

# **Continuum Mechanics Modeling of Composite Materials**

Kontinuumsmechanische Modellierung  
von Verbundwerkstoffen

## **Habilitationsschrift**

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Dipl.Ing. Dr.techn. Heinz Pettermann

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# Abstract

The present thesis — “Habilitationsschrift” — is a compilation of six original, peer reviewed articles in scientific journals and one contribution to conference proceedings. It is concerned with computational (i.e. numerical as well as analytical) investigations of matrix–inclusion type composites based on continuum mechanics of materials approaches.

Analytical and numerical models are presented and extensions to standard methods are introduced; specific features, advantages, and shortcomings are discussed. The models are applied to homogenization as well as localization, to computational materials characterization, and to structural analyses of components made from composite materials.

Four papers focus on the analytical Mori–Tanaka type mean field methods. They address elastic models and bounds, thermo-elastic behavior incorporating inclusion orientation distributions, an incremental thermo-elasto-plastic formulation and its implementation as constitutive material law, as well as the application of the latter in structural analyses.

Numerical unit cell approaches utilizing the finite element method are covered by three papers. Various types of unit cells and the formulation of the boundary conditions are presented in terms of piezo-elastic continuous fiber reinforced composites, in terms of the simulation of a bending experiment taking into account creep deformations, and in terms of a multi-inclusion model for tribological problems.

# Zusammenfassung

Die vorliegende Habilitationsschrift ist eine Zusammenstellung von sechs “peer-reviewed” Originalartikeln in wissenschaftlichen Fachzeitschriften und einem Beitrag in einem Tagungsband. Rechnerische (d.h. numerische als auch analytische) Untersuchungen von Matrix-Inklusions-Verbundwerkstoffen auf der Basis von Kontinuumsmethoden der Werkstoffmechanik werden behandelt.

Es werden analytische und numerische Modelle vorgestellt und Erweiterungen von Standardmethoden eingeführt; spezifische Eigenheiten, Vorteile und Nachteile werden diskutiert. Angewandt werden die Modelle zur Homogenisierung sowie Lokalisierung, zur rechnerischen Materialcharakterisierung und zur Strukturberechnung von Komponenten aus Verbundwerkstoffen.

Vier Artikel betrachten analytische “mean field” Methoden vom Mori-Tanaka-Typ. Sie behandeln elastische Modelle und Schranken, thermoelastisches Verhalten unter Einbeziehung von Orientierungsverteilungen der Inklusionen, eine inkrementelle, thermoelastoplastische Formulierung und deren Implementierung als konstitutives Materialgesetz sowie die Anwendung des Letzteren im Rahmen von Strukturberechnungen.

Numerische Einheitszellenansätze unter Verwendung von Finite Elemente Methoden werden von drei Artikeln abgedeckt. Verschiedene Typen von Einheitszellen und die Formulierung der Randbedingungen werden anhand von piezoelastischen, kontinuierlich faserverstärkten Verbundwerkstoffen, anhand der Simulation eines Biegeversuches unter Berücksichtigung der Kriechdeformationen und anhand eines Multiinklusionsmodelles für tribologische Anwendungen präsentiert.

# On the Compilation of this Thesis (Habilitationsschrift)

The present thesis — “Habilitationsschrift” — consists of two parts.

One part gives an overview of the scientific field which the thesis is associated to and, in particular, the relation of the thesis to this field.

The other part — which forms the thesis proper — is a compilation of six original papers already published in international, peer reviewed journals and one paper in conference proceedings. The contributions are closely connected to each other and selected such, to present a consistent view on a scientific area.

## On the Selection

The scope of the thesis is computational modeling in mechanics of heterogeneous materials. Analytical as well as numerical models are presented. Pertinent papers are arranged to give a concise and consistent overview.

First, analytical methods are treated based on the Eshelby concept of inclusions in a matrix material. In Section 2.1 various predictive models and bounds on elastic properties of composites are presented and their relation to the micro-topology of inhomogeneous materials is discussed. An extension to thermo-elastic behavior under consideration of the orientation distribution of short fibers is shown in Section 2.2. Section 2.3 shows the extension to thermo-elasto-plastic behavior applicable to metal matrix composites and its implementation into a finite element code as constitutive material law. This tool is utilized to predict the response of a functionally graded composite, Section 2.4. Even if the latter two papers involve numerical methods, viz. the finite element method, the modeling of the composite’s response is based on analytical approaches.

Next, numerical methods are employed for the simulation of composite materials. The models belong to the group of ‘periodic micro-field approaches’ that employ unit cells. The

computational tool for solving the pertinent problems is the finite element method. Section 3.1 presents the most general case of required boundary conditions on such unit cells and the application to piezo-elastic fibers embedded in a dielectric matrix material. In Section 3.2 a four point bending test is investigated for studying the creep response of continuous fiber reinforced metals. Finally, a tribological setup is analyzed by unit cells containing multiple randomly positioned inclusions, Section 3.3. The specific form of the boundary conditions and the need for statistical evaluation of the stress fields are discussed.

## Compiled Papers

The item number refers to the section where the papers are reprinted.

2.1 Pettermann H.E., Böhm H.J., Alcalá J.:

*Normalized Diagrams for Micro-Mechanical Estimates of the Elastic Response of Composite Materials;*

Metall.Mater.Trans.A **33A**, 3187-3199, 2002.

2.2 Duschlbauer D., Pettermann H.E., Böhm H.J.:

*Mori–Tanaka Based Evaluation of Inclusion Stresses in Composites with Nonaligned Reinforcements;*

Scripta Mater. **48**, 223-228, 2003.

2.3 Pettermann H.E., Plankensteiner A.F., Böhm H.J., Rammerstorfer F.G.:

*A Thermo–Elasto–Plastic Constitutive Material Law Based on an Incremental Mori–Tanaka Approach;*

Computers and Structures **71**, 197-214, 1999.

2.4 Pettermann H.E.:

*Numerical Simulations of a Compositionally Graded Structure Using a Hierarchical Approach;*

Mat.Sci.Engin. **A276**, 277-282, 2000.

3.1 Pettermann H.E., Suresh S.:

*A Comprehensive Unit Cell Model: A Study of Coupled Effects in Piezoelectric 1-3 Composites;*

Int.J.Sol.Struct. **37**, 5447-5464, 2000.

3.2 Daxner T., Rammerstorfer F.G., Segurado J., Pettermann H.E.:

*Creep Deformation of MMCs in Four Point Bending Mode - Numerical Simulations at Various Length Scales;*

J.Engng.Mater.Technol. **125**, 50-55, 2003.

3.3 Segurado J., Merstallinger A., Pettermann H.E.:

*Numerical Simulations in Tribology - A Micro-Mechanics of Materials Approach;*

in Proceedings of the WTC2001, Vienna, Austria, Sept. 3-7, (Eds: J.Franek, W.J. Bartz, A. Pauschitz), The Austrian Tribology Society, 2001.

# Chapter 1

## Introduction

Mechanics of materials, in present notion, started some one-hundred years ago with pioneering work by Reuss and Voigt. It was developed further with time and was applied increasingly. In recent years research activities were given a boost because of the the tremendous multiplication of computational resources. The activities have also been accelerated by the introduction of novel high performance materials like composites, layered compounds, and foam-type structures. However, not only these are subject to intense research, but also 'conventional' materials such as metals, alloys, ceramics, and polymers.

Computational modeling aims at understanding the physical mechanisms which govern the behavior of a material. Once having gained such knowledge, it can be utilized for design, improvement, and tailoring of materials. Moreover, components and structures made from such materials can be investigated in greater detail with respect to their loading response. And, thinking about product development, the number of prototypes can be reduced by guiding the way towards promising solutions.

Mechanics of materials is an interdisciplinary field combining elements from mathematics, mechanics, and materials science.

The present thesis is devoted to computational (i.e. numerical and analytical) modeling of heterogeneous materials, primarily to matrix–inclusion type composites. The modeling of the entire behavior is far beyond the scope of this work, which would require the treatment of a huge number of different properties, mechanisms, and phenomena. Considerations are focused primarily on the thermo-elasto-plastic behavior as response to quasistatic mechanical and temperature loading.

Analytical as well as numerical methods are employed within the framework of continuum mechanics of materials. Theoretical foundations and applications are presented for both approaches; advantages and drawbacks are addressed. Although the models have been set

up for simulation of metal matrix composites, application is not restricted to that family of materials. As long as the assumptions underlying the modeling are met different material systems can be investigated equivalently.

## 1.1 Aims and Scope

A primary task in mechanics of materials is the prediction of materials' behavior. This means, on the one hand, to estimate the effective (or overall) properties from the composition, commonly referred to as *homogenization*. On the other hand, most approaches allow for *localization*, i.e. to estimate the local load state within the individual constituents as response to an overall applied (far field) load.

A number of mechanisms are active, coupled to each other and interacting with each other, building a complex system which governs the behavior. This, in particular, applies to non-linear problems. Typically, not all possible mechanisms can be introduced into a simulation. Thus, one has to decide which phenomena are of relevance and which can be neglected without introducing too much of an error. Of course, such considerations must be closely related to the type of the investigated problem as well as to the questions posed. Last but not least, the models for the individual mechanisms should be reviewed critically. All models come with explicit and implicit assumptions, the latter often being not immediately obvious. Being aware of these issues, the capabilities as well as the limitations of a particular modeling approach can be assessed, which is important for avoiding incorrect conclusions from an insufficiently realistic simulation.

Understanding the physics as well as the mathematics of the models (at least to a certain extent) provides the basis for gaining proper results from modeling and simulation. As mentioned above, prediction of overall properties can be regarded as the first step. Identification of the governing mechanisms and assessing their effect on the material behavior leads one step further. Bringing together this knowledge with service requirements allows for *functional oriented materials design*. Such tools at hand can guide the way to promising candidate materials with the potential to markedly reducing the number of prototypes and development time. This applies not only to materials but can be extended straightforward to structures and components made from composite materials.

## Transition between Length Scales

The length-scale at which a problem is considered is of great importance in mechanics of materials. Each material has features of a structure when studied at sufficiently high spatial resolution, and any structure has material type features when viewed from afar. Typically, a material is an inhomogeneous agglomeration of constituents, provided the viewer zooms in close enough, e.g. different or differently oriented grains in a polycrystal, particles and matrix material in a composite, gravel and cement in concrete, etc. At the length scale of the constituents, their behavior is described by some continuum type material models. At the scale of micro-mechanical investigations, the interaction of the various phases is taken into account. This way, for the greater length-scale, a unique constitutive behavior is extracted which typically cannot be captured fully by standard closed form continuum models.

An illustrative way for denoting these different length-scales are the *micro*, *meso*, and *macro* scale. Among these the level of components or structural parts is called macro scale. At the meso scale subdomains are regarded with locally varying loads and/or compositions. Finally, the interaction of the constituents is accounted for at the micro scale. Within the present thesis mechanics of materials, typically, provides the transition from the micro to the meso scale (homogenization) and vice versa (localization).

## Relation to Experiments

Another, not yet widely utilized application of mechanics of materials is the support of experimental materials characterization. Each evaluation of the raw data gained by an experiment involves some physical model. Such models are established and well understood for standard materials. The model assumptions comply with the behavior of the materials as well as with the deformation, stress, and strain modes they have been developed for. However, as soon as non-standard materials or non-standard test procedures are involved the evaluation of the experiment should be reconsidered. Some assumptions may be violated, with the potential danger of obtaining erroneous results.

Verification and validation of the theoretical models are important issues in modeling and simulation. The predictive capabilities of a model should be verified by recourse to other simulation approaches and by recourse to experimental data. One has to keep in mind, however, that experimental characterization often yields an incomplete picture of the material's behavior, because only rather simple load cases can be captured. Even for linear elastic response considerable experimental effort may be necessary to quantify all parameters, e.g. orthotropic materials necessitate nine independent moduli.

