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**UNIVERSITÀ  
DEL SALENTO**

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## Scientific Program - Timetable

Sun day 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15 30 45		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	10:15 30 45	Registration		von Mises prize lecture		
	11:15 30 45		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	12:15 30 45		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	13:15 30 45		Lunch	Lunch	Lunch	
		Opening				
		Univ. Chorus Performance				Closing
	14:15 30 45	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	15:15 30 45	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
Registration pre-opening	16:15 30 45	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	17:15 30 45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	18:15 30 45		Public lecture Francesco D'Andria			
	19:15 30 45	Opening reception at Castle of Charles V				
	20:15 30 45			Conference dinner at Hotel Tiziano		
	21:15 30 45					

# GAMM 2015

Università del Salento

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## **S06: Material modelling in solid mechanics**

The section focuses on constitutive modeling of natural and artificial materials subjected to elastic and inelastic deformation processes. The aim is to compare new constitutive models formulated on phenomenological and micromechanics basis to determine their validity limits also by means of the simulation of the experimental data. A wide range of open problems will be considered in the Section, from multi-scale modeling of heterogeneous materials, to the implementation of constitutive models in numerical applications until to the virtual testing of structural systems.

# A novel stabilization technique for X-FEM like enriched formulations

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The extended Finite Element Method, introduced by Ted Belytschko and coworkers and reviewed in [1], is considered nowadays an almost mature technology, so that various commercial implementations exist. Nonetheless, there are several fundamental aspects normally overlooked, that can be considerably improved in view of large scale application of the method. Typical examples are blending to standard finite elements, where effective solutions have been found, and efficient quadrature in enriched elements that is still an open problem although many contributions exist.

Among these fundamental aspects, a major one is played by the so-called "stabilization", i.e. the fact that, in some circumstances, the X-FEM formulation turns out into an indeterminate system of equations. This is evidenced by the blow up of the condition number in linear equations solving with the consequent ill-conditioning. Typically, the problem arises when a discontinuity comes close to enrichment nodes, and an element is split into two parts, one of which is very small.

Although this problem arises frequently in practical applications, it is surprisingly faced by few publications. Proposed techniques for its solution include modification of the enrichment structure [2], use of system preconditioners, eigenvalue decomposition of the element stiffness matrix [3]. While the proposed literature approaches are based on the idea of correcting the enrichment space to solve the problem, here a markedly different approach is presented. An analytic study of the problem has been done to see how the structure of the problem changes in these degenerate cases. Then, to ensure optimal conditioning, computational speed in large scale applications and to keep the lightweight structure of the original X-FEM enrichment, the standard and enrichment variables are constrained by small penalty terms in the global variational problem. This contribution presents the development of this new stabilization approach as well as the results on some benchmark problems.

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# Automatic Implementation of Elasto-plastic Incremental Formulations at Finite Strains using Hyper-Dual Numbers

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Numerical simulation of standard dissipative materials undergoing finite strains remains an important and challenging topic in computational mechanics. For their implicit finite element implementation, the stresses and consistent tangent moduli are required. Whereas the precision quality of the stress calculation determines the physical accuracy of the numerical simulation, the accuracy of the algorithmic tangent moduli influences the convergence behavior in an iterative solution scheme as well as the detection of material instabilities in localization analysis, cf. e.g., [1]. For conventional material formulations, evolution equations are defined for the variables associated with the dissipative material behavior. Ortiz et al.[2] recasted the inelasticity theory as an equivalent optimization problem where the incremental stress potential within time interval  $[t_n, t_{n+1}]$  is minimized with respect to the internal variables. The scheme is referred to as incremental variational formulation (IVF). The IVF provides a general numerical framework which is suitable for the implementation of a broad range of constitutive models and their thermodynamical consistency is a priori guaranteed, cf. e.g., [3]. One of the important advantages of IVFs is their quasi-hyperelastic potential structure which allows to investigate the existence of minimizers by analyzing generalized convexity conditions, cf. e.g., [1]. On the other hand, the main disadvantage is that their implementation requires more effort than classical formulations. This is partially due to higher-order derivatives e.g. of the incremental stress potential with respect to the internal variables which are additionally required for solving the inner minimization problem in terms of the Newton-Raphson method. Therefore, numerical approximations of the derivatives may be a useful alternative reducing the implementation time in particular for scientific development purposes. However, often-used numerical differentiation schemes, such as the finite difference method, will end up in a comparably poor accuracy being also sensitive with respect to perturbation values, especially for the higher-order derivatives. Fike [4] developed a method for exact and automatic first- and second-order derivative calculations independent on the choice of perturbation values using hyper dual numbers (HDNs). Tanaka et al. [5] exploited this for a numerical scheme to implement hyperelastic materials. There, it is shown that the numerical calculation of stresses and tangent moduli is almost identical to the implementation of the analytic derivatives in the sense of computer accuracy. In this contribution, a novel implementation of IVFs using HDNs is presented to arrive at a fully automatic and robust scheme with computer accuracy. This implementation scheme provides a compact model-independent framework, which means that once the framework is implemented, any other standard dissipative material model can be incorporated by solely modifying the energy functions, i.e., the Helmholtz free energy function, the dissipation potential function and additional side constraints such as e.g. the yield function in the case of plasticity. Its uncomplicated implementation for associative finite strain elasto-plasticity and performance is illustrated by some representative numerical examples.

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# Efficient time integration in multiplicative inelasticity

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Models of multiplicative inelasticity are widely used to simulate the phenomenological behaviour of, for example, polymeric or metallic materials. Typical specific examples are models of multiplicative viscoelasticity, elastoplasticity or viscoplasticity. Within numerical simulations, a time stepping scheme of the constitutive equations is needed. Beside stability and accuracy of the numerical algorithm, its efficiency is one crucial aspect.

In Shutov et. al. [1], a famous model of Maxwell fluid, which is based on the multiplicative decomposition of the deformation gradient and includes a Neo-Hookean hyperelasticity relation as well as an incompressible viscous flow rule, has been considered. More precisely, a time stepping algorithm for implicit time integration of the inelastic flow rule has been presented. The integration algorithm is based on a backward Euler time discretisation, is iteration free and prevents error accumulation.

In this contribution, the basic idea of Shutov et. al. [1] is applied to more general models of multiplicative inelasticity. Here, models of multiplicative viscoelasticity, elastoplasticity and viscoplