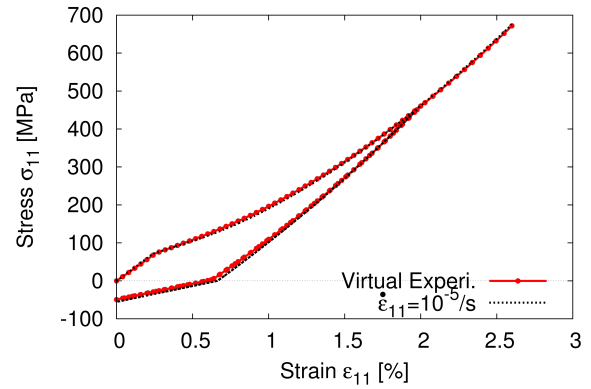


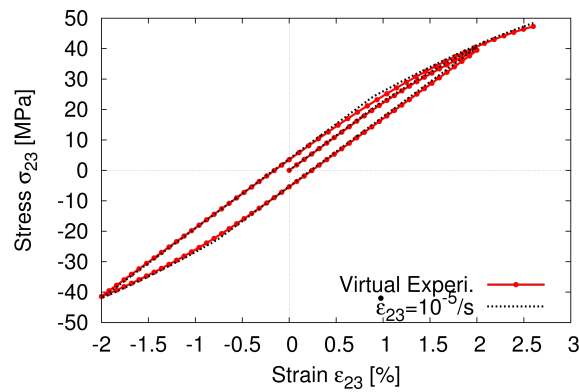
Figure 6.4.: Fit of constitutive model to rate-dependent virtual experiments; (a) transverse tension; (b) transverse compression; (c) longitudinal tension; (d) longitudinal compression; (e) transverse biaxial tension; (f) transverse biaxial compression.



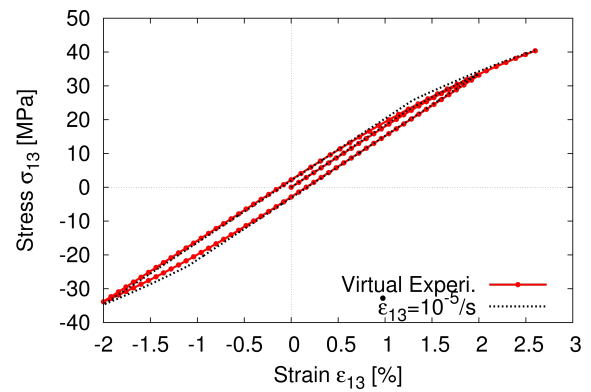
(a) Transverse cyclic load



(b) Longitudinal cyclic load

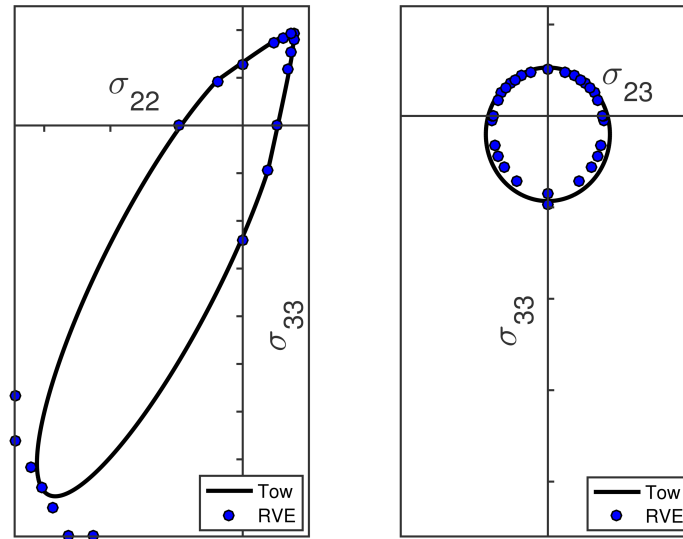


(c) Transverse shear cyclic load

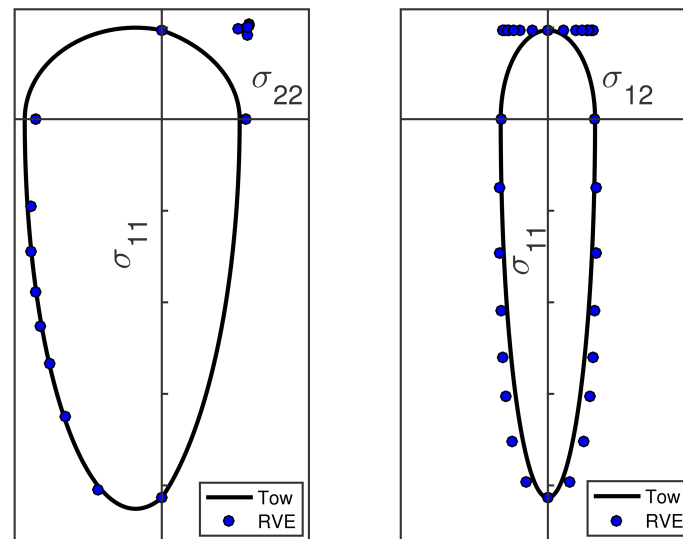


(d) Longitudinal shear cyclic load

Figure 6.5.: Fit of constitutive model to virtual experiments; (a) cyclic loading in transverse fibre direction; (b) cyclic loading in longitudinal fibre direction; (c) cyclic shear in the plane transverse to fibre direction; (d) cyclic shear in the plane of the fibre.



(a) Yield surface in 22/33 and 23/33 stress space



(b) Yield surface in 11/22 and 12/11 stress space

Figure 6.6.: Comparison between the identified yield surface from the unidirectional composite RVE and the tow constitutive model in stress space.

Table 6.1.: Identified tow constitutive model material parameters

μ_f^t [MPa]	α_f^t	E_F^c [MPa]	E_T^t [MPa]	E_T^c [MPa]	G_{FT} [MPa]
1981	9.79	8363.81	5829.88	6017.29	1799.75
G_{TT} [MPa]	ν_{FT}	ν_{TT}^t	ν_{TT}^c	γ_3	γ_4
2244.35	0.41	0.28	0.46	0.049	0.003
γ_5	γ_6	τ_3 [sec]	τ_4 [sec]	τ_5 [sec]	τ_6 [sec]
0.006	0.043	3056	0.122	11480	2278
ν_{FT}^p	ν_{TT}^p	ν_{TF}^p	$\nu_{FT}^{p45^\circ}$	Y_F^t [MPa]	Y_F^c [MPa]
0.3	0.39	0.1	0.35	71.014	150
Y_T^t [MPa]	Y_T^c [MPa]	Y_{BTT}^t [MPa]	Y_{BTT}^c [MPa]	Y_{STT} [MPa]	Y_{SFT} [MPa]
33.99	59.54	40	156	19	22.5
H_F^t [MPa]	H_F^{nl} [MPa]	c_F	Q_2 [MPa]	β_2	Q_3 [MPa]
21378.69	1.759×10^{10}	3.595	225.4	1115.74	3.65
β_3	Q_4 [MPa]	β_4 [MPa]	Q_5 [MPa]	β_5	Q_6 [MPa]
73.14	8.21	1976.795	8.35	152.99	400
β_6	Q_7 [MPa]	β_7	Q_8 [MPa]	β_8	b_1
274.85	10.87	2841.16	7.65	1132.08	174.13
c_1 [MPa]	b_2	c_2 [MPa]	b_3	c_3 [MPa]	$\eta_{1,2,3}^{t,c} = \eta_{4,5}$ [sec]
4066.81	260.78	9397.024	226.7	6892.9	1E9
$p_2^{t,c}$	$p_3^{t,c}$	p_4	p_5		
17.5	19.5	14.8	18		

is done by reading the elastic strain I_4 corresponding to the stress component I_4^* (assuming $\beta = 0$) from an elastic uniaxial stress-strain curve generated by subjecting the unidirectional composite RVE to either longitudinal tension or compression depending on the desired off-axis load direction. For the comparison between the constitutive model and the RVE, the isotropic hardening material parameter for longitudinal shear is set to $Q_7 = 0.0001$ (see **Remark 1** for explanation).

Displayed in Figure 6.7 are off-axis tension and compression in the plane of isotropy as well as off-axis tension and compression in the plane parallel to the longitudinal fibre direction.

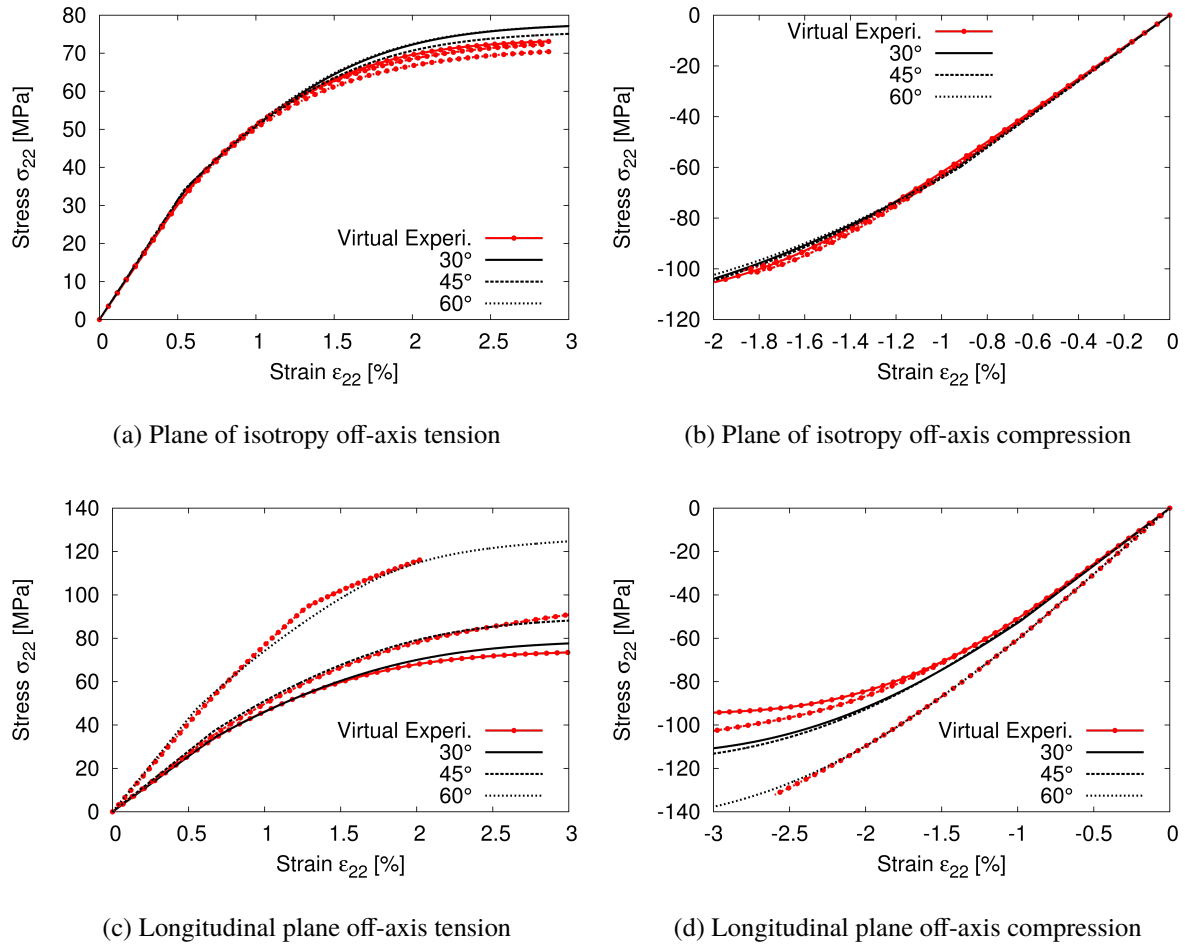


Figure 6.7.: Validation of the constitutive model against virtual experiments; (a) off-axis tension in the plane transverse to fibre direction; (b) off-axis compression in the plane transverse to fibre direction; (c) off-axis tension in the plane parallel to the longitudinal fibre direction; (d) off-axis compression in the plane parallel to the longitudinal fibre direction.

The constitutive model shows a relatively good agreement with the RVE for all off-axis load cases.

6.6. Mesomechanical analyses

This section deals with the study of the deformation behaviour of the plain weave composite as well as the determination of the composite yield surface.

6.6.1. Plain weave deformation behaviour

To study the deformation behaviour of the plain weave composite RUC, the RUC is subjected to rate dependent in-plane tension, in-plane compression, in-plane biaxial tension, in-plane biaxial compression, in-plane shear, out-of-plane tension, out-of-plane compression and out-of-plane shear. The applied far field strain tensors for the tensile load cases are defined in Table 6.2. A change of sign in Table 6.2 results in the compression load cases. Additionally, in-plane and out-of-plane load-unload-compression-reload tests as well as cyclic in-plane and out-of-plane shear tests are conducted on the plain weave RUC. For each of the load cases, homogenized stress-strain curves are provided. Furthermore, a shot of the field distribution of accumulated plastic strain in the RUC is also provided. The accumulated plastic strain shot corresponds to the red marking on the stress-strain curves.

Table 6.2.: Far field tensor applied for each load case

Load case	Far field strain tensor [10^{-2}]	Diagram
In-plane tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1$	
Out-of-plane tension	$\epsilon^0 = \mathbf{e}_3 \otimes \mathbf{e}_3$	
In-plane shear	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_2$	
Out-of-plane shear	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_3$	
In-plane biaxial tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2$	
Out-of-plane biaxial tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_3 \otimes \mathbf{e}_3$	
In-plane combined shear tension	$\epsilon^0 = \mathbf{e}_1 \otimes \mathbf{e}_1 + (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1)$	
Out-of-plane combined shear tension	$\epsilon^0 = \mathbf{e}_3 \otimes \mathbf{e}_3 + (\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1)$	

Displayed in Figure 6.8 are rate dependent stress-strain plots for in-plane tension and compression as well as their corresponding accumulated plastic strain distribution. From the obtained stress-strain plots, the effect of viscoelasticity as well as viscoplasticity is observed,

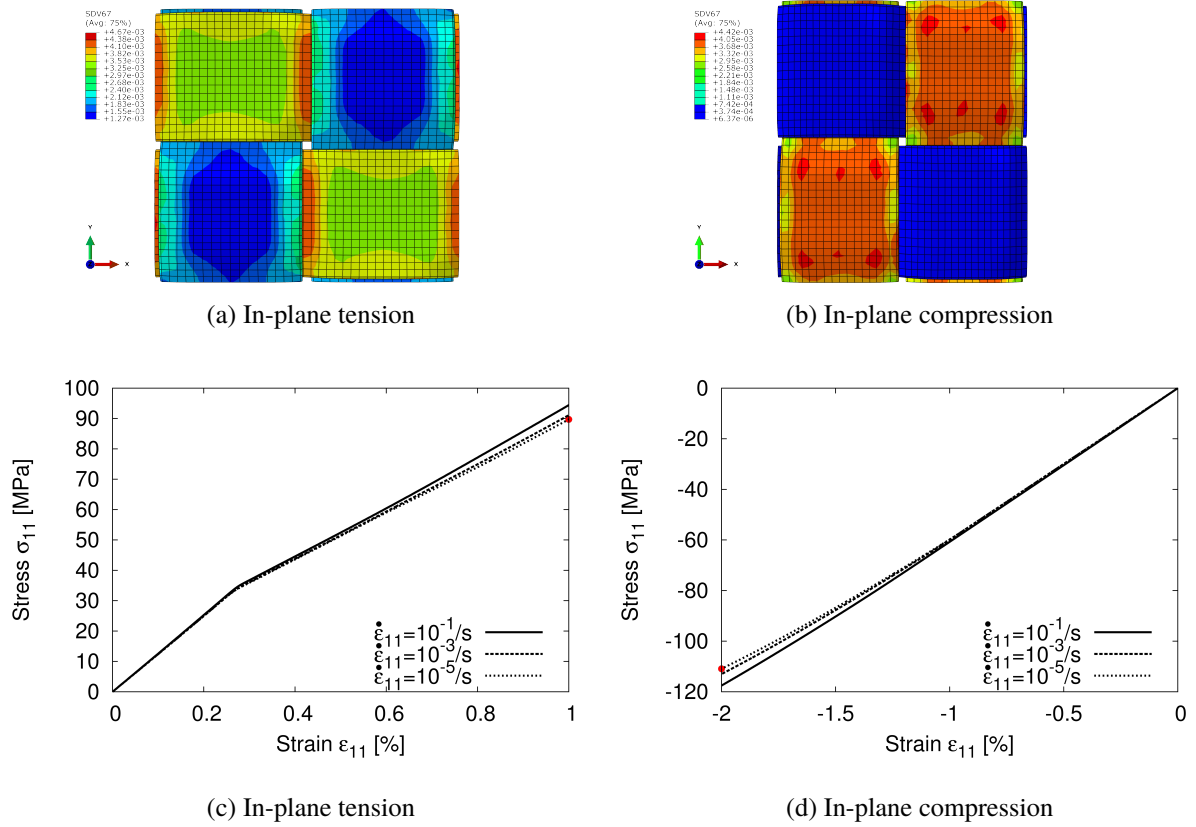


Figure 6.8.: Accumulated plastic strain plots and homogenized stress-strain curves for in-plane tension and compression.

although this is minimal. The material shows a different response in tension and in compression. From the accumulated plastic strain distribution for in-plane tension (see Figure 6.11a), the highest plastic strains occur in the crimp regions (the areas where bending of the yarns occur due to undulation) of the weft yarns (tows in x-direction) whereas the lowest plastic strains occur in the centre of the warp yarns (tows in y-direction). For in-plane compression (see Figure 6.11b), the highest plastic strains occur in the warp yarns which experience transverse tension whereas the weft yarns which are under compression in the longitudinal tow direction experience the lowest plastic strains. The in-plane cyclic response of the material is also shown in Figure 6.12a. From the obtained in-plane load-unload-compression-reload curve, the role of kinematic hardening is not evident since the applied far field strain does not result in plastic yielding in the compression load cycle. The volumetric deformation of the plain weave composite due to in-plane tension is also shown in Figure 6.13a. The plot shows a more pronounced lateral contraction in z-direction ($\epsilon_{33}/\epsilon_{11}$) as compared to y-direction ($\epsilon_{22}/\epsilon_{11}$).

Figure 6.9 shows rate dependent stress-strain curves for out-of-plane tension and out-of-

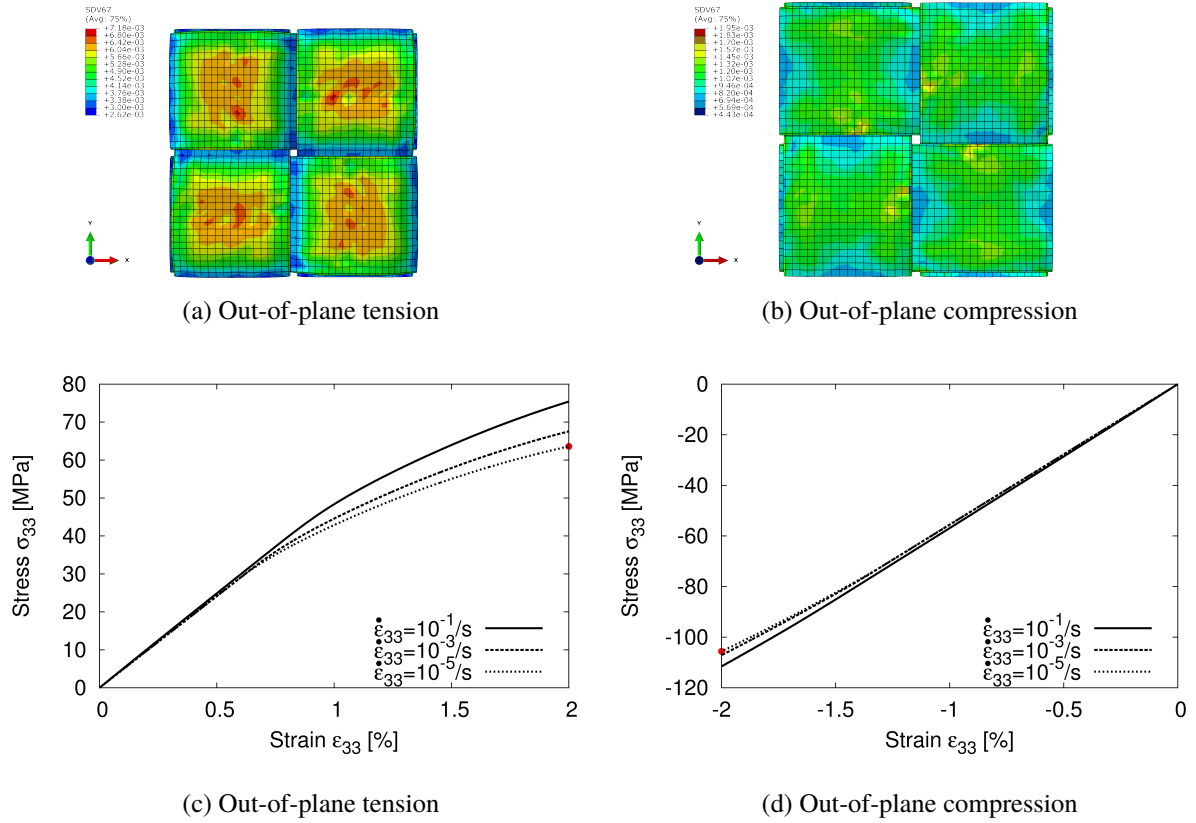


Figure 6.9.: Accumulated plastic strain plots and homogenized stress-strain curves for out-of-plane tension and compression.

plane compression as well as their corresponding accumulated plastic strain distribution. The material shows a different response in tension and in compression. Furthermore, both load cases exhibit viscoelastic and viscoplastic effects due to a change in elastic and plastic strain as a result of increasing strain rate. The accumulated plastic strain distribution in the weft and warp yarns appear to be equally distributed for both tension and compression (see Figures 6.9a and 6.9b). This is due to the fact that the load is mainly carried by the matrix. The out-of-plane cyclic response of the material is displayed in Figure 6.12a. The plot shows a combined isotropic-kinematic hardening effect as a result of a reduced yield stress in the compression cycle. The volumetric deformation of the composite under out-of-plane tension is also displayed in Figure 6.13b.

Figure 6.10 shows rate dependent in-plane biaxial tension and compression response as well as their corresponding accumulated plastic strain distribution. The material response differs for tension and compression. The material displays a viscoelastic-viscoplastic response for biaxial compression (see Figure 6.10c). However for biaxial tension, the rate dependent response is

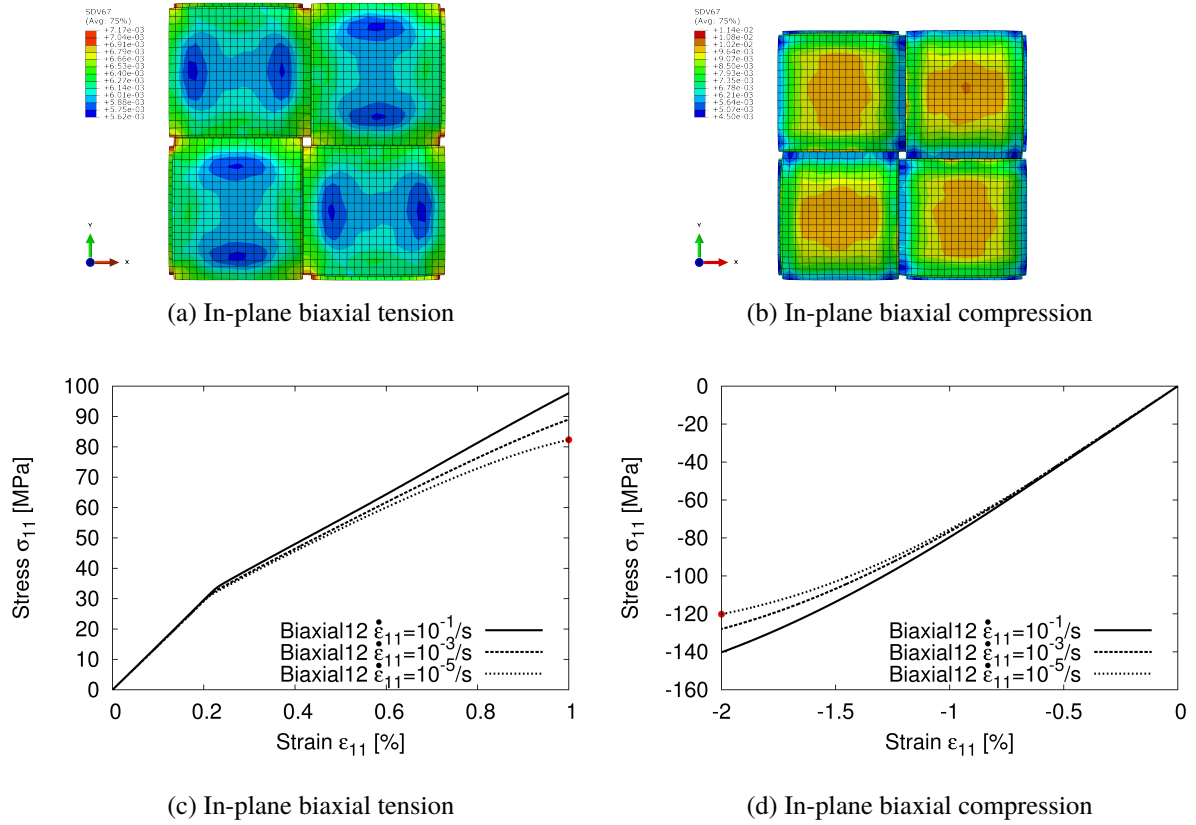


Figure 6.10.: Accumulated plastic strain plots and homogenized stress-strain curves for in-plane biaxial tension and compression.

predominantly viscoplastic (see Figure 6.10d). The corresponding accumulated plastic strain distribution for biaxial tension show the crimp regions experience higher plastic deformation as compared to the centre of the yarns (see Figure 6.10a). For biaxial compression, the opposite is the case. The centre of the yarns undergo a higher plastic deformation as compared to the crimp regions (see Figure 6.10b).

Figure 6.11 shows rate-dependent in-plane and out-of-plane shear response as well as their corresponding accumulated plastic strain distribution. Both load cases exhibit rate dependent elastic and plastic response. Furthermore for cyclic tests (see Figures 6.12c and 6.12d), a combined isotropic-kinematic hardening behaviour is observed. This is attributed to the yield stress reduction in compression. The accumulated plastic strain distribution for in-plane shear (see Figure 6.11a) shows a higher plastic deformation in the crimp regions of the yarns as compared to the centre of the yarns. For out-of-plane shear, the warp yarns (y-direction) undergo a higher plastic deformation as a result of matrix dominated response (see Figure 6.11b).

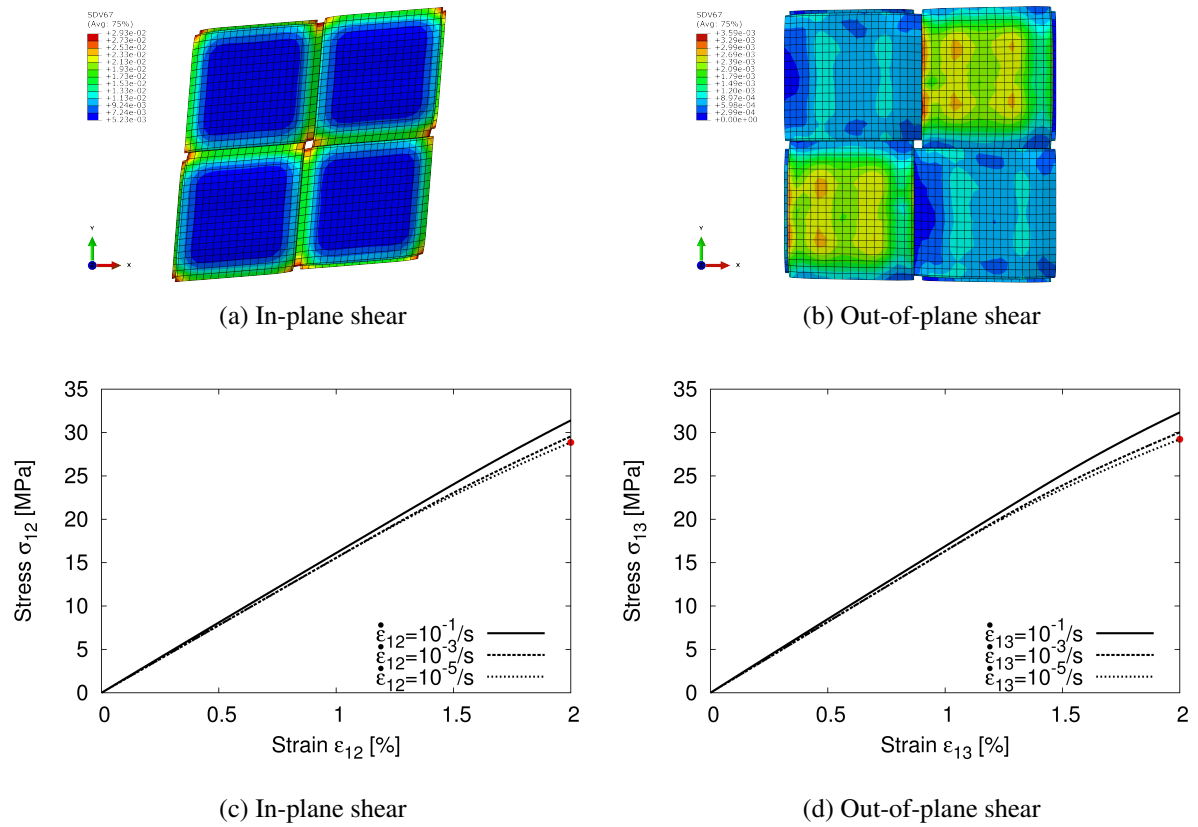


Figure 6.11.: Accumulated plastic strain plots and homogenized stress-strain curves for transverse shear and longitudinal shear.

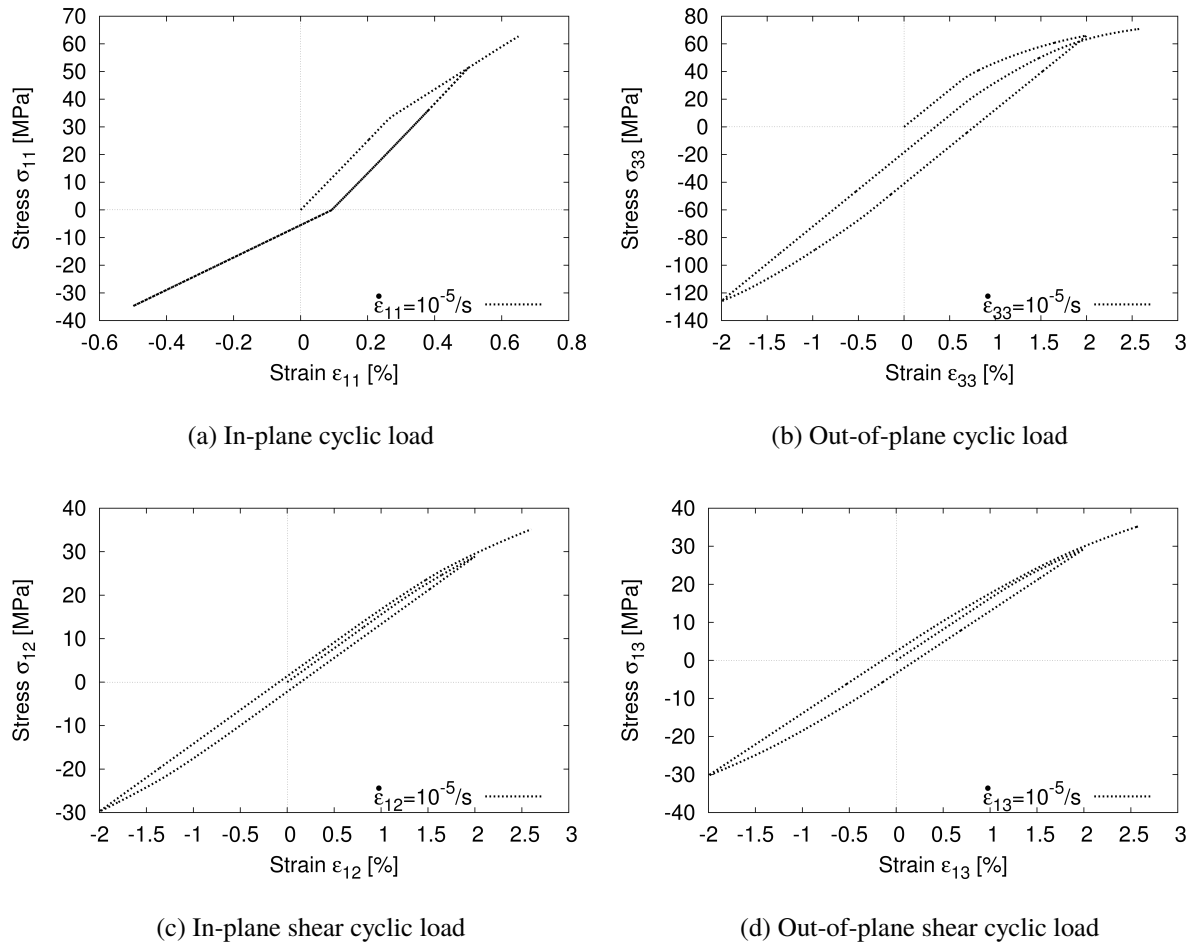


Figure 6.12.: Homogenized stress-strain curves for in-plane cyclic load, out-of-plane cyclic load, in-plane shear cyclic load and out-of-plane shear cyclic load.

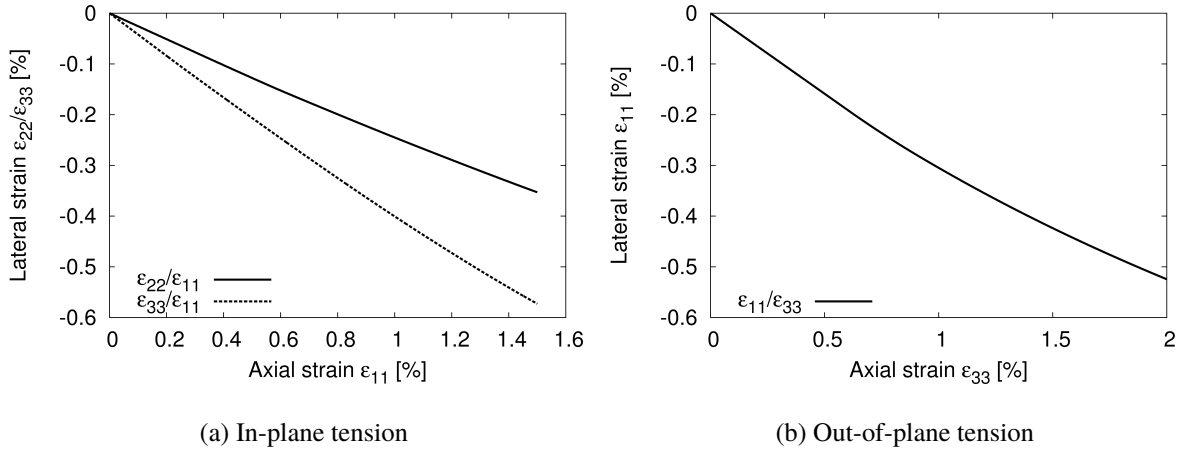


Figure 6.13.: Homogenized lateral strain versus axial strain plots for in-plane tension and out-of-plane tension.

6.6.2. Plain weave composite yield surface identification

For the purpose of recommendations concerning a continuum mechanical model development of the plain weave flax fibre/epoxy composite RUC, knowledge regarding the shape of the composite yield surface is generated. This is undertaken by subjecting the plain weave composite RUC to various biaxial tensile and compressive tests as well as combined shear tension and combined shear compression tests (see Table 6.2 for a graphical illustration of the applied far field strains). The employed load combinations are similar to the load combinations used in Bedzra et al. [2020] for the identification of the yield surface of the unidirectional flax fibre/epoxy composite (refer to Bedzra et al. [2020] for details). Displayed in Figure 6.14 are identified yield surfaces of the plain weave composite in 11/22, 12/22, 11/33 and 13/33 stress space. Due to geometrical and material symmetry, it is not necessary to identify the yield surfaces in 22/33 and 23/33 stress space. For comparison purposes, the yield function of the derived anisotropic continuum model of the tow is also plotted.

From Figure 6.14, it can be observed that the tow yield function is in a reasonably good agreement with the identified yield surfaces from the plain weave composite RUC except in the case of 11/33 stress space where a discrepancy can be observed as a result of the inability to control biaxial yielding. An idea will be to extend the tow constitutive model to take into account biaxial yielding in 11/33 stress space. However from the non-quadratic nature of the identified RUC yield surfaces in principal stress space (11/22 and 11/33 stress space), it will be advisable to construct a multi-surface yield function (see e.g. Bedzra et al. [2017a]) or a non-quadratic yield function (see e.g. Bedzra et al. [2019]) for the continuum mechanical model

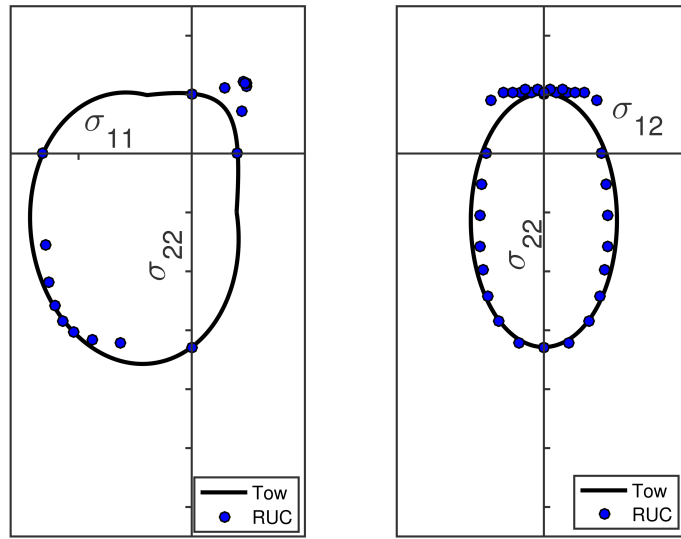
of the flax fibre/epoxy plain weave composite instead. The current plain weave composite assumes a similar material property for the weft and warp yarns. In general the weft and warp yarns may possess different material characteristics as such, it will be better to develop a general orthotropic continuum mechanical model for the plain weave composite as opposed to a transversely isotropic continuum model.

6.6.3. Conclusion and future work

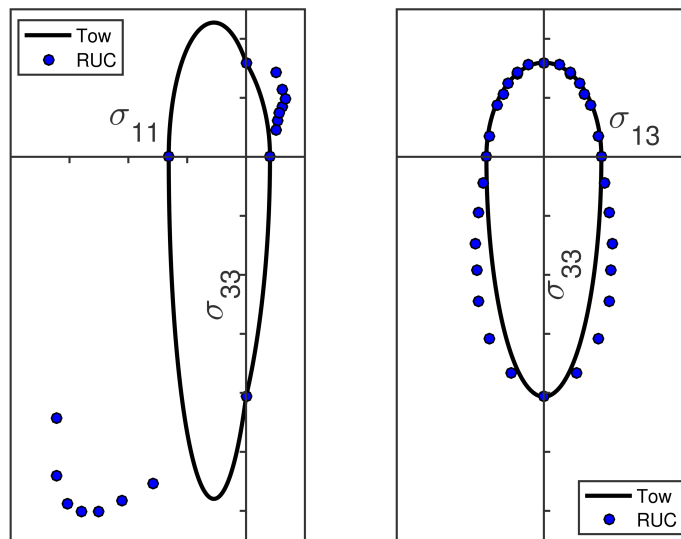
A systematic approach for creating a continuum model of a unidirectional flax fibre/epoxy composite which is integrated into the tows of a plain weave flax fibre/epoxy composite repeating unit cell has been proposed. Continuum models are more computationally efficient and easier to interface with complex structures as opposed to models which seek to directly capture the response of the composite microstructure.

The first step of the approach relies on the development of a representative volume element of the microstructure of the flax fibre/epoxy unidirectional composite. The next step relies on the subsection of the microstructure to the necessary deformation states required to generate the deformation profile of the composite and to also identify the yield surface of the composite. Once this information is obtained, a continuum model is developed for the composite and validated against other load states subjected to the microstructure. Although the continuum model does not directly model the individual fibre filament and matrix interaction, it contains information about the deformation behaviour of the composite microstructure. This constitutive model is then assigned to the tows of a plain weave flax fibre/epoxy composite repeating unit cell mesostructure and the deformation profile as well as the yield surface of the plain weave composite is identified through virtual experiments.

As part of future research, a continuum model will be developed for the plain weave mesostructure which will be assigned to plies (or laminar) of different laminate configurations in order to study their deformation behaviour and to also serve as the material model of the laminate for computations on the scale of the structure. Furthermore, the generated representative volume element of the unidirectional flax fibre/epoxy composite as well as the plain weave composite repeating unit cell will be experimentally validated to better validate the existing tow model and the continuum model to be developed for the plain weave composite. Additionally, tow damage and matrix damage as well as decohesion at matrix/filament or matrix/tow interface will be taken into account through implementation of nonlocal damage models for the matrix, fibre filaments, the matrix/filament interface, the tow, the matrix/tow interface and the continuum model to be developed for the plain weave composite. Other potential avenues for future research will be an extension of the generated models to finite



(a) Yield surface in 11/22 and 12/22 stress space



(b) Yield surface in 11/33 and 13/33 stress space

Figure 6.14.: Comparison between the identified yield surface from the unidirectional composite RVE and the tow constitutive model in stress space.

deformation for applications to structural fabrics (such as air beams or pneumatic membranes).

7 | Conclusions and Outlook

The objective of this dissertation was the development and implementation of general anisotropic constitutive models for unidirectional composites as well as textile composites using a hierarchical multi-scale modelling approach. As part of this objective, several constitutive models were developed.

In Chapter 2, an anisotropic elastoplastic constitutive model for woven tungsten fibre reinforced copper matrix was developed. This was done by first setting up a finite element model of a repeating unit cell of a plain weave composite, where the tows and the matrix were modelled as isotropic elastoplastic materials. The elastic response of the composite was modelled by means of an anisotropic strain energy function. Based on the identified yield surface, an anisotropic yield function was constructed from multiple yield functions defined in terms of structural tensors pointing in three privilege directions of the material. The strength of each of the yield surface was taken to harden with respect to the equivalent plastic strain, thus providing anisotropic strain hardening of the yield surface. The material parameters of the model were obtained by fitting the derived constitutive model to uniaxial stress-strain as well as shear stress-strain data generated from a finite element model of the composite. With the fitted parameters, the model was shown to be predictive of other in-plane stress-strain response of the composite material. From the obtained simulation results, it was shown that the fibre orientations played an important role in the deformation process. The presented constitutive model was developed on the assumption that the tows were isotropic materials; however, the tows are in actual fact transversely isotropic materials. Furthermore, the model did not account for the effect of plastic Poisson's ratio as well as out-of-plane plastic response. These questions should be addressed in future works.

In Chapter 3, a constitutive model, based on the multi-surface model developed in Chapter 2, for the in-plane anisotropic elastoplastic behaviour of paper and paperboard was developed and was compared to a non-quadratic counterpart of the constitutive model. The material parameters for both constitutive models were identified by fitting the models to uniaxial stress-strain curves as well as lateral strain versus axial strain curves obtained from actual experiments. With the identified material parameters, both constitutive models were compared

to experimentally obtained off-axis stress-strain curves. Both plasticity models were in a good agreement with the experimental results, although the multi-surface model slightly over predicted one of the off-axis tensile tests. Furthermore, both models were employed in the finite element analysis of a paperboard with a circular hole under tension. The numerically predicted force-displacement curves and local strain fields were compared to experimental results. Again, both constitutive models were in a good agreement with the experimental results. Also, the convergence behaviour of both models was studied using a stand-alone stress-driven algorithm. From the comparison, the multi-surface model showed a superior rate of convergence to the non-quadratic model. However, implementation of the non-quadratic model was less laborious as compared to the multi-surface model due to the active set search that had to be undertaken. The non-quadratic modelling approach should be employed, due to the ease of implementation, when developing a constitutive model for the textile composite material in future works.

In Chapter 4, an anisotropic elastoplastic material model for unidirectional tungsten fibre reinforced copper was also developed by first setting up a finite element model of the unidirectional composite. It was subjected to various biaxial tensile tests as well as combined shear tensile tests. From these virtual experiments, the initial yield surface of the unidirectional composite was identified in principal stress-space. To capture the yield surface, a Hill type yield function was employed. To capture the anisotropic hardening behaviour of the composite, multiple isotropic hardening functions were employed. After parameter identification, the model was validated by comparing the predicted yield surface to the yield surface obtained from the finite element model of the unidirectional composite. Although the yield surface predicted by the constitutive model was in a good agreement with the yield surface obtained from the composite in regions corresponding to combined shear tensile tests, the same could not be said for regions corresponding to biaxial tensile tests. This was due to the fact that the yield function could not be controlled in biaxial yielding. Furthermore, the ability of the constitutive model to capture lateral versus axial strain response obtained from the composite was investigated. From the investigations, the constitutive model showed an excellent agreement with the finite element model of the composite for uniaxial tension in the fibre direction. However, the same could not be said for uniaxial tension in the transverse fibre direction. This was attributed to the lack of control of the plastic Poisson's ratios.

Finally in Chapter 6, a general non-associative anisotropic viscoelastic-viscoplastic constitutive model for unidirectional fibre reinforced polymer composite materials, taking into account the recommendations made in Chapter 4, was developed. This was achieved by first developing a constitutive model for the fibre and matrix of interest, which were flax fibre and

epoxy matrix. Next, a finite element model of a unidirectional composite was setup in Chapter 5. The composite was subjected to various virtual biaxial experiments, based on which the yield surface of the composite was identified in stress-space. To capture the deformation behaviour of the composite, a non-associative anisotropic viscoelastic-viscoplastic continuum model was developed. The evolution of the yield surface of the constitutive model during plastic strain was described by multiple isotropic and kinematic hardening functions, thus providing anisotropic strain hardening of the yield surface. The material parameters of the continuum model were identified by fitting it to uniaxial and biaxial tensile and compressive stress-strain curves generated from the unidirectional composite. The constitutive model was validated by comparing the predicted yield surface to the yield surface obtained from the unidirectional composite, as well as off-axis tension and compression tests carried out in various directions of the plane parallel to the longitudinal fibre direction and the plane transverse to the longitudinal fibre direction (plane of isotropy). The constitutive model was in a very good agreement with the corresponding virtual experiments conducted on the finite element model of the composite. Next, the constitutive model was assigned to the tows of a plain weave flax fibre/epoxy composite repeating unit cell and the deformation behaviour of the composite was studied as well as the yield surface of the composite was identified.

As part of future research, a continuum model will be developed for the plain weave mesostructure which will be assigned to plies (or laminar) of different laminate configurations in order to study their deformation behaviour and to also serve as the material model of the laminate for computations on the scale of the structure. Furthermore, the generated representative volume element of the unidirectional flax fibre/epoxy composite as well as the plain weave composite repeating unit cell generated in Chapters 5 and 6, respectively, will be experimentally validated to better validate the existing tow model and the continuum model to be developed for the plain weave composite. Additionally, tow damage and matrix damage as well as decohesion at matrix/filament or matrix/tow interface will be taken into account through implementation of nonlocal damage models for the matrix, fibre filaments, the matrix/filament interface, the tow, the matrix/tow interface and the continuum model to be developed for the plain weave composite. Other potential avenues for future research will be an extension of the generated models to finite deformation for applications to structural fabrics (such as air beams or pneumatic membranes).

Appendix for article 1

A.1. Linearization of the constitutive equation

Assuming $\mathcal{J}_{act}$ is active set 8, the local system of equations, consisting of the discretized evolution equations and the yield functions, is given below (see C.8):

$$\begin{aligned} \mathbf{r}(\boldsymbol{\varepsilon}^p, \bar{\lambda}_1, \bar{\lambda}_2, \bar{\lambda}_3) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \sum_{i=1}^3 \left(\bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \right) = \mathbf{0}, \\ r_j &= \Phi_j = 0, \quad j = 1, 2, 3. \end{aligned} \quad (\text{A.1})$$

Consider first the linearization of the plastic flow rule:

$$\begin{aligned} \Delta \mathbf{r} &= \Delta \left(\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \sum_{i=1}^3 \left(\bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \right) \right), \\ &= \Delta \boldsymbol{\varepsilon}^p - \Delta \boldsymbol{\varepsilon}_n^p - \sum_{i=1}^3 \Delta \bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} - \sum_{i=1}^3 \bar{\lambda}_i \Delta \left(\frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \right). \end{aligned} \quad (\text{A.2})$$

The tensor $\boldsymbol{\varepsilon}_n^p$ is known. Therefore, $\Delta \boldsymbol{\varepsilon}_n^p$ vanishes and this leads to the intermediate result:

$$\begin{aligned} \Delta \mathbf{r} &= \Delta \boldsymbol{\varepsilon}^p - \sum_{i=1}^3 \Delta \bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \\ &\quad - \sum_{i=1}^3 \bar{\lambda}_i \frac{\Delta \left((\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i \right) \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} - (\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i \Delta \left(\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} \right)}{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}. \end{aligned} \quad (\text{A.3})$$

Consider now the linearization of the term $\Delta((\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i)$ taking into account the stress-strain relation $\boldsymbol{\sigma} = \mathcal{C}_{\text{ani}}([\boldsymbol{\varepsilon}] - [\boldsymbol{\varepsilon}^p])$ and making use of the prior knowledge of the tensor $\boldsymbol{\varepsilon}$ results in

$$\Delta((\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i) = \frac{\partial((\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i)}{\partial \boldsymbol{\sigma}} \cdot \Delta \boldsymbol{\sigma} = -(\mathbf{V}^i \otimes \mathbf{V}^i) : \mathcal{C}_{\text{ani}}[\Delta \boldsymbol{\varepsilon}^p]. \quad (\text{A.4})$$

Next, the term $\Delta\left(\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}\right)$ is linearized as follows:

$$\Delta\left(\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}\right) = \frac{1}{2\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \frac{\partial((\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2)}{\partial \boldsymbol{\sigma}} \cdot \Delta \boldsymbol{\sigma} = -\frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i \cdot \mathcal{C}_{\text{ani}}[\Delta \boldsymbol{\varepsilon}^p]}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}. \quad (\text{A.5})$$

Finally the linearized plastic flow rule takes the form

$$\begin{aligned} \Delta \mathbf{r} = \Delta \boldsymbol{\varepsilon}^p - \sum_{i=1}^3 \Delta \bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}} \\ + \sum_{i=1}^3 \bar{\lambda}_i \frac{(\mathbf{V}^i \otimes \mathbf{V}^i) : \mathcal{C}_{\text{ani}}[\Delta \boldsymbol{\varepsilon}^p] \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} - \sum_{i=1}^3 \bar{\lambda}_i \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2 (\mathbf{V}^i \otimes \mathbf{V}^i) : \mathcal{C}_{\text{ani}}[\Delta \boldsymbol{\varepsilon}^p]}{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2 \sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}. \end{aligned} \quad (\text{A.6})$$

and is further simplified as:

$$\Delta \mathbf{r} = \underbrace{(\mathcal{I})}_{\frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}_p}}[\Delta \boldsymbol{\varepsilon}^p] + \sum_{i=1}^3 \underbrace{\left(-\frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}\right)}_{\frac{\partial \mathbf{r}}{\partial \bar{\lambda}_i}} \Delta \bar{\lambda}_i. \quad (\text{A.7})$$

The linearization of the yield functions are performed analogously. The resulting linearized local system of equations is summarized as:

$$\begin{aligned} \Delta \mathbf{r} &= \frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}_p}[\Delta \boldsymbol{\varepsilon}_p] + \sum_{i=1}^3 \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_i} \Delta \bar{\lambda}_i, \\ \Delta r_j &= \frac{\partial r_j}{\partial \boldsymbol{\varepsilon}_p} \cdot \Delta \boldsymbol{\varepsilon}_p + \sum_{i=1}^3 \frac{\partial r_j}{\partial \bar{\lambda}_i} \Delta \bar{\lambda}_i, \quad j = 1, 2, 3. \end{aligned} \quad (\text{A.8})$$

where the following expressions hold:

$$\begin{aligned}
\frac{\partial \mathbf{r}}{\partial \varepsilon_p} &= \mathcal{I}, \\
\frac{\partial \mathbf{r}}{\partial \bar{\lambda}_i} &= -\frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathbf{V}^i}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}, \\
\frac{\partial r_j}{\partial \varepsilon_p} &= -\frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i) \mathcal{C}_{\text{ani}}[\mathbf{V}^i]}{\sqrt{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2}}, \\
\frac{\partial r_j}{\partial \bar{\lambda}_i} &= -a_i Q_i \beta_i e^{-\beta_i (\kappa_n + \sum_{i=1}^3 \bar{\lambda}_i \sqrt{a_i})}.
\end{aligned} \tag{A.9}$$

For the case where there is plastification in all yield functions, the resulting system of equations consists of 9 nonlinear scalar equations which are solved iteratively by means of the Newton method. The local Gauss point iteration is performed in every time step until the root-mean-square value of the total residuum becomes smaller than a prescribed tolerance. The variables that have to be updated during the iteration are ε^p and $\bar{\lambda}_i$.

$$\begin{bmatrix} \frac{\partial \mathbf{r}}{\partial \varepsilon_p} & \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_1} & \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_2} & \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_3} \\ \frac{\partial r_1}{\partial \varepsilon_p} & \frac{\partial r_1}{\partial \bar{\lambda}_1} & \frac{\partial r_1}{\partial \bar{\lambda}_2} & \frac{\partial r_1}{\partial \bar{\lambda}_3} \\ \frac{\partial r_2}{\partial \varepsilon_p} & \frac{\partial r_2}{\partial \bar{\lambda}_1} & \frac{\partial r_2}{\partial \bar{\lambda}_2} & \frac{\partial r_2}{\partial \bar{\lambda}_3} \\ \frac{\partial r_3}{\partial \varepsilon_p} & \frac{\partial r_3}{\partial \bar{\lambda}_1} & \frac{\partial r_3}{\partial \bar{\lambda}_2} & \frac{\partial r_3}{\partial \bar{\lambda}_3} \end{bmatrix} \begin{bmatrix} \Delta \varepsilon^p \\ \Delta \bar{\lambda}_1 \\ \Delta \bar{\lambda}_2 \\ \Delta \bar{\lambda}_3 \end{bmatrix} = - \begin{bmatrix} \mathbf{r} \\ r_1 \\ r_2 \\ r_3 \end{bmatrix}. \tag{A.10}$$

A.2. Consistent tangent

For the calculation of the tangential stiffness matrix in a finite element computation, the derivation of the consistent tangent operator is required. The fourth order tensor $\mathcal{C}_{\text{cons}}$ is derived based on Simo et al. [1988]; Simo and Hughes [1998] and it represents a relation between the increments $\Delta \boldsymbol{\sigma}$ and $\Delta \boldsymbol{\varepsilon}$ as follows:

$$\Delta \boldsymbol{\sigma} = \mathcal{C}_{\text{cons}} [\Delta \boldsymbol{\varepsilon}]. \tag{A.11}$$

Since the stress tensor $\boldsymbol{\sigma}$ is a function of $\boldsymbol{\varepsilon}$ and ε^p , it is possible to express the increment $\Delta \boldsymbol{\sigma}$ as

$$\Delta \boldsymbol{\sigma} = \mathcal{C}_{\text{ani}} ([\Delta \boldsymbol{\varepsilon}] - [\Delta \varepsilon^p]). \tag{A.12}$$

Also taking the discrete flow rule ($\epsilon_p = \epsilon_n^p + \sum_{i=1}^3 \bar{\lambda}_i \frac{\partial \Phi_i}{\partial \sigma}$) into account, the relation between the increments $\Delta \epsilon^p$, $\Delta \sigma$, and $\Delta \bar{\lambda}_i$ is obtained from the converged local Gauss point iteration as follows:

$$\begin{aligned} \Delta \epsilon^p &= \frac{\partial \epsilon_p}{\partial \Delta \sigma} [\Delta \sigma] + \sum_{i=1}^3 \frac{\partial \epsilon_p}{\partial \bar{\lambda}_i} \Delta \bar{\lambda}_i \\ &= \sum_{i=1}^3 \bar{\lambda}_i \frac{\partial^2 \Phi_i}{\partial \sigma^2} [\Delta \sigma] + \sum_{i=1}^3 \frac{\partial \Phi_i}{\partial \sigma} \Delta \bar{\lambda}_i. \end{aligned} \quad (\text{A.13})$$

Substituting equation (A.13) into (A.12) yields

$$\underbrace{\left(\mathbf{c}_{\text{ani}}^{-1} + \sum_{i=1}^3 \bar{\lambda}_i \frac{\partial^2 \Phi_i}{\partial \sigma^2} \right)}_{\mathcal{E}^{-1}} [\Delta \sigma] = \Delta \epsilon - \sum_{i=1}^3 \frac{\partial \Phi_i}{\partial \sigma} \Delta \bar{\lambda}_i. \quad (\text{A.14})$$

and after rearranging leads to

$$\Delta \sigma = \mathcal{E} \left([\Delta \epsilon] - \left[\sum_{i=1}^3 \frac{\partial \Phi_i}{\partial \sigma} \Delta \bar{\lambda}_i \right] \right). \quad (\text{A.15})$$

Consider now the linearization of the yield function taking into account the converged local Gauss point iteration. This leads to the following:

$$\Delta r_j = \frac{\partial \Phi_j}{\partial \sigma} \cdot \Delta \sigma + \sum_{i=1}^3 \frac{\partial \Phi_j}{\partial \bar{\lambda}_i} \Delta \bar{\lambda}_i = 0 \quad j = 1, 2, 3. \quad (\text{A.16})$$

Substituting equation (A.15) into (A.16) and rearranging results in

$$\Delta \bar{\lambda}_i = g_{ij}^{-1} \frac{\partial \Phi_j}{\partial \sigma} \cdot \mathcal{E} [\Delta \epsilon], \quad (\text{A.17})$$

where

$$g_{ij} = \left(\frac{\partial \Phi_i}{\partial \sigma} \cdot \mathcal{E} \left[\frac{\partial \Phi_j}{\partial \sigma} \right] - \frac{\partial \Phi_i}{\partial \bar{\lambda}_j} \right). \quad (\text{A.18})$$

Remark. As a result of the Jacobian matrix g_{ij} being ill conditioned in when multiple yield functions are active, the global Newton iteration does not lead to convergence. To overcome this problem, g_{ij} is rewritten as

$$\bar{g}_{ij} = g_{ij} + \varepsilon \delta_{ij}. \quad (\text{A.19})$$

The second term in (A.19) regularizes the Jacobian matrix. For more details on how to choose ε , the reader is referred to Schröder and Miehe [1997]; Miehe and Schröder [2001].

Finally, substituting equation (A.17) into (A.15) leads to

$$\Delta \sigma = \underbrace{\left(\varepsilon - \sum_{i=1}^3 \sum_{j=1}^3 \bar{g}_{ij}^{-1} \varepsilon \left[\frac{\partial \Phi_i}{\partial \sigma} \right] \otimes \varepsilon \left[\frac{\partial \Phi_j}{\partial \sigma} \right] \right)}_{\mathcal{C}_{\text{cons}}} [\Delta \varepsilon]. \quad (\text{A.20})$$

A.3. Relation between coefficients of strain energy function and elasticity constants

The coefficients of the strain energy function are related to the elasticity constants as follows:

$$\begin{aligned} K_1^{\text{iso}} &= \frac{E_3 (1 - \nu_{12}\nu_{21})}{8D}, \\ K_1^{\text{ani1}} &= \frac{E_1 (1 - \nu_{23}\nu_{32}) + E_3 (1 - 2\nu_{13} - \nu_{12}\nu_{21} - 2\nu_{12}\nu_{23})}{8D} - \frac{1}{2}G_{13}, \\ K_1^{\text{ani2}} &= \frac{E_2 (1 - 2\nu_{32} - \nu_{13}\nu_{31} - 2\nu_{12}\nu_{31}) + E_3 (1 - \nu_{12}\nu_{12})}{8D} - \frac{1}{2}G_{23}, \\ K^{\text{kop1}} &= -\frac{E_3 (1 - \nu_{13} - \nu_{12}\nu_{21} - \nu_{12}\nu_{23})}{4D} - \frac{1}{2}(G_{12} - G_{13} - G_{23}), \\ K^{\text{kop2}} &= \frac{E_2 (\nu_{32} + \nu_{12}\nu_{31}) - E_3 (1 - \nu_{12}\nu_{21})}{4D} - \frac{1}{2}(G_{12} - G_{13} - G_{23}), \\ K^{\text{kop12}} &= \frac{E_1 (\nu_{21} + \nu_{23}\nu_{31}) - E_2 (\nu_{32} + \nu_{12}\nu_{31}) + E_3 (1 - \nu_{13} - \nu_{12}\nu_{21} - \nu_{12}\nu_{23})}{4D}, \\ &\quad + \frac{1}{2}(G_{12} - G_{13} - G_{23}), \\ K_2^{\text{iso}} &= \frac{1}{2}(G_{12} - G_{13} - G_{23}), \\ K_2^{\text{ani1}} &= \frac{1}{2}(G_{12} - G_{23}), \\ K_2^{\text{ani2}} &= \frac{1}{2}(G_{12} - G_{13}), \end{aligned} \quad (\text{A.21})$$

where

$$D = 1 - \nu_{12}\nu_{21} - \nu_{13}\nu_{31} - \nu_{23}\nu_{32} - 2\nu_{12}\nu_{23}\nu_{31}. \quad (\text{A.22})$$

Appendix for article 2

B.1. Fulfilment of the Clausius-Duhem inequality

In the following, it is shown that the evolution equations actually fulfil the Clausius-Duhem inequality. With $\dot{\lambda} \geq 0$, substituting $\dot{\varepsilon}_p$ and $\dot{\kappa}$ into the Clausius-Duhem inequality yields:

$$\boldsymbol{\sigma} \cdot \dot{\lambda} \left(\sum_{i=1}^3 \frac{2k}{\|\mathbf{K}\|} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-1} \frac{\mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right) + \sum_{i=1}^3 R_i^{nq} \dot{\lambda} \geq 0. \quad (\text{B.1})$$

The result in (B.1) can be simplified as:

$$\dot{\lambda} \sum_{i=1}^3 \left(\frac{2k}{\|\mathbf{K}\|} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-1} \frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} + R_i^{nq} \right) = \dot{\lambda} \left(\frac{2k}{\|\mathbf{K}\|} (\Phi + 1) + \sum_{i=1}^3 R_i^{nq} \right) \geq 0. \quad (\text{B.2})$$

$\mathbf{K}$ and its norm $\|\mathbf{K}\|$ is given as:

$$\begin{aligned} \mathbf{K} &= \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} = \sum_{i=1}^3 \frac{2k}{(s_i^0 - R_i^{nq})} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-1} \mathbf{V}^i, \\ \|\mathbf{K}\| &= \sqrt{\sum_{i=1}^3 \frac{4k^2}{(s_i^0 - R_i^{nq})^2} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{4k-2} \mathbf{V}^i \cdot \mathbf{V}^i}. \end{aligned} \quad (\text{B.3})$$

Taking into account the fact that $\mathbf{V}^i \cdot \mathbf{V}^i = 1$, (B.3) can be further simplified as:

$$\begin{aligned} \|\mathbf{K}\| &= \sqrt{\sum_{i=1}^3 \frac{4k^2}{(s_i^0 - R_i^{nq})^2} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{4k} \left(\frac{(s_i^0 - R_i^{nq})}{\boldsymbol{\sigma} \cdot \mathbf{V}^i} \right)^2} \\ &= \sqrt{\sum_{i=1}^3 \frac{4k^2}{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)^2} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{4k}}. \end{aligned} \quad (\text{B.4})$$

By employing (B.4), the term $2k/\|\mathbf{K}\|$ is obtained as:

$$\frac{2k}{\|\mathbf{K}\|} = \sum_{i=1}^3 (\boldsymbol{\sigma} \cdot \mathbf{V}^i)^{1-2k} (s_i^0 - R_i^{nq})^{2k}. \quad (\text{B.5})$$

Substitution of (B.5) into (B.2) results in:

$$\dot{\lambda} \sum_{i=1}^3 \left((\Phi + 1) (\boldsymbol{\sigma} \cdot \mathbf{V}^i)^{1-2k} (s_i^0 - R_i^{nq})^{2k} + R_i^{nq} \right) \geq 0. \quad (\text{B.6})$$

Taking into account the Kuhn-Tucker condition as well as making use of the prior knowledge of $(\boldsymbol{\sigma} \cdot \mathbf{V}^i = (s_i^0 - R_i^{nq}))$ at yield, the final form of the Clausius-Duhem inequality is obtained as:

$$\dot{\lambda} \sum_{i=1}^3 s_i^0 \geq 0. \quad (\text{B.7})$$

This inequality is sufficiently satisfied since s_i^0 is positive.

B.2. Linearization of non-quadratic constitutive equations

The local system of equations, consisting of the discretized evolution equation together with the yield function, is given below (see (C.8)):

$$\begin{aligned} \mathbf{r}(\boldsymbol{\varepsilon}^p, \bar{\lambda}) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda} \frac{\mathbf{K}}{\|\mathbf{K}\|} = \mathbf{0}, \\ r &= \Phi = 0. \end{aligned} \quad (\text{B.8})$$

Linearization of the residuums leads to the following system of equations

$$\begin{aligned}\Delta \mathbf{r} &= \frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}_p} [\Delta \boldsymbol{\varepsilon}_p] + \frac{\partial \mathbf{r}}{\partial \bar{\lambda}} \Delta \bar{\lambda}, \\ \Delta r &= \frac{\partial r}{\partial \boldsymbol{\varepsilon}_p} \cdot \Delta \boldsymbol{\varepsilon}_p + \frac{\partial r}{\partial \bar{\lambda}} \Delta \bar{\lambda}.\end{aligned}\tag{B.9}$$

where the following expressions hold:

$$\begin{aligned}\frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}_p} &= \mathcal{I} - \bar{\lambda} \left(\frac{\mathcal{I}}{\sqrt{\mathbf{K} \cdot \mathbf{K}}} - \frac{(\mathbf{K} \otimes \mathbf{K})}{(\mathbf{K} \cdot \mathbf{K}) \sqrt{\mathbf{K} \cdot \mathbf{K}}} \right) : \frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}_p}, \\ \frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}_p} &= \sum_{i=1}^3 \frac{2k(2k-1)}{(s_i^0 - R_i^{nq})} \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-2} (\mathbf{V}^i \otimes \mathbf{V}^i) : \mathcal{C}_{\text{ani}}, \\ \frac{\partial \mathbf{r}}{\partial \bar{\lambda}} &= -\frac{\mathbf{K}}{\sqrt{\mathbf{K} \cdot \mathbf{K}}}, \\ \frac{\partial r}{\partial \boldsymbol{\varepsilon}_p} &= -\mathcal{C}_{\text{ani}}^T [\mathbf{K}], \\ \frac{\partial r}{\partial \bar{\lambda}} &= \sum_{i=1}^3 2k \left(\frac{\boldsymbol{\sigma} \cdot \mathbf{V}^i}{(s_i^0 - R_i^{nq})} \right)^{2k-1} \frac{(\boldsymbol{\sigma} \cdot \mathbf{V}^i)}{(s_i^0 - R_i^{nq})^2} \frac{\partial R_i^{nq}}{\partial \bar{\lambda}},\end{aligned}\tag{B.10}$$

with $\partial_{\bar{\lambda}} R_i^{nq}$ ($i = 1, 2$) expressed as

$$\begin{aligned}\frac{\partial R_i^{nq}}{\partial \bar{\lambda}} &= -\frac{1}{2k} \left(\frac{\Omega}{A_i} \right)^{\frac{(1-2k)}{2k}} \left(\frac{\partial \Omega}{\partial \bar{\lambda}} \frac{1}{A_i} - \frac{\Omega}{(A_i)^2} \frac{\partial A_i}{\partial \bar{\lambda}} \right), \\ \frac{\partial \Omega}{\partial \bar{\lambda}} &= -2k ((\sigma_{y1} - R_1)(\sigma_{y2} - R_2))^{(2k-1)} \left(\frac{\partial R_1}{\partial \bar{\lambda}} (\sigma_{y2} - R_2) + (\sigma_{y1} - R_1) \frac{\partial R_2}{\partial \bar{\lambda}} \right) \Omega_1, \\ \frac{\partial A_1}{\partial \bar{\lambda}} &= -2k \left(V_{22}^2 ((\sigma_{y2} - R_2) V_{22}^2)^{2k-1} \frac{\partial R_2}{\partial \bar{\lambda}} - V_{11}^2 ((\sigma_{y1} - R_1) V_{11}^2)^{2k-1} \frac{\partial R_1}{\partial \bar{\lambda}} \right), \\ \frac{\partial A_2}{\partial \bar{\lambda}} &= -2k \left(V_{11}^1 ((\sigma_{y1} - R_1) V_{11}^1)^{2k-1} \frac{\partial R_1}{\partial \bar{\lambda}} - V_{22}^1 ((\sigma_{y2} - R_2) V_{22}^1)^{2k-1} \frac{\partial R_2}{\partial \bar{\lambda}} \right), \\ \frac{\partial R_i}{\partial \bar{\lambda}} &= -Q_i \beta_i e^{-\beta_i (\kappa_n + \bar{\lambda})},\end{aligned}\tag{B.11}$$

and $\partial_{\bar{\lambda}} R_3^{nq}$ expressed as

$$\begin{aligned} \frac{\partial R_3^{nq}}{\partial \bar{\lambda}} &= V_{12}^3 \left(\frac{\partial R_{45^\circ}}{\partial \bar{\lambda}} (A_3)^{1/2k} - \frac{1}{2k} (\sigma_{y12}^{45^\circ} - R_{45^\circ}) (A_3)^{\frac{(1-2k)}{2k}} \frac{\partial A_3}{\partial \bar{\lambda}} \right), \\ \frac{\partial A_3}{\partial \bar{\lambda}} &= k B_1 \left(\frac{\frac{1}{2} (\sigma_{y12}^{45^\circ} - R_{45^\circ}) B_1}{(s_1^0 - R_1^{nq})} \right)^{2k-1} \left(\frac{\partial R_{45^\circ}}{\partial \bar{\lambda}} \frac{1}{(s_1^0 - R_1^{nq})} - \frac{(\sigma_{y12}^{45^\circ} - R_{45^\circ})}{(s_1^0 - R_1^{nq})^2} \frac{\partial R_1^{nq}}{\partial \bar{\lambda}} \right) \\ &\quad + k B_2 \left(\frac{\frac{1}{2} (\sigma_{y12}^{45^\circ} - R_{45^\circ}) B_2}{(s_2^0 - R_2^{nq})} \right)^{2k-1} \left(\frac{\partial R_{45^\circ}}{\partial \bar{\lambda}} \frac{1}{(s_2^0 - R_2^{nq})} - \frac{(\sigma_{y12}^{45^\circ} - R_{45^\circ})}{(s_2^0 - R_2^{nq})^2} \frac{\partial R_2^{nq}}{\partial \bar{\lambda}} \right), \\ \frac{\partial R_{45^\circ}}{\partial \bar{\lambda}} &= -Q_{45^\circ} \beta_{45^\circ} e^{-\beta_{45^\circ} (\kappa_n + \bar{\lambda})}. \end{aligned} \quad (\text{B.12})$$

The resulting system of equations is solved iteratively by means of the Newton method. The local Gauss point iteration is performed in every time step until the root mean square value of the total residuum becomes smaller than a prescribed tolerance. The variables that have to be updated during the iteration are ε^p and $\bar{\lambda}$.

$$\begin{bmatrix} \frac{\partial \mathbf{r}}{\partial \varepsilon_p} & \frac{\partial \mathbf{r}}{\partial \bar{\lambda}} \\ \frac{\partial r_1}{\partial \varepsilon_p} & \frac{\partial r_1}{\partial \bar{\lambda}} \end{bmatrix} \begin{bmatrix} \Delta \varepsilon^p \\ \Delta \bar{\lambda} \end{bmatrix} = - \begin{bmatrix} \mathbf{r} \\ r \end{bmatrix}. \quad (\text{B.13})$$

B.3. Determination of consistent tangent operator for non-quadratic plasticity model

In order to determine the tangential stiffness matrix necessary for finite element computation, the consistent tangent operator $\mathcal{C}_{\text{nonq}}$ is required. It represents a relation between $\Delta \boldsymbol{\sigma}$ and $\Delta \boldsymbol{\varepsilon}$:

$$\Delta \boldsymbol{\sigma} = \mathcal{C}_{\text{nonq}} [\Delta \boldsymbol{\varepsilon}]. \quad (\text{B.14})$$

Since the stress tensor $\boldsymbol{\sigma}$ is a function of $\boldsymbol{\varepsilon}$ and ε_p , the increment $\Delta \boldsymbol{\sigma}$ can be expressed as:

$$\Delta \boldsymbol{\sigma} = \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} [\Delta \boldsymbol{\varepsilon}] + \frac{\partial \boldsymbol{\sigma}}{\partial \varepsilon_p} [\Delta \varepsilon_p] = \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} + \frac{\partial \boldsymbol{\sigma}}{\partial \varepsilon_p} : \frac{\partial \varepsilon_p}{\partial \boldsymbol{\varepsilon}} \right) [\Delta \boldsymbol{\varepsilon}]. \quad (\text{B.15})$$

The relation between the increments $\Delta \boldsymbol{\varepsilon}$ and $\Delta \varepsilon_p$ is obtained from the converged solution of the local Gauss point iteration and is given as:

$$\Delta \varepsilon_p = \frac{\partial \varepsilon_p}{\partial \boldsymbol{\varepsilon}} [\Delta \boldsymbol{\varepsilon}] = -\mathcal{A}_p^{-1} : \mathcal{A}_\varepsilon [\Delta \boldsymbol{\varepsilon}], \quad (\text{B.16})$$

where the fourth order tensors $\mathcal{A}_p$ and $\mathcal{A}_\epsilon$ are defined as follows:

$$\begin{aligned}\mathcal{A}_p &= \frac{\partial \mathbf{r}}{\partial \boldsymbol{\epsilon}_p} - \frac{\partial \mathbf{r}}{\partial \bar{\lambda}} \otimes \left(\frac{\partial r}{\partial \bar{\lambda}} \right)^{-1} \frac{\partial r}{\partial \boldsymbol{\epsilon}_p}, \\ \mathcal{A}_\epsilon &= \frac{\partial \mathbf{r}}{\partial \boldsymbol{\epsilon}} - \frac{\partial \mathbf{r}}{\partial \bar{\lambda}} \otimes \left(\frac{\partial r}{\partial \bar{\lambda}} \right)^{-1} \frac{\partial r}{\partial \boldsymbol{\epsilon}}.\end{aligned}\tag{B.17}$$

The residuum $\mathbf{r}$ and r are defined in (C.8).

Finally, the consistent tangent is computed by

$$\mathcal{C}_{\text{nonq}} = \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} - \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}_p} : \mathcal{A}_p^{-1} : \mathcal{A}_\epsilon.\tag{B.18}$$

B.4. Identification of initial yield constants for both multi-surface and non-quadratic plasticity models

To identify the yield surface parameters r_i^0 , s_i^0 , R_i^{mt} , and R_i^{nq} for both constitutive models, it is assumed that the yield stress in MD-direction σ_{y1} , CD-direction σ_{y2} , 45° to MD-direction $\sigma_{y12}^{45^\circ}$, as well as their corresponding hardening stresses R_1 , R_2 , and R_{45° , have been identified. Furthermore, let V_{11}^1 , V_{22}^1 and V_{11}^2 , V_{22}^2 represent (1, 1) and (2, 2) components of the tensor $\mathbf{V}^1$ and $\mathbf{V}^2$, respectively.

For uniaxial tension in MD-direction, the multi-surface yield function Φ_1 results in

$$\Phi_1 = \sqrt{((\sigma_{y1} - R_1) V_{11}^1)^2} - (r_1^0 - R_1^{mt}) = 0.\tag{B.19}$$

Furthermore, for uniaxial tension in CD-direction, Φ_2 results in

$$\Phi_2 = \sqrt{((\sigma_{y2} - R_2) V_{22}^2)^2} - (r_2^0 - R_2^{mt}) = 0.\tag{B.20}$$

The solution of (B.19) and (B.20), taking into account $R_i(\kappa = 0) = 0$ and $R_i^{mt}(\kappa = 0) = 0$, leads to the parameters r_1^0 , r_2^0 , R_1^{mt} , and R_2^{mt} which are given by

$$\begin{aligned}r_1^0 &= \sigma_{y1} V_{11}^1, & R_1^{mt} &= R_1 V_{11}^1 \\ r_2^0 &= \sigma_{y2} V_{22}^2, & R_2^{mt} &= R_2 V_{22}^2.\end{aligned}\tag{B.21}$$

In the case of the non-quadratic yield function, uniaxial tension in MD-direction results in

$$\Phi = \left(\frac{(\sigma_{y1} - R_1) V_{11}^1}{(s_1^0 - R_1^{nq})} \right)^{2k} + \left(\frac{(\sigma_{y1} - R_1) V_{11}^2}{(s_2^0 - R_2^{nq})} \right)^{2k} - 1 = 0. \quad (\text{B.22})$$

Similarly, for uniaxial tension in CD-direction, the yield function results in

$$\Phi = \left(\frac{(\sigma_{y2} - R_2) V_{22}^1}{(s_2^0 - R_2^{nq})} \right)^{2k} + \left(\frac{(\sigma_{y2} - R_2) V_{22}^2}{(s_1^0 - R_1^{nq})} \right)^{2k} - 1 = 0. \quad (\text{B.23})$$

By solving Equation (B.22) and (B.23) simultaneously, taking into account $R_i(\kappa = 0) = 0$ and $R_i^{nq}(\kappa = 0) = 0$, direct relations between $s_i^0 (i = 1, 2)$ and uniaxial yield stresses σ_{y1}, σ_{y2} , as well as R_1^{nq}, R_2^{nq} , and R_1, R_2 , are obtained as follows:

$$\begin{aligned} R_1^{nq} &= s_1^0 - \left(\frac{\Omega}{A_1} \right)^{1/2k}, \quad A_1 = ((\sigma_{y2} - R_2) V_{22}^2)^{2k} - ((\sigma_{y1} - R_1) V_{11}^2)^{2k}, \\ R_2^{nq} &= s_2^0 - \left(\frac{\Omega}{A_2} \right)^{1/2k}, \quad A_2 = ((\sigma_{y1} - R_1) V_{11}^1)^{2k} - ((\sigma_{y2} - R_2) V_{22}^1)^{2k}, \\ s_1^0 &= \left(\frac{\Omega^0}{(\sigma_{y2} V_{22}^2)^{2k} - (\sigma_{y1} V_{11}^2)^{2k}} \right)^{1/2k}, \quad s_2^0 = \left(\frac{\Omega^0}{(\sigma_{y1} V_{11}^1)^{2k} - (\sigma_{y2} V_{22}^1)^{2k}} \right)^{1/2k}, \end{aligned} \quad (\text{B.24})$$

where

$$\begin{aligned} \Omega &= ((\sigma_{y1} - R_1) (\sigma_{y2} - R_2))^{2k} \Omega_1, \quad \Omega^0 = (\sigma_{y1} \sigma_{y2})^{2k} \Omega_1, \\ \Omega_1 &= \left[(V_{11}^1 V_{22}^2)^{2k} - (V_{11}^2 V_{22}^1)^{2k} \right]. \end{aligned} \quad (\text{B.25})$$

The yield surface parameters r_3^0, s_3^0, R_1^{mt} , and R^{nq} , can easily be identified with an additional experimental stress-strain curve for shear in MD-CD plane. However, a shear stress-strain curve maybe difficult to obtain for paper material. Instead an off-axis 45° to MD direction tensile stress-strain curve as done in Xia et al. [2002] is used to compute r_3^0, s_3^0, R_1^{mt} , and R^{nq} . To accomplish this, the uniaxial stress state in the off-axis direction is transformed to the material directions by performing a tensor rotation which results in the following non-zero stress components:

$$\boldsymbol{\sigma} = \frac{(\sigma_{y12}^{45^\circ} - R_{45^\circ})}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (\text{B.26})$$

Substituting B.26 into the third yield function Φ_3 of the multi-surface plasticity model results

in

$$\Phi_3 = \sqrt{((\sigma_{y12}^{45^\circ} - R_{45^\circ}) V_{12}^3)^2 - (r_3^0 - R_3^{mt})} = 0, \quad (\text{B.27})$$

where V_{12}^3 is the $(1, 2)$ component of the tensor $\mathbf{V}^3$. The solution of (B.27), taking into account $R_{45^\circ}(\kappa = 0) = 0$ and $R_3^{mt}(\kappa = 0) = 0$, results in

$$r_3^0 = \sigma_{y12}^{45^\circ} V_{12}^3, \quad R_3^{mt} = R_{45^\circ} V_{12}^3. \quad (\text{B.28})$$

Again substituting (B.26) into the non-quadratic yield function, taking into account $R_i^{nq}(\kappa = 0) = 0$ and $R_{45^\circ}(\kappa = 0) = 0$, and making use of the prior knowledge of s_i^0 ($i = 1, 2$) and R_i^{nq} ($i = 1, 2$), the yield surface parameters s_3^0 and R_3^{nq} are computed as

$$\begin{aligned} R_3^{nq} &= s_3^0 - (\sigma_{y12}^{45^\circ} - R_{45^\circ}) V_{12}^3 (A_3)^{1/2k}, \\ A_3 &= 1 - \left(\frac{\frac{1}{2} (\sigma_{y12}^{45^\circ} - R_{45^\circ}) B_1}{(s_1^0 - R_1^{nq})} \right)^{2k} - \left(\frac{\frac{1}{2} (\sigma_{y12}^{45^\circ} - R_{45^\circ}) B_2}{(s_2^0 - R_2^{nq})} \right)^{2k}, \\ B_1 &= (V_{11}^1 + V_{22}^1), \quad B_2 = (V_{11}^2 + V_{22}^2), \\ s_3^0 &= \sigma_{y12}^{45^\circ} V_{12}^3 \left(1 - \left(\frac{\frac{1}{2} \sigma_{y12}^{45^\circ} B_1}{s_1^0} \right)^{2k} - \left(\frac{\frac{1}{2} \sigma_{y12}^{45^\circ} B_2}{s_2^0} \right)^{2k} \right)^{1/2k}. \end{aligned} \quad (\text{B.29})$$

Appendix for article 4

C.1. Fulfilment of the Clausius-Duhem inequality for epoxy matrix

In the following, restrictions concerning the material parameters of the epoxy matrix material are derived. The derivative of the plastic potential g_m with respect to σ yields the following expression for the plastic evolution equation (6.10) as

$$\dot{\epsilon}_p = \dot{\lambda}_p \frac{\mathcal{B}_m[\beta]}{\|\mathcal{B}_m[\beta]\|}, \quad \mathcal{B}_m := \partial_{\sigma\sigma}^2 g_m = 3\mathcal{P} + \frac{2}{9}\alpha_m(\mathbf{1} \otimes \mathbf{1}), \quad \mathcal{P} = \mathcal{I} - \frac{1}{3}(\mathbf{1} \otimes \mathbf{1}). \quad (\text{C.1})$$

Also from (5.13) the following derivatives are obtained

$$\frac{\partial \psi_{ve1}^m}{\partial \epsilon_1^{ee}} = \gamma_1 \mathcal{C}_{el}[\epsilon_1^{ee}] \quad \text{and} \quad \frac{\partial \psi_{ve2}^m}{\partial \epsilon_2^{ee}} = \gamma_1 \mathcal{C}_{el}[\epsilon_2^{ee}]. \quad (\text{C.2})$$

With $\dot{\lambda}_p \geq 0$, substituting (C.1), C.2, (6.10)₂, (6.10)₃ and (6.11) into the Clausius-Duhem inequality (5.8) yields

$$\frac{\gamma_1}{\tau_1} \mathcal{C}_{el}[\epsilon_1^{ee}] \cdot \epsilon_1^{ee} + \frac{\gamma_2}{\tau_2} \mathcal{C}_{el}[\epsilon_2^{ee}] \cdot \epsilon_2^{ee} + \dot{\lambda}_p \left(\frac{\beta \cdot \mathcal{B}_m[\beta]}{\|\mathcal{B}_m[\beta]\|} + \frac{b}{c} \chi \cdot \chi + R_m^t + R_m^c \right) \geq 0. \quad (\text{C.3})$$

The first and second term satisfy the inequality if the ratio of the viscoelastic material parameters $\gamma_{1,2}$ and $\tau_{1,2}$ are positive and the fourth order elastic stiffness tensor $\mathcal{C}_{el}$ is positive semi-definite. This is the case if the physical meaning of the material parameters of $\mathcal{C}_{el}$ are taken into account. The third term satisfy the inequality if $\mathcal{B}_m$ is positive semi-definite. This places the following restriction on the parameter α_m

$$\frac{2}{3}\alpha_m \geq 0. \quad (\text{C.4})$$

The fourth term also satisfies the inequality if the ratio of the kinematic hardening parameters b and c is positive. Finally, since $\tilde{\sigma}_y^t$ and $\tilde{\sigma}_y^c$ are functions of R_m^t and R_m^c , respectively, the Clausius-Duhem inequality is satisfied if $\tilde{\sigma}_t \geq 0$ and $\tilde{\sigma}_c \geq 0$.

C.2. Numerical aspects of epoxy matrix constitutive model

C.2.1. Viscoelasticity

In the following, all variables without subscripts are evaluated at time t_{n+1} . The evolution equations for viscoelasticity (6.11) is then discretized following the approach in ??? where $\partial \epsilon_e / \partial s$ is assumed to be constant within the time interval $s \in [t_n, t_{n+1}]$. This results in

$$\begin{aligned}
 \mathbf{h}_{1,2} &= \int_{-\infty}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau_{1,2}}\right) \frac{\partial \epsilon^e(s)}{\partial s} ds \\
 &= \exp\left(\frac{-\Delta t}{\tau_{1,2}}\right) \underbrace{\int_{-\infty}^{t_n} \exp\left(-\frac{t_n-s}{\tau_{1,2}}\right) \frac{\partial \epsilon^e(s)}{\partial s} ds}_{\mathbf{h}_{n1,2}} + \int_{t_n}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau_{1,2}}\right) \frac{\partial \epsilon^e(s)}{\partial s} ds \\
 &= \exp\left(\frac{-\Delta t}{\tau_{1,2}}\right) \mathbf{h}_{n1,2} + \frac{\Delta \epsilon^e}{\Delta t} \int_{t_n}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau_{1,2}}\right) ds \\
 &= \exp\left(\frac{-\Delta t}{\tau_{1,2}}\right) \mathbf{h}_{n1,2} + \frac{\tau_{1,2}}{\Delta t} \left(1 - \exp\left(\frac{-\Delta t}{\tau_{1,2}}\right)\right) \Delta \epsilon^e.
 \end{aligned} \tag{C.5}$$

Furthermore, as a result of the recursive determination of the variables $\mathbf{h}_{1,2}$, the variables ϵ_n^e and $\mathbf{h}_{n1,2}$ have to be stored in a database. Making use of (5.14) and (D.23), the stress at any time t can be computed by

$$\boldsymbol{\sigma}(t) = \mathcal{C}_e [\epsilon^e + \gamma_1 \mathbf{h}_1 + \gamma_2 \mathbf{h}_2]. \tag{C.6}$$

For the finite element implementation of viscoelasticity, the tangent operator $\mathcal{C}_{\text{vis}}$ which represents a relation between $\Delta \boldsymbol{\sigma}$ and $\Delta \epsilon^e$ is required. This is obtained by taking the derivative of (C.6) with respect to the elastic strain ϵ^e , which results in

$$\mathcal{C}_{\text{vis}} = \frac{\partial \boldsymbol{\sigma}}{\partial \epsilon^e} = \mathcal{C}_{\text{el}} \left(1 + \gamma_1 \frac{\tau_1}{\Delta t} \left(1 - e^{\left(\frac{-\Delta t}{\tau_1}\right)} \right) + \gamma_2 \frac{\tau_2}{\Delta t} \left(1 - e^{\left(\frac{-\Delta t}{\tau_2}\right)} \right) \right). \tag{C.7}$$

C.2.2. Viscoplasticity

The plastic evolution equations are discretized by means of a standard backward Euler integration scheme and are summarized together with the yield function in residuum format as $(\bar{\lambda}_p := \dot{\lambda}_p \Delta t)$:

$$\begin{aligned} \mathbf{r}_1 &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\partial_{\boldsymbol{\sigma}} g_m}{\|\partial_{\boldsymbol{\sigma}} g_m\|} = \mathbf{0}, \\ \mathbf{r}_2 &= \boldsymbol{\varepsilon}^{pi} - \boldsymbol{\varepsilon}_n^{pi} - \bar{\lambda}_p \frac{b}{c} \boldsymbol{\chi} = \mathbf{0}, \\ r_3 &= \Phi^m = 0. \end{aligned} \tag{C.8}$$

Due to the symmetry of the internal variables, the symmetric tensors $\mathbf{r}_1$ and $\mathbf{r}_2$ can be represented in Voigt form as six-dimensional arrays. Thus, the resulting system of equations consist of 13 nonlinear scalar equations which are solved iteratively using e.g. Newton's method. This local iteration is performed in every time step until the root mean square of the total residuum becomes smaller than a prescribed tolerance. In order to employ Newton's method, the consistent linearization of (C.8) with respect to $\boldsymbol{\varepsilon}^p$, $\boldsymbol{\varepsilon}^{pi}$ and $\bar{\lambda}_p$ has to be undertaken. For the linearization of the constitutive equations, the reader is referred to C.2.3.