For non-conservative inelastic behavior the situation is even more complex. The material response depends on the history of loading, because a certain load state is not uniquely tied to an associated deformation. A proper constitutive material law defining the complete behavior is required for modeling such materials.

If the agreement between experiment and prediction is not satisfactory, identification of the reasons is of high interest. Fitting some parameters may help to resolve a few specific load cases, however, such a trial and error procedure does not provide a deeper understanding of the material. Additionally, by just fitting some parameters the entire complex non-linear behavior may be changed beyond control.

Besides the choice of proper constitutive models for the constituents, reliable constituent material parameters are required. An incomplete set of material parameters can be a potential source of problems. In addition, the in-situ behavior of many materials when acting as constituents of a composite is known to differ from the behavior of bulk samples. If the parameters (or part of them) are not well known, the reliability of the predictions may be compromised.

The quality of the predictions in terms of capturing the mechanisms and understanding the physics of the behavior of a composite, however, tends to depend on the employed approach and the modeled constitutive behavior of the constituents rather than on input data.

## 1.2 Approaches

A number of different approaches are described in the literature showing different grades of complexity and various fields of applicability. References to related publications are cited in the papers compiled in Section 2 and 3.

The decision on the particular model employed for an investigation is a trade-off between the accuracy and the effort in terms of man as well as CPU power. Depending on the problem and the questions posed this choice is of major importance for successful modeling. Computationally expensive approaches are applied for numerical materials characterization at a high level of detail. They are much too costly, however, for analysis of larger compounds and components. To make the latter feasible, less accurate but computationally less demanding methods are employed.

The methods discussed in the present work are based on micro mechanical considerations. The interaction of the constituents is modeled by mechanical means rather than extracted phenomenologically. These approaches allow for homogenization as well as for localization, the importance of which was discussed above.

Note that the methods employed in the present work do not have an intrinsic absolute length scale, i.e. the size of the inclusions is determined in a relative way only.

A family of analytical methods is presented in Section 2. Their advantage are the low computational costs which make them ideal for just-in-time predictions of a composite's response. They show great flexibility with respect to composition and loading scenarios. Besides computational materials characterization they can be implemented as constitutive material laws into finite element codes (and other numerical tools). The latter allows for structural analyses of composite components, where at any location (i.e. in each Gauss point) the composite's behavior is given individually as response to the local loading situation. The low computational effort inherent the analytical methods, however, is contrasted by a limitation in accuracy.

Alternatively, numerical methods are discussed in Section 3. Various micro-topologies are investigated by means of the finite element method. Local fluctuating fields are resolved in great detail giving a quite accurate picture of the composite's response. Essential for these so-called unit cell models is the correct formulation of the boundary conditions. Over or under constraining must be strictly avoided to obtain the mechanical response accurately. Such numerical approaches require considerable personnel as well as computational power. Thus, they are less flexible with respect to varying input parameters.

A combined application of both methods is considered profitable in computational materials research. Experience is gained mutually, advantages of both can be deployed, disadvantages can be circumvented, and limitations can be assessed.

## **Material Behavior and Properties**

The present approaches are not restricted to special classes of composite materials. The basic methods are general in formulation which make them applicable to a wide range of materials. Restrictions are introduced, however, by assigning a specific constitutive behavior to constituents. As long as the constituent materials can be modeled sufficiently accurate (i.e. the assumptions on their behavior hold) and the micro to meso transfer works consistently the validity of the simulation is maintained.

The materials investigated are primarily composites with matrix-inclusion type topology. The shape of the inhomogeneities cover the range from continuous fibers, short fibers, particles, platelets to thin disks. The spatial orientations of those are not restricted to specific arrangements when employing the analytical methods. The symmetry of the composite's overall behavior is typically orthotropic or transversally isotropic. The inclusion materials are usually taken to be transversally isotropic or isotropic while the matrix material is

isotropic. The latter assumptions make sense for thermo-elastic behavior, but must be handled with care when inelastic response of constituents is involved. The interfaces between the constituents are treated as perfectly bonded.

The resulting overall properties are determined by the constituents' behavior as well as by topological features and, possibly, by residual micro stresses. The combination of these being responsible for the load distribution at the micro scale and, consequently, for the composite's response.

The discussed analytical as well as numerical methods and tools allow for the investigation of a number of different properties. The present work focuses on constituents with thermo-elasto-plastic behavior, in particular thermal expansion, elasticity, (metal) plasticity, creep, and piezo-elasticity. The considered far fields are associated to the aforementioned constitutive laws and restricted to quasistatic loading. Beyond the scope to the present work is the treatment of damage, fracture, decohesion, interfacial sliding and the like as well as the treatment of dynamic effects.

Besides the mechanical properties the methods have the capabilities to handle problems like transport phenomena (e.g. heat and electric conduction, diffusion) and magneto-static problems.

## Chapter 2

# Analytical Mechanics of Heterogeneous Materials

The methods discussed in this chapter belong to the group of *mean field approaches* operating on the basis of averaged fields within each constituent. The interaction between the constituents is given in terms of closed form solutions which are derived from (micro) mechanical considerations. All models are closely related to the Eshelby concept treating a dilute inclusion embedded in a matrix material, and they are extended to capture non-dilute concentrations and multi-phase materials, too. Within the present work the so-called Mori–Tanaka methods (also referred to as ‘equivalent inclusion — average strain’ models) are adopted.

The Mori–Tanaka formulations result in low computational effort. This makes them ideal tools for immediate predictions of the overall material behavior and ideal for parameter studies with varying input data. Intrinsicly, they state the complete behavior of a composite material, i.e. to give the response to any loading scenario. As such they can serve as constitutive laws within finite element codes allowing for structural analyses of composite components.

In the following sections the relation of the Mori–Tanaka methods to other models and bounds is discussed and arbitrary inclusion orientations are introduced. Thermo-elasto-plastic formulations are derived, implemented, and applied to structural analyses.

## 2.1 Elastic Predictions and Bounds

In this section various models and bounds for elastic predictions of two-phase composites are reviewed. The methods comprise rules of mixture, Hashin–Shtrikman type bounds, Mori–Tanaka type models, and classical self-consistent schemes. Their relations among each other and to specific micro-topologies are discussed as well as their range of applicability.

The predictions are cast into the form of normalized diagrams. For isotropic behavior plots for extracting the Young’s and the shear modulus are presented. For transversally isotropic predictions the two principal Young’s moduli are given.

Pages 9 – 21

Pettermann H.E., Böhm H.J., Alcalá J.:

*Normalized Diagrams for Micro-Mechanical Estimates of the Elastic Response of Composite Materials;*

Metall.Mater.Trans.A **33A**, 3187-3199, 2002.

## 2.2 Thermo–Elastic Short Fiber Reinforced Composites

The Mori–Tanaka mean field approach for thermo-elastic problems is presented in this section. In extension of the standard method considering aligned inclusions, non-aligned inclusion orientations are incorporated. An expanded formulation is introduced allowing for an enhanced localization procedure. The local fields within any individually oriented inclusion can be obtained as response to overall thermo-elastic loading.

Pages 23 – 28

Duschlbauer D., Pettermann H.E., Böhm H.J.:

*Mori–Tanaka Based Evaluation of Inclusion Stresses in Composites with Nonaligned Reinforcements;*

Scripta Mater. **48**, 223-228, 2003.

## 2.3 Thermo–Elasto–Plastic Constitutive Law — FEM Implementation

An extension of the standard Mori–Tanaka method is presented in this section to capture thermo-elasto-plastic behavior. An incremental formulation is adopted for the description of the (metal) plasticity of the matrix phase as well as for the overall behavior. It is implemented into a commercial finite element code as constitutive material law. An Euler backward scheme is developed to obtain fast convergence and numerical stability. Temperature dependent material data can be handled as well as arbitrary loading sequences. Computational material characterization and an analysis of a selectively fiber reinforced component are performed to demonstrate the applicability of the approach.