The scalar evolution equation for accumulated plastic strain (6.10)₃ is also descritized by means of the backward Euler integration scheme as:

$$\kappa = \kappa_n + \bar{\lambda}_p. \tag{C.9}$$

The accumulated plastic strain κ is computed at the end of each local Newton iteration via the converged value of the plastic multiplier $\bar{\lambda}_p$. Furthermore, for the calculation of the tangential stiffness matrix in a finite element computation, the derivation of the consistent tangent operator is required. The consistent tangent operator $\mathcal{C}_{\text{cons}}^m$ represents a relation between $\Delta \boldsymbol{\sigma}$ and $\Delta \boldsymbol{\varepsilon}$. It is given without derivation in C.2.4.

C.2.3. Linearization of matrix material constitutive equations

The local system of equations, consisting of the discretized evolution equation together with the yield function, is given below (see (C.8)):

$$\begin{aligned}
 \mathbf{r}_1(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}^{pi}, \bar{\lambda}_p) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\mathbf{K}_m}{\|\mathbf{K}_m\|} = \mathbf{0}, \quad \mathbf{K}_m = \mathcal{B}_m[\boldsymbol{\beta}], \\
 \mathbf{r}_2(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}^{pi}, \bar{\lambda}_p) &= \boldsymbol{\varepsilon}^{pi} - \boldsymbol{\varepsilon}_n^{pi} - \bar{\lambda}_p \frac{b}{c} \boldsymbol{\chi} = \mathbf{0}, \\
 r_3(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}^{pi}, \bar{\lambda}_p) &= \Phi^m = 0.
 \end{aligned} \tag{C.10}$$

Linearization of the residuals leads to the following system of equations

$$\begin{aligned}
 \Delta \mathbf{r}_1 &= \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^p} [\Delta \boldsymbol{\varepsilon}^p] + \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^{pi}} [\Delta \boldsymbol{\varepsilon}^{pi}] + \frac{\partial \mathbf{r}_1}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p, \\
 \Delta \mathbf{r}_2 &= \frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^p} [\Delta \boldsymbol{\varepsilon}^p] + \frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^{pi}} [\Delta \boldsymbol{\varepsilon}^{pi}] + \frac{\partial \mathbf{r}_2}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p, \\
 \Delta r_3 &= \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^p} \cdot \Delta \boldsymbol{\varepsilon}^p + \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^{pi}} \cdot \Delta \boldsymbol{\varepsilon}^{pi} + \frac{\partial r_3}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p.
 \end{aligned} \tag{C.11}$$

where the following expressions hold:

$$\begin{aligned}
\frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^p} &= \mathcal{I} - \bar{\lambda}_p \left(\frac{\mathcal{I}}{\sqrt{\mathbf{K}_m \cdot \mathbf{K}_m}} - \frac{(\mathbf{K}_m \otimes \mathbf{K}_m)}{(\mathbf{K}_m \cdot \mathbf{K}_m) \sqrt{\mathbf{K}_m \cdot \mathbf{K}_m}} \right) : \frac{\partial \mathbf{K}_m}{\partial \boldsymbol{\varepsilon}^p}, \\
\frac{\partial \mathbf{K}_m}{\partial \boldsymbol{\varepsilon}^p} &= - \left(3\mathcal{P} + \frac{2}{9} \alpha_m (\mathbf{1} \otimes \mathbf{1}) \right) : (\mathcal{C}_{\text{vis}} + c\mathcal{I}), \\
\frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^{pi}} &= -\bar{\lambda}_p \left(\frac{\mathcal{I}}{\sqrt{\mathbf{K}_m \cdot \mathbf{K}_m}} - \frac{(\mathbf{K}_m \otimes \mathbf{K}_m)}{(\mathbf{K}_m \cdot \mathbf{K}_m) \sqrt{\mathbf{K}_m \cdot \mathbf{K}_m}} \right) : \frac{\partial \mathbf{K}_m}{\partial \boldsymbol{\varepsilon}^{pi}}, \\
\frac{\partial \mathbf{K}_m}{\partial \boldsymbol{\varepsilon}^{pi}} &= \left(3\mathcal{P} + \frac{2}{9} \alpha_m (\mathbf{1} \otimes \mathbf{1}) \right) : (c\mathcal{I}), \\
\frac{\partial \mathbf{r}_1}{\partial \bar{\lambda}^p} &= -\frac{\mathbf{K}_m}{\sqrt{\mathbf{K}_m \cdot \mathbf{K}_m}}, \\
\frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^p} &= -\bar{\lambda}_p b \mathcal{I}, \\
\frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^{pi}} &= \mathcal{I} (1 + \bar{\lambda}_p b), \\
\frac{\partial \mathbf{r}_2}{\partial \bar{\lambda}_p} &= -\frac{b}{c} \boldsymbol{\chi}, \\
\frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^p} &= -(\mathcal{C}_{\text{vis}} + c\mathcal{I})^T [(6\beta^D + 2(\tilde{\sigma}_c - \tilde{\sigma}_t) \mathbf{1})], \\
\frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^{pi}} &= (c\mathcal{I}) [(6\beta^D + 2(\tilde{\sigma}_y^c - \tilde{\sigma}_y^t) \mathbf{1})], \\
\frac{\partial r_3}{\partial \bar{\lambda}_p} &= 2 \left(\frac{\partial \tilde{\sigma}_y^c}{\partial \bar{\lambda}_p} - \frac{\partial \tilde{\sigma}_y^t}{\partial \bar{\lambda}_p} \right) (\boldsymbol{\beta} \cdot \mathbf{1}) - 2 \left(\tilde{\sigma}_y^c \frac{\partial \tilde{\sigma}_y^t}{\partial \bar{\lambda}_p} + \frac{\partial \tilde{\sigma}_y^c}{\partial \bar{\lambda}_p} \tilde{\sigma}_y^t \right), \\
\frac{\partial \tilde{\sigma}_y^t}{\partial \bar{\lambda}_p} &= Q^t \beta^t e^{-\beta^t (\kappa_n + \bar{\lambda}_p)} \left(\frac{\bar{\lambda}_p}{\Delta t} \eta^t + 1 \right)^{1/p^t} + (\sigma_{yt} - R_m^t) \frac{1}{p^t} \left(\frac{\eta^t}{\Delta t} \right) \left(\frac{\bar{\lambda}_p}{\Delta t} \eta^t + 1 \right)^{1/p^t - 1}.
\end{aligned} \tag{C.12}$$

The derivative of $\partial_{\bar{\lambda}_p} \tilde{\sigma}_y^c$ can be determined analogously to $\partial_{\bar{\lambda}_p} \tilde{\sigma}_y^t$. The resulting system of equations

$$\begin{bmatrix} \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^p} & \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^{pi}} & \frac{\partial \mathbf{r}_1}{\partial \bar{\lambda}_p} \\ \frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^p} & \frac{\partial \mathbf{r}_2}{\partial \boldsymbol{\varepsilon}^{pi}} & \frac{\partial \mathbf{r}_2}{\partial \bar{\lambda}_p} \\ \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^p} & \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}^{pi}} & \frac{\partial r_3}{\partial \bar{\lambda}_p} \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{\varepsilon}^p \\ \Delta \boldsymbol{\varepsilon}^{pi} \\ \Delta \bar{\lambda}_p \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ r_3 \end{bmatrix}, \tag{C.13}$$

is solved iteratively by means of the Newton's method until the root mean square value of the total residuum becomes smaller than a prescribed tolerance. The variables that have to be updated during the local Gauss point iteration are $\boldsymbol{\varepsilon}^p$, $\boldsymbol{\varepsilon}^{pi}$, and $\bar{\lambda}_p$.

C.2.4. Matrix material consistent tangent operator

The consistent tangent operator for the matrix material $\mathcal{C}_{\text{cons}}^m$ is obtained as

$$\mathcal{C}_{\text{cons}}^{\text{mat}} = \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} - \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}_p} : \mathcal{A}_p^{-1} : \mathcal{A}_\varepsilon, \quad (\text{C.14})$$

where $\mathcal{A}_p$ and $\mathcal{A}_\varepsilon$ are defined as

$$\begin{aligned} \mathcal{A}_p &= \mathcal{T}_{1p} - \mathcal{T}_{1pi} : \mathcal{T}_{2pi}^{-1} : \mathcal{T}_{2p}, \\ \mathcal{A}_\varepsilon &= \mathcal{T}_{1\varepsilon} - \mathcal{T}_{1pi} : \mathcal{T}_{2pi}^{-1} : \mathcal{T}_{2\varepsilon}, \end{aligned} \quad (\text{C.15})$$

with the fourth order tensors $\mathcal{T}_{1p}$, $\mathcal{T}_{2p}$, $\mathcal{T}_{1pi}$, $\mathcal{T}_{2pi}$, $\mathcal{T}_{1\varepsilon}$, and $\mathcal{T}_{2\varepsilon}$ in turn expressed as ($j = 1, 2$)

$$\begin{aligned} \mathcal{T}_{jp} &= \frac{\partial \mathbf{r}_j}{\partial \boldsymbol{\varepsilon}_p} - \frac{\partial \mathbf{r}_j}{\partial \bar{\lambda}_p} \otimes \left(\frac{\partial r_3}{\partial \bar{\lambda}_p} \right)^{-1} \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}_p}, \\ \mathcal{T}_{jpi} &= \frac{\partial \mathbf{r}_j}{\partial \boldsymbol{\varepsilon}_{pi}^1} - \frac{\partial \mathbf{r}_j}{\partial \bar{\lambda}_p} \otimes \left(\frac{\partial r_3}{\partial \bar{\lambda}_p} \right)^{-1} \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}_{pi}^1}, \\ \mathcal{T}_{j\varepsilon} &= \frac{\partial \mathbf{r}_j}{\partial \boldsymbol{\varepsilon}} - \frac{\partial \mathbf{r}_j}{\partial \bar{\lambda}_p} \otimes \left(\frac{\partial r_3}{\partial \bar{\lambda}_p} \right)^{-1} \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}}. \end{aligned} \quad (\text{C.16})$$

C.3. Relation between strain energy function parameters and transverse isotropic elasticity constants

The coefficients of the strain energy function ψ_e^f are related to the elasticity constants as follows

$$\begin{aligned} K_1^{\text{iso}} &= -\frac{E_T (1 - \nu_{FT}\nu_{TF})}{8D_1D_2}, \\ K_2^{\text{iso}} &= -\frac{E_T}{4D_2}, \\ K_1^{\text{ani1}} &= -\frac{E_F (1 - 2\nu_{TF} - (\nu_{TT})^2 - 2\nu_{TF}\nu_{TT}) + E_T (2\nu_{TT} + 3\nu_{FT}\nu_{TF} - 1)}{8D_1D_2}, \\ K_2^{\text{ani1}} &= -\frac{E_T - 2G_{FT}D_2}{4D_2}, \\ K^{\text{kop1}} &= -\frac{E_F\nu_{TF}D_2 - E_T(\nu_{TT} + \nu_{FT}\nu_{TF})}{4D_1D_2}, \\ D_1 &= \nu_{TT} + 2\nu_{FT}\nu_{TF} - 1, \quad D_2 = 1 + \nu_{TT}, \quad \nu_{TF} = \frac{E_T}{E_F}\nu_{FT}, \quad E_F = E_F^t\chi_e^t + E_F^c\chi_e^c. \end{aligned} \quad (\text{C.17})$$

C.4. Plastic potential parameter identification for flax fibre

Consider a uniaxial tensile load in the longitudinal fibre direction ($\mathbf{n}_1 = [1, 0, 0]^T$ and $\boldsymbol{\sigma} \cdot \mathbf{M}_1 = \sigma_{11}$), from the evolution equation for plasticity (5.27)₁, the following relation is established:

$$\Delta \boldsymbol{\varepsilon}_p = \frac{\bar{\lambda}_p}{\|\partial_{\boldsymbol{\sigma}} g_f\|} \begin{bmatrix} (2\alpha_f + \frac{8}{9}) \sigma_{11} & 0 & 0 \\ 0 & -\frac{4}{9} \sigma_{11} & 0 \\ 0 & 0 & -\frac{4}{9} \sigma_{11} \end{bmatrix}. \quad (\text{C.18})$$

The plastic strain in the fibre direction can be related to the plastic strain in the transverse fibre direction as

$$\Delta \varepsilon_{22}^p = -\nu_{FT}^p \Delta \varepsilon_{11}^p. \quad (\text{C.19})$$

By substituting the plastic strain components in (C.18) into (C.19), the parameter α_f can be identified as

$$\alpha_f = \frac{2}{9} \frac{(1 - 2\nu_{FT}^p)}{\nu_{FT}^p}. \quad (\text{C.20})$$

C.5. Fulfilment of the Clausius-Duhem inequality for flax fibre

In the following, restrictions concerning the parameters of the flax fibre material are derived. The derivation of g_f with respect to $\boldsymbol{\sigma}$ yields the following expression for the plastic evolution equation (5.27)₁ as

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda}_p \frac{\mathcal{B}_f[\boldsymbol{\sigma}]}{\|\mathcal{B}_f[\boldsymbol{\sigma}]\|}, \quad \mathcal{B}_f = \partial_{\boldsymbol{\sigma}\boldsymbol{\sigma}}^2 g_f = 2(\mathcal{P}[\mathbf{M}_1] \otimes \mathcal{P}[\mathbf{M}_1]) + 2\beta_{fib}(\mathbf{M}_1 \otimes \mathbf{M}_1). \quad (\text{C.21})$$

With $\dot{\lambda}_p \geq 0$, substituting (C.21) and (5.27)₂ into (5.25) yields

$$\dot{\lambda}_p \left(\frac{\boldsymbol{\sigma} \cdot \mathcal{B}_f[\boldsymbol{\sigma}]}{\|\mathcal{B}_f[\boldsymbol{\sigma}]\|} + R_f \right) \geq 0. \quad (\text{C.22})$$

The first term satisfies the Clausius-Duhem inequality if $\mathcal{B}_f$ is positive semi-definite (that is if the eigenvalues of $\mathcal{B}_f$ is greater or equal to zero). This requirement places the following restrictions on the parameter α_f

$$\alpha_f \geq 0. \quad (\text{C.23})$$

Finally, since R_F is a function of ζ , the Clausius-Duhem inequality is fulfilled if $\zeta \geq 0$ which is the case by definition.

C.6. Numerical aspects of flax fibre constitutive model

C.6.1. Anisotropic plasticity

The evolution equations are discretized by means of a standard backward Euler integration scheme. As done for the matrix material, all variables without subscripts are assumed to be evaluated at time t_{n+1} . The discretized evolution equations together with the yield function are then summarized in residuum format as ($\bar{\lambda}_p := \dot{\lambda}_p \Delta t$):

$$\begin{aligned} \mathbf{r} &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\partial_{\boldsymbol{\sigma}} g_f}{\|\partial_{\boldsymbol{\sigma}} g_f\|}, \\ r &= \Phi^f = 0. \end{aligned} \quad (\text{C.24})$$

Again due to the symmetry of the internal variables, the symmetric tensor $\mathbf{r}$ can be represented in Voigt form as a six dimensional array. This result in 7 nonlinear scalar equations which have to be solved iteratively using e.g. Newton's method at each Gauss point. To employ Newton's method, the consistent linearization of (C.24) with respect to $\boldsymbol{\varepsilon}_p$ and $\bar{\lambda}_p$ has to be carried out. For the linearization of the constitutive equations, the reader is referred to C.6.2

The scalar evolution equation for accumulated plastic strain $\dot{\kappa}$ (5.27)₂ is discretized analogously to (C.9) by means of the backward Euler integration scheme. As done for the case of the matrix material, κ is computed at the end of each local Newton iteration via the converged value of the plastic multiplier $\bar{\lambda}_p$. Thus, κ is only updated when the local Newton iteration has converged. The corresponding consistent tangent operator $\mathcal{C}_{\text{cons}}^f$ is derived in C.6.3.