Pages 30 – 47

Pettermann H.E., Plankensteiner A.F., Böhm H.J., Rammerstorfer F.G.:

*A Thermo–Elasto–Plastic Constitutive Material Law Based on an Incremental Mori–Tanaka Approach;*

Computers and Structures **71**, 197-214, 1999.

## 2.4 Multi-Scale Analysis of Functionally Graded Composites

The computational tool developed in Section 2.3 is employed to predict the behavior of a component with spatially varying composition. A hierarchical approach is utilized acting on different length scales. The transition between the macro and the meso scale is handled by a finite element program. The Mori–Tanaka based constitutive law captures the transition between the meso and the micro scale. It provides the tool for predicting the load distribution between inclusions and matrix (localization) and for extracting the incremental response of the composite on the meso scale (homogenization).

Pages 49 – 54

Pettermann H.E.:

*Numerical Simulations of a Compositionally Graded Structure Using a Hierarchical Approach;*

Mat.Sci.Engin. **A276**, 277-282, 2000.

## Chapter 3

# Numerical Mechanics of Heterogeneous Materials

The methods presented in this chapter belong to the group of *unit cell approaches* operating on a subregion of the composite material. Depending on the individual problems investigated various subregions are selected to capture the relevant mechanisms.

The inclusion–matrix topology is modeled explicitly and analyzed by the finite element method. This way the local fluctuating fields can be resolved in great detail. Such approaches are well suited for in-depth studies of local mechanisms governing the behavior of the composite. The high methodical accuracy, however, involves a trade-off with the man power requirement for setting up the models and with the computational needs for numerically solving the problems.

Unit cells of various size and various types of periodicity are introduced. Consistent boundary conditions appropriate for the different applications are described in detail. The dependence of the local fields on the particular micro topology is discussed. Constituents are treated which show elasto-plastic, creep, and piezo-elastic material behavior.

### 3.1 Unit Cell Approach for Piezo–Elastic Composites

The present section is concerned with aligned continuous piezo-elastic fibers embedded in a dielectric matrix material. The consistent formulation of the boundary conditions is discussed and the most general case for 3/D periodic unit cells is given. Typical for a homogenization task the effect of fiber content, shape, and arrangement on the overall properties is investigated. The complete set of piezo-elastic material data is extracted for each composite under consideration.

Pages 57 – 74

Pettermann H.E., Suresh S.:

*A Comprehensive Unit Cell Model: A Study of Coupled Effects in Piezoelectric 1-3 Composites;*

Int.J.Sol.Struct. **37**, 5447-5464, 2000.

## 3.2 Computational Simulation of a Four Point Bending Experiment

The response of a continuous fiber reinforced aluminum specimen in a four point bending experiment is investigated. Elasto-plastic and, in particular, creep behavior are considered. Various topologies are modeled giving rise to different load distributions between the constituents. By such localization procedures local load states are identified as well as their effect on the overall response. This way the experimental results can be interpreted in a more comprehensive manner.

Pages 76 – 81

Daxner T., Rammerstorfer F.G., Segurado J., Pettermann H.E.:

*Creep Deformation of MMCs in Four Point Bending Mode - Numerical Simulations at Various Length Scales;*

J.Engng.Mater.Technol. **125**, 50-55, 2003.

### 3.3 Multi-Inclusion Unit Cells for Tribological Problems

A tribological setup consisting of a particle reinforced composite and a rigid counter body is analyzed. Plane multi-inclusion unit cells with spatially random particle arrangements are set up. The free surface where frictional contact takes place necessitates a specific set of boundary conditions at the opposite side. A series of randomly generated unit cells is evaluated for the stress distribution by statistical means.

Pages 83 – 86

Segurado J., Merstallinger A., Pettermann H.E.:

*Numerical Simulations in Tribology - A Micro-Mechanics of Materials Approach*;  
in Proceedings of the WTC2001, Vienna, Austria, Sept. 3-7, (Eds: J.Franek, W.J. Bartz,  
A. Pauschitz), The Austrian Tribology Society, 2001.