C.6.2. Linearization of flax fibre constitutive equations

The local system of equations, consisting of the discretized evolution equation together with the yield function, is given below (see (C.24)):

$$\begin{aligned} \mathbf{r}(\boldsymbol{\varepsilon}^p, \bar{\lambda}_p) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\mathbf{K}_f}{\|\mathbf{K}_f\|} = \mathbf{0}, \quad \mathbf{K}_f = \mathcal{B}_f[\boldsymbol{\sigma}], \\ r(\boldsymbol{\varepsilon}^p, \bar{\lambda}_p) &= \Phi^f = 0. \end{aligned} \quad (\text{C.25})$$

Linearization of the residuum leads to the following system of equations

$$\begin{aligned}\Delta \mathbf{r} &= \frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}^p} [\Delta \boldsymbol{\varepsilon}^p] + \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p, \\ \Delta r &= \frac{\partial r}{\partial \boldsymbol{\varepsilon}^p} \cdot \Delta \boldsymbol{\varepsilon}^p + \frac{\partial r}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p.\end{aligned}\tag{C.26}$$

where the following expressions hold:

$$\begin{aligned}\frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}^p} &= \mathcal{I} - \bar{\lambda}_p \left(\frac{\mathcal{I}}{\sqrt{\mathbf{K}_f \cdot \mathbf{K}_f}} - \frac{(\mathbf{K}_f \otimes \mathbf{K}_f)}{(\mathbf{K}_f \cdot \mathbf{K}_f) \sqrt{\mathbf{K}_f \cdot \mathbf{K}_f}} \right) : \frac{\partial \mathbf{K}_f}{\partial \boldsymbol{\varepsilon}^p}, \\ \frac{\partial \mathbf{K}_f}{\partial \boldsymbol{\varepsilon}^p} &= -\mathcal{B}_f : \mathcal{C}_{\text{ani}}^f, \\ \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_p} &= -\frac{\mathbf{K}_f}{\sqrt{\mathbf{K}_f \cdot \mathbf{K}_f}}, \\ \frac{\partial r}{\partial \boldsymbol{\varepsilon}^p} &= -\left(\mathcal{C}_{\text{ani}}^f\right)^T : \mathcal{A}_f[\boldsymbol{\sigma}], \quad \mathcal{A}_f = 2\zeta \frac{\partial \langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle}{\partial \boldsymbol{\sigma}}, \\ \frac{\partial \langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle}{\partial \boldsymbol{\sigma}} &= \frac{1}{2} (1 + \text{sign}(\boldsymbol{\sigma} \cdot \mathbf{M}_1)) \mathbf{M}_1, \quad \text{sign}(\boldsymbol{\sigma} \cdot \mathbf{M}_1) = \frac{\boldsymbol{\sigma} \cdot \mathbf{M}_1}{|\boldsymbol{\sigma} \cdot \mathbf{M}_1|}, \\ \frac{\partial r}{\partial \bar{\lambda}_p} &= \frac{1}{2} \boldsymbol{\sigma} \cdot \frac{\partial \mathcal{A}_f}{\partial \bar{\lambda}_p}[\boldsymbol{\sigma}], \quad \frac{\partial \mathcal{A}_f}{\partial \bar{\lambda}_p} = 2 \frac{\partial \zeta}{\partial \bar{\lambda}_p} \left(\frac{\partial \langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle \boldsymbol{\sigma} \cdot \mathbf{M}_1 \rangle}{\partial \boldsymbol{\sigma}} \right), \\ \frac{\partial \zeta}{\partial \bar{\lambda}_p} &= -2 (Y_F^t - R_F)^{-3} (H_F^l + H_F^{nl} c_F \kappa^{(c_F-1)}).\end{aligned}\tag{C.27}$$

The resulting system of equations is solved iteratively by means of Newton's method. The variables that have to be updated during the iteration are $\boldsymbol{\varepsilon}_p$ and $\bar{\lambda}_p$.

$$\begin{bmatrix} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\varepsilon}^p} & \frac{\partial \mathbf{r}}{\partial \bar{\lambda}_p} \\ \frac{\partial r}{\partial \boldsymbol{\varepsilon}^p} & \frac{\partial r}{\partial \bar{\lambda}_p} \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{\varepsilon}^p \\ \Delta \bar{\lambda}_p \end{bmatrix} = - \begin{bmatrix} \mathbf{r} \\ r \end{bmatrix}.\tag{C.28}$$

C.6.3. Determination of flax fibre consistent tangent operator

In order to determine the tangential stiffness matrix necessary for finite element computation, the consistent tangent operator $\mathcal{C}_{\text{cons}}^f$ is required. It represents a relation between $\Delta \boldsymbol{\sigma}$ and $\Delta \boldsymbol{\varepsilon}$:

$$\Delta \boldsymbol{\sigma} = \mathcal{C}_{\text{cons}}^f [\Delta \boldsymbol{\varepsilon}].\tag{C.29}$$

Since the stress tensor $\boldsymbol{\sigma}$ is a function of $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}_p$, the increment $\Delta\boldsymbol{\sigma}$ can be expressed as:

$$\Delta\boldsymbol{\sigma} = \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} [\Delta\boldsymbol{\varepsilon}] + \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}^p} [\Delta\boldsymbol{\varepsilon}^p] = \left(\frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} + \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}^p} : \frac{\partial\boldsymbol{\varepsilon}^p}{\partial\boldsymbol{\varepsilon}} \right) [\Delta\boldsymbol{\varepsilon}]. \quad (\text{C.30})$$

The relation between the increments $\Delta\boldsymbol{\varepsilon}$ and $\Delta\boldsymbol{\varepsilon}^p$ is obtained by solving the following system of equations

$$\begin{aligned} \frac{\partial\boldsymbol{r}}{\partial\boldsymbol{\varepsilon}} [\Delta\boldsymbol{\varepsilon}] + \frac{\partial\boldsymbol{r}}{\partial\boldsymbol{\varepsilon}^p} [\Delta\boldsymbol{\varepsilon}^p] + \frac{\partial\boldsymbol{r}}{\partial\bar{\lambda}^p} \Delta\bar{\lambda}^p &= \mathbf{0}, \\ \frac{\partial r}{\partial\boldsymbol{\varepsilon}} \cdot \Delta\boldsymbol{\varepsilon} + \frac{\partial r}{\partial\boldsymbol{\varepsilon}^p} \cdot \Delta\boldsymbol{\varepsilon}^p + \frac{\partial r}{\partial\bar{\lambda}^p} \Delta\bar{\lambda}^p &= 0, \end{aligned} \quad (\text{C.31})$$

taking into account the converged solution of the local Gauss point iteration ($\boldsymbol{r} = \mathbf{0}, r = 0$), as

$$\Delta\boldsymbol{\varepsilon}^p = \frac{\partial\boldsymbol{\varepsilon}^p}{\partial\boldsymbol{\varepsilon}} [\Delta\boldsymbol{\varepsilon}] = -\boldsymbol{\mathcal{A}}_p^{-1} : \boldsymbol{\mathcal{A}}_\varepsilon [\Delta\boldsymbol{\varepsilon}], \quad (\text{C.32})$$

where the fourth order tensors $\boldsymbol{\mathcal{A}}_p$ and $\boldsymbol{\mathcal{A}}_\varepsilon$ are defined as follows:

$$\begin{aligned} \boldsymbol{\mathcal{A}}_p &= \frac{\partial\boldsymbol{r}}{\partial\boldsymbol{\varepsilon}^p} - \frac{\partial\boldsymbol{r}}{\partial\bar{\lambda}^p} \otimes \left(\frac{\partial r}{\partial\bar{\lambda}^p} \right)^{-1} \frac{\partial r}{\partial\boldsymbol{\varepsilon}^p}, \\ \boldsymbol{\mathcal{A}}_\varepsilon &= \frac{\partial\boldsymbol{r}}{\partial\boldsymbol{\varepsilon}} - \frac{\partial\boldsymbol{r}}{\partial\bar{\lambda}^p} \otimes \left(\frac{\partial r}{\partial\bar{\lambda}^p} \right)^{-1} \frac{\partial r}{\partial\boldsymbol{\varepsilon}}. \end{aligned} \quad (\text{C.33})$$

Finally, the consistent tangent is computed by

$$\boldsymbol{\mathcal{C}}_{\text{cons}}^f = \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} - \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}^p} : \boldsymbol{\mathcal{A}}_p^{-1} : \boldsymbol{\mathcal{A}}_\varepsilon. \quad (\text{C.34})$$

The residuum $\boldsymbol{r}$ and r are defined in (C.25).

Appendix for article 5

D.1. Relation between strain energy function parameters and elasticity constants

The coefficients of the strain energy function ψ_{tow}^e are related to the elasticity constants as follows

$$\begin{aligned}
 K_1^{\text{iso}} &= -\frac{E_T (1 - \nu_{FT}\nu_{TF})}{8D_1D_2}, \\
 K_2^{\text{iso}} &= -\frac{E_T}{4D_2}, \\
 K_1^{\text{ani1}} &= -\frac{E_F (1 - 2\nu_{TF} - (\nu_{TT})^2 - 2\nu_{TF}\nu_{TT}) + E_T (2\nu_{TT} + 3\nu_{FT}\nu_{TF} - 1)}{8D_1D_2}, \\
 K_2^{\text{ani1}} &= -\frac{E_T - 2G_{FT}D_2}{4D_2}, \\
 K^{\text{kop1}} &= -\frac{E_F\nu_{TF}D_2 - E_T (\nu_{TT} + \nu_{FT}\nu_{TF})}{4D_1D_2}, \\
 K^{\text{ani2}} &= -\frac{2G_{TT}D_2 - E_T}{4D_2}, \\
 D_1 &= \nu_{TT} + 2\nu_{FT}\nu_{TF} - 1, \quad D_2 = 1 + \nu_{TT}, \quad \nu_{TF} = \frac{E_T}{E_F}\nu_{FT}, \quad E_F = E_F^t\chi_{el}^{1t} + E_F^c\chi_{el}^{1c}, \\
 E_T &= E_T^t\chi_e^{2t} + E_T^c\chi_e^{2c}, \quad \nu_{TT} = \nu_{TT}^t\chi_e^{2t} + \nu_{TT}^c\chi_e^{2c}.
 \end{aligned} \tag{D.1}$$

D.2. Relation between yield surface parameters and hardening functions

Consider the case where the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ coincides with the longitudinal fibre direction and $\chi_i = 0$. By making use of the yield function (6.30) and the following load cases $(\tilde{Y}_{STT} = \sigma_{23})$, $(\tilde{Y}_{SFT} = \sigma_{12})$, $(\tilde{Y}_F^t = \sigma_{11})$, $(\tilde{Y}_T^t = \sigma_{22})$, $(2\tilde{Y}_{BTT}^t = \sigma_{22} + \sigma_{33})$, $(\tilde{Y}_F^c = -\sigma_{11})$, $(\tilde{Y}_T^c = -\sigma_{22})$ and $(2\tilde{Y}_{BTT}^c = -(\sigma_{22} + \sigma_{33}))$, the yield surface parameters are obtained as

$$\begin{aligned}\zeta_1 &= \frac{1}{(\tilde{Y}_{STT})^2}, \quad \zeta_2 = \frac{1}{(\tilde{Y}_{SFT})^2}, \quad \zeta_5^{t,c} = \frac{1}{(\tilde{Y}_F^{t,c})^2}, \\ \zeta_3^{t,c} &= \frac{1}{\Omega^{t,c}} \left[\left(2\tilde{Y}_{BTT}^{t,c} \right)^2 \left(1 - \frac{\zeta_1}{4} (\tilde{Y}_T^{t,c})^2 \right) - (\tilde{Y}_T^{t,c})^2 \right], \\ \zeta_4^{t,c} &= \frac{1}{\Omega^{t,c}} \left[|\tilde{Y}_T^{t,c}| - |2\tilde{Y}_{BTT}^{t,c}| \left(1 - \frac{\zeta_1}{4} (\tilde{Y}_T^{t,c})^2 \right) \right],\end{aligned}\tag{D.2}$$

where

$$\Omega^{t,c} = \left(2\tilde{Y}_{BTT}^{t,c} \right)^2 |\tilde{Y}_T^{t,c}| - (\tilde{Y}_T^{t,c})^2 |2\tilde{Y}_{BTT}^{t,c}|.\tag{D.3}$$

D.3. Relation between flow potential parameters and plastic Poisson's ratios

Consider the case where the unit vector $\mathbf{n}_1 = [1, 0, 0]^T$ coincides with the longitudinal fibre direction and $\chi_i = 0$.

By making use of the plastic strain evolution equation (6.10)₁, the plastic strain tensor for a uniaxial tension in the longitudinal fibre direction can be computed as

$$\Delta \boldsymbol{\varepsilon}_p = \frac{\bar{\lambda}_p}{\|\partial_{\boldsymbol{\sigma}} g_{UD}\|} \begin{bmatrix} (2\alpha_4 + \frac{8}{9}) \sigma_{11} & 0 & 0 \\ 0 & -\frac{4}{9} \sigma_{11} & 0 \\ 0 & 0 & -\frac{4}{9} \sigma_{11} \end{bmatrix}.\tag{D.4}$$

Furthermore, the plastic strain in the longitudinal fibre direction can be related to the plastic strain in the transverse fibre direction as

$$\Delta \varepsilon_{22}^p = -\nu_{FT}^p \Delta \varepsilon_{11}^p.\tag{D.5}$$

By substituting the plastic strain components of (D.4) into (D.5), the parameter α_4 is obtained as

$$\alpha_4 = \frac{2(1 - 2\nu_{FT}^p)}{9\nu_{FT}^p}. \quad (\text{D.6})$$

Next consider the case where the tow is subjected to a uniaxial tension in transverse longitudinal tow direction. The plastic strain tensor yields

$$\Delta\epsilon_p = \frac{\bar{\lambda}_p}{\|\partial_{\sigma}g_{UD}\|} \begin{bmatrix} -\frac{4}{9}\sigma_{22} & 0 & 0 \\ 0 & \left(\frac{\alpha_1}{2} + \frac{2}{9} + 2\alpha_3\right)\sigma_{22} & 0 \\ 0 & 0 & \left(-\frac{\alpha_1}{2} + \frac{2}{9} + 2\alpha_3\right)\sigma_{22} \end{bmatrix}. \quad (\text{D.7})$$

Again relating the plastic strain in the direction of loading to the plastic strains in the lateral direction yields

$$\begin{aligned} \Delta\epsilon_{33}^p &= -\nu_{TT}^p \Delta\epsilon_{22}^p, \\ \Delta\epsilon_{11}^p &= -\nu_{TF}^p \Delta\epsilon_{22}^p. \end{aligned} \quad (\text{D.8})$$

By substituting the plastic strain components of (D.7) into (D.8) and solving simultaneously, α_1 and α_3 can be obtained as

$$\alpha_1 = \frac{4(1 + \nu_{TT}^p)}{9\nu_{TF}^p} \quad \text{and} \quad \alpha_3 = \frac{1(1 - \nu_{TF}^p - \nu_{TT}^p)}{9\nu_{TF}^p}, \quad (\text{D.9})$$

respectively.

Next consider a uniaxial tension (σ'_{45°) at an angle 45° in the plane parallel to the longitudinal fibre direction. By performing a coordinate transformation using the relation

$$\sigma = Q^T \sigma' Q, \quad Q = \cos \theta (\mathbf{e}_1 \otimes \mathbf{e}_1) + \cos \theta (\mathbf{e}_2 \otimes \mathbf{e}_2) + \sin \theta (\mathbf{e}_1 \otimes \mathbf{e}_2 - \mathbf{e}_2 \otimes \mathbf{e}_1), \quad (\text{D.10})$$

where $\mathbf{e}_i$ ($i = 1, 2, 3$) are the basis vectors of the cartesian coordinate system, the nonzero components of the stress tensor in the reference coordinate are obtained as:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{bmatrix} = \frac{\sigma'_{45^\circ}}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}. \quad (\text{D.11})$$

Substituting the resulting stress tensor D.11 into the plastic evolution equation yields the

following plastic strain tensor

$$\Delta \varepsilon_p = \frac{\bar{\lambda}_p}{\|\partial_{\sigma} g_{UD}\|} \begin{bmatrix} \left(\frac{2}{9} + \alpha_4\right) \sigma'_{45^\circ} & \frac{\alpha_2}{2} \sigma'_{45^\circ} & 0 \\ \frac{\alpha_2}{2} \sigma'_{45^\circ} & \left(\frac{\alpha_1}{4} - \frac{1}{9} + \alpha_3\right) \sigma'_{45^\circ} & 0 \\ 0 & 0 & \left(-\frac{\alpha_1}{4} - \frac{1}{9} + \alpha_3\right) \sigma'_{45^\circ} \end{bmatrix}. \quad (D.12)$$

The plastic strain in the direction of loading $\Delta \varepsilon_{45^\circ}^p$ can be related to the plastic strain at right angle to the direction of loading $\Delta \varepsilon_{45^\circ + \frac{\pi}{2}}^p$ as

$$\Delta \varepsilon_{45^\circ + \frac{\pi}{2}}^p = -\nu_{FT}^{p45^\circ} \Delta \varepsilon_{45^\circ}^p, \quad (D.13)$$

where

$$\Delta \varepsilon_{45^\circ}^p = \frac{\Delta \varepsilon_{11}^p}{2} + \frac{\Delta \varepsilon_{22}^p}{2} + \Delta \varepsilon_{12}^p \quad \text{and} \quad \Delta \varepsilon_{45^\circ + \frac{\pi}{2}}^p = \frac{\Delta \varepsilon_{11}^p}{2} + \frac{\Delta \varepsilon_{22}^p}{2} - \Delta \varepsilon_{12}^p. \quad (D.14)$$

Substituting the plastic strain components in (D.12) into (D.14), the parameter α_2 is obtained as

$$\alpha_2 = \left(\frac{\alpha_1}{4} + \alpha_3 + \alpha_4 + \frac{1}{9} \right) \left(\frac{1 + \nu_{FT}^{p45^\circ}}{1 - \nu_{FT}^{p45^\circ}} \right). \quad (D.15)$$

D.4. Fulfilment of the Clausius-Duhem inequality

In the following, restrictions concerning the material parameters of the tow constitutive model are derived. The derivative of the plastic potential g_{UD} with respect to σ yields the following expressions for the plastic evolution equation (6.10)₁

$$\dot{\varepsilon}_p = \dot{\lambda}_p \frac{\mathcal{B}[\beta]}{\|\mathcal{B}[\beta]\|}, \quad (D.16)$$

where

$$\begin{aligned} \mathcal{B} := \partial_{\sigma\sigma}^2 g_{UD} = & 2\mathcal{P}[\mathbf{M}_1] \otimes \mathcal{P}[\mathbf{M}_1] + \alpha_1 \mathcal{P}_p + (\alpha_2 - \alpha_1) \mathcal{E}^1 : \mathcal{P}_p + 2\alpha_3 (\mathbf{1} - \mathbf{M}_1) \otimes (\mathbf{1} - \mathbf{M}_1) \\ & + 2\alpha_4 (\mathbf{M}_1 \otimes \mathbf{M}_1), \end{aligned} \quad (D.17)$$

with the fourth order tensors $\mathcal{P}$ and $\mathcal{P}_p$ defined as

$$\begin{aligned}\mathcal{P} &:= \partial_{\sigma} \beta^D = \mathcal{I} - \frac{1}{3} (\mathbf{1} \otimes \mathbf{1}), \\ \mathcal{P}_p &:= \partial_{\sigma} \beta_p = \mathcal{I} - \frac{1}{2} (\mathbf{1} \otimes \mathbf{1}) + \frac{1}{2} (\mathbf{M}_1 \otimes \mathbf{1} + \mathbf{1} \otimes \mathbf{M}_1) - \frac{3}{2} (\mathbf{M}_1 \otimes \mathbf{M}_1).\end{aligned}\quad (\text{D.18})$$

Furthermore from (6.23) the following derivatives are obtained

$$\begin{aligned}\frac{\partial \psi_{1,2}^{ve}}{\partial \boldsymbol{\varepsilon}_{1,2}^{ee}} &= \gamma_{1,2} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_1) [\boldsymbol{\varepsilon}_{1,2}^{ee}], \quad \frac{\partial \psi_{3,4}^{ve}}{\partial \boldsymbol{\varepsilon}_{3,4}^{ee}} = \gamma_{3,4} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_2) [\boldsymbol{\varepsilon}_{3,4}^{ee}], \\ \frac{\partial \psi_{5,6}^{ve}}{\partial \boldsymbol{\varepsilon}_{5,6}^{ee}} &= \gamma_{5,6} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_3) [\boldsymbol{\varepsilon}_{5,6}^{ee}].\end{aligned}\quad (\text{D.19})$$

With $\dot{\lambda}_p \geq 0$, substituting (D.16), (D.19), (6.10)₂, (6.10)₃ and (6.11) into the Clausius-Duhem inequality (6.8) yields

$$\begin{aligned}& \sum_{i=1}^2 \frac{\gamma_i}{\tau_i} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_1) [\boldsymbol{\varepsilon}_i^{ee}] \cdot \boldsymbol{\varepsilon}_i^{ee} + \sum_{i=3}^4 \frac{\gamma_i}{\tau_i} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_2) [\boldsymbol{\varepsilon}_i^{ee}] \cdot \boldsymbol{\varepsilon}_i^{ee} \\ & + \sum_{i=5}^6 \frac{\gamma_i}{\tau_i} \text{sym}(\mathcal{C}_{\text{ani}} : \mathcal{H}_3) [\boldsymbol{\varepsilon}_i^{ee}] \cdot \boldsymbol{\varepsilon}_i^{ee} + \dot{\lambda}_p \left(\frac{\boldsymbol{\beta} \cdot \boldsymbol{\beta} [\boldsymbol{\beta}]}{\|\boldsymbol{\beta} [\boldsymbol{\beta}]\|} + \sum_{i=1}^3 \frac{b_i}{c_i} \boldsymbol{\chi}_i \cdot \boldsymbol{\chi}_i + \sum_{i=1}^8 R_i \right) \geq 0.\end{aligned}\quad (\text{D.20})$$

The first six terms satisfy the inequality if the ratio of the viscoelastic material parameters γ_i and τ_i are positive and the fourth order anisotropic elastic stiffness tensor $\mathcal{C}_{\text{ani}}$ is positive semi-definite since $\mathcal{H}_i$ are just projections. This is the case if the physical meaning of the material parameters of $\mathcal{C}_{\text{ani}}$ are taken into account. The seventh term satisfies the inequality if $\boldsymbol{\beta}$ is positive semi-definite. This places the following restrictions on the flow potential parameters

$$\alpha_1 \geq 0, \quad \alpha_2 \geq 0, \quad \alpha_3 \geq 0 \quad \text{and} \quad \alpha_4 \geq 0. \quad (\text{D.21})$$

The kinematic hardening terms satisfy the inequality if the ratio of the kinematic hardening parameters b_i and c_i are positive. Finally, since the yield surface parameters ζ_i are functions of the hardening functions $\tilde{Y}_F^{t,c}$, $\tilde{Y}_T^{t,c}$, $\tilde{Y}_{BT}^{t,c}$, $\tilde{Y}_{STT}$ and $\tilde{Y}_{SFT}$ which themselves are function of the isotopic hardening stresses R_i , the Clausius-Duhem inequality is satisfied if

$$\tilde{Y}_F^{t,c} \geq 0, \quad \tilde{Y}_T^{t,c} \geq 0, \quad \tilde{Y}_{BT}^{t,c} \geq 0, \quad \tilde{Y}_{STT} \geq 0 \quad \text{and} \quad \tilde{Y}_{SFT} \geq 0. \quad (\text{D.22})$$

D.5. Numerical aspects

D.5.1. Anisotropic viscoelasticity

In the following all variables without subscripts are evaluated at time t_{n+1} . The evolution equations for viscoelasticity (6.11) is discretized analogously to the approach adopted in Bedzra et al. [2020] following Simo and Hughes [1998]; Kaliske and Rothert [1997]; Miled et al. [2011], where $\partial \epsilon_e / \partial s$ is assumed to be constant within the time interval $s \in [t_n, t_{n+1}]$. This results in

$$\mathbf{h}_i = \exp\left(\frac{-\Delta t}{\tau_i}\right) (\mathbf{h}_i)_n + \frac{\tau_i}{\Delta t} \left(1 - \exp\left(\frac{-\Delta t}{\tau_i}\right)\right) \Delta \epsilon^e. \quad (\text{D.23})$$

As a result of the recursive determination of the variable $\mathbf{h}_i$, the variables ϵ_n^e and $(\mathbf{h}_i)_n$ have to be stored in a database. Making use of (6.25) and (D.23), the stress at any time t can be computed by

$$\begin{aligned} \boldsymbol{\sigma}(t) = & \mathbf{C}_{\text{ani}} [\epsilon^e] + \sum_{i=1}^2 \gamma_i \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_1) [\mathbf{h}_i] + \sum_{i=3}^4 \gamma_i \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_2) [\mathbf{h}_i] \\ & + \sum_{i=5}^6 \gamma_i \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_3) [\mathbf{h}_i]. \end{aligned} \quad (\text{D.24})$$

For finite element computation of viscoelasticity, the tangent operator $\mathbf{C}_{\text{vis}}$ which represents the relation between $\Delta \boldsymbol{\sigma}$ and $\Delta \epsilon^e$ is required. This is obtained from (D.24) as

$$\begin{aligned} \mathbf{C}_{\text{vis}} = & \mathbf{C}_{\text{ani}} + \sum_{i=1}^2 \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_1) \frac{\gamma_i \tau_i}{\Delta t} \left(1 - \exp\left(\frac{-\Delta t}{\tau_i}\right)\right) \\ & + \sum_{i=3}^4 \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_2) \frac{\gamma_i \tau_i}{\Delta t} \left(1 - \exp\left(\frac{-\Delta t}{\tau_i}\right)\right) \\ & + \sum_{i=5}^6 \text{sym}(\mathbf{C}_{\text{ani}} : \mathcal{H}_3) \frac{\gamma_i \tau_i}{\Delta t} \left(1 - \exp\left(\frac{-\Delta t}{\tau_i}\right)\right). \end{aligned} \quad (\text{D.25})$$

D.5.2. Numerical aspects of anisotropic viscoplasticity

The plastic evolution equations are discretized by means of a standard backward Euler integration scheme and are summarized together with the yield function in residuum format as

$(\bar{\lambda}_p := \dot{\lambda}_p \Delta t)$:

$$\begin{aligned} \mathbf{r}_1 &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\partial_{\boldsymbol{\sigma}} g_{\text{UD}}}{\|\partial_{\boldsymbol{\sigma}} g_{\text{UD}}\|} = \mathbf{0}, \\ \mathbf{r}_k &= \boldsymbol{\varepsilon}_i^{pi} - (\boldsymbol{\varepsilon}_i^{pi})_n - \bar{\lambda}_p \frac{b_i}{c_i} \boldsymbol{\chi}_i = \mathbf{0}, \quad \forall \quad i = 1, 2, 3, \quad k = 2, 3, 4 \\ r_5 &= \Phi^{UD} = 0. \end{aligned} \tag{D.26}$$

Due to the symmetry of the internal variables, the symmetric tensors $\mathbf{r}_1$ and $\mathbf{r}_k$ ($k = 2, 3, 4$) can be represented in Voigt form as six-dimensional arrays. Thus, the resulting system of equations consist of 25 nonlinear scalar equations which are solved iteratively by Newton's method. The local iteration is performed in every time step until the root mean square of the total residuum becomes smaller than a prescribed tolerance. In order to employ Newton's method, the consistent linearization of (D.26) with respect to $\boldsymbol{\varepsilon}^p$, $\boldsymbol{\varepsilon}_i^{pi}$ ($i = 1, 2, 3$) and $\bar{\lambda}_p$ has to be carried out. For the linearization of the constitutive equations, the reader is referred to D.5.3.

The scalar evolution equation for accumulated plastic strain $(6.10)_4$ is also discretized by the backward Euler integration scheme as:

$$\kappa = \kappa_n + \bar{\lambda}_p. \tag{D.27}$$

The accumulated plastic strain κ is computed at the end of each local Newton iteration via the converged value of the plastic multiplier $\bar{\lambda}_p$. Furthermore for the calculation of the tangential stiffness matrix in a finite element computation, the derivation of the consistent tangent operator is required. The consistent tangent operator can be derived by following the approach outlined for the flax fibre material model in Bedzra et al. [2020].

D.5.3. Linearization of tow constitutive equations

The local system of equations, consisting of the discretized evolution equations together with the yield function, is given below (see (D.26)):

$$\begin{aligned} \mathbf{r}_1(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}_i^{pi}, \bar{\lambda}_p) &= \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_n^p - \bar{\lambda}_p \frac{\mathbf{K}}{\|\mathbf{K}\|} = \mathbf{0}, \quad \mathbf{K} = \mathcal{B}[\boldsymbol{\beta}], \\ \mathbf{r}_k(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}_i^{pi}, \bar{\lambda}_p) &= \boldsymbol{\varepsilon}_i^{pi} - (\boldsymbol{\varepsilon}_i^{pi})_n - \bar{\lambda}_p \frac{b_i}{c_i} \boldsymbol{\chi}_i = \mathbf{0}, \quad \forall \quad i = 1, 2, 3, \quad k = 2, 3, 4, \\ r_5(\boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}_i^{pi}, \bar{\lambda}_p) &= \Phi^{UD} = 0. \end{aligned} \tag{D.28}$$

Linearization of the residuum leads to the following systems of equations

$$\begin{aligned}
\Delta \mathbf{r}_1 &= \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}^p} [\Delta \boldsymbol{\varepsilon}^p] + \sum_{i=1}^3 \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}_i^{pi}} [\Delta \boldsymbol{\varepsilon}_i^{pi}] + \frac{\partial \mathbf{r}_1}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p, \\
\Delta \mathbf{r}_k &= \frac{\partial \mathbf{r}_k}{\partial \boldsymbol{\varepsilon}^p} [\Delta \boldsymbol{\varepsilon}^p] + \sum_{i=1}^3 \frac{\partial \mathbf{r}_k}{\partial \boldsymbol{\varepsilon}_i^{pi}} [\Delta \boldsymbol{\varepsilon}_i^{pi}] + \frac{\partial \mathbf{r}_k}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p, \quad \forall \quad k = 2, 3, 4, \\
\Delta r_5 &= \frac{\partial r_5}{\partial \boldsymbol{\varepsilon}^p} \cdot \Delta \boldsymbol{\varepsilon}^p + \sum_{i=1}^3 \frac{\partial r_5}{\partial \boldsymbol{\varepsilon}_i^{pi}} \cdot \Delta \boldsymbol{\varepsilon}_i^{pi} + \frac{\partial r_5}{\partial \bar{\lambda}_p} \Delta \bar{\lambda}_p,
\end{aligned} \tag{D.29}$$

where the following expressions hold:

$$\begin{aligned}
\frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}_p} &= \mathbf{I} - \bar{\lambda}_p \left(\frac{\mathbf{I}}{\sqrt{\mathbf{K} \cdot \mathbf{K}}} - \frac{(\mathbf{K} \otimes \mathbf{K})}{(\mathbf{K} \cdot \mathbf{K}) \sqrt{\mathbf{K} \cdot \mathbf{K}}} \right) : \frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}^p}, \\
\frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}^p} &= -\mathbf{B} : \left(\mathbf{c}_{\text{vis}} + \sum_{i=1}^3 c_i \mathbf{H}_i \right), \\
\frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}_i^{pi}} &= -\bar{\lambda}_p \left(\frac{\mathbf{I}}{\sqrt{\mathbf{K} \cdot \mathbf{K}}} - \frac{(\mathbf{K} \otimes \mathbf{K})}{(\mathbf{K} \cdot \mathbf{K}) \sqrt{\mathbf{K} \cdot \mathbf{K}}} \right) : \frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}_i^{pi}}, \\
\frac{\partial \mathbf{K}}{\partial \boldsymbol{\varepsilon}_i^{pi}} &= c_i \mathbf{B} : \mathbf{H}_i, \\
\frac{\partial \mathbf{r}_1}{\partial \bar{\lambda}_p} &= -\frac{\mathbf{K}}{\sqrt{\mathbf{K} \cdot \mathbf{K}}}, \\
\frac{\partial \mathbf{r}_k}{\partial \boldsymbol{\varepsilon}^p} &= -\bar{\lambda}_p b_i \mathbf{H}_i, \\
\frac{\partial \mathbf{r}_k}{\partial \boldsymbol{\varepsilon}_i^{pi}} &= \mathbf{I} + \bar{\lambda}_p b_i \mathbf{H}_i, \\
\frac{\partial \mathbf{r}_k}{\partial \bar{\lambda}_p} &= -\frac{b_i}{c_i} \boldsymbol{\chi}_i, \\
\frac{\partial r_5}{\partial \boldsymbol{\varepsilon}^p} &= - \left(\mathbf{c}_{\text{vis}} + \sum_{i=1}^3 c_i \mathbf{H}_i \right)^T [\mathcal{A}[\boldsymbol{\beta}] + \mathbf{b}], \\
\frac{\partial r_5}{\partial \boldsymbol{\varepsilon}_i^{pi}} &= (c_i \mathbf{H}_i)^T [\mathcal{A}[\boldsymbol{\beta}] + \mathbf{b}], \\
\frac{\partial r_5}{\partial \bar{\lambda}_p} &= \frac{1}{2} \boldsymbol{\beta} \cdot \frac{\partial \mathcal{A}}{\partial \bar{\lambda}_p} [\boldsymbol{\beta}] + \frac{\partial \mathbf{b}}{\partial \bar{\lambda}_p} \cdot \boldsymbol{\beta}.
\end{aligned} \tag{D.30}$$

The fourth-order tensor $\mathcal{A}$ and the second order tensor $\mathbf{b}$ are expressed as

$$\begin{aligned}
\mathcal{A} &:= \zeta_1 \mathcal{P}_p + (\zeta_2 - \zeta_1) \boldsymbol{\varepsilon}^1 : \mathcal{P}_p + 2\zeta_4^t \frac{\partial \langle I_9^* \rangle_+}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle I_9^* \rangle_+}{\partial \boldsymbol{\sigma}} + 2\zeta_4^c \frac{\partial \langle I_9^* \rangle_-}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle I_9^* \rangle_-}{\partial \boldsymbol{\sigma}} \\
&\quad + 2\zeta_5^t \frac{\partial \langle I_4^* \rangle_+}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle I_4^* \rangle_+}{\partial \boldsymbol{\sigma}} + 2\zeta_5^c \frac{\partial \langle I_4^* \rangle_-}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \langle I_4^* \rangle_-}{\partial \boldsymbol{\sigma}} = \partial_{\boldsymbol{\sigma}\boldsymbol{\sigma}}^2 \Phi^{\text{UD}}, \\
\mathbf{b} &= \zeta_3^t \frac{\partial \langle I_9^* \rangle_+}{\partial \boldsymbol{\sigma}} + \zeta_3^c \frac{\partial \langle I_9^* \rangle_-}{\partial \boldsymbol{\sigma}}, \\
\frac{\partial \langle I_9^* \rangle_+}{\partial \boldsymbol{\sigma}} &= \frac{1}{2} (1 + \text{sign}(I_9^*)) (\mathbf{1} - \mathbf{M}_1), \\
\frac{\partial \langle I_9^* \rangle_-}{\partial \boldsymbol{\sigma}} &= \frac{1}{2} (-1 + \text{sign}(I_9^*)) (\mathbf{1} - \mathbf{M}_1), \\
\frac{\partial \langle I_4^* \rangle_+}{\partial \boldsymbol{\sigma}} &= \frac{1}{2} (1 + \text{sign}(I_4^*)) \mathbf{M}_1, \\
\frac{\partial \langle I_4^* \rangle_-}{\partial \boldsymbol{\sigma}} &= \frac{1}{2} (-1 + \text{sign}(I_4^*)) \mathbf{M}_1.
\end{aligned} \tag{D.31}$$

Furthermore $\partial_{\bar{\lambda}_p} \mathcal{A}$ and $\partial_{\bar{\lambda}_p} \mathbf{b}$ can be obtained by taking the derivatives of the yield surface parameters ζ_i defined in D.2 with respect to $\bar{\lambda}_p$.

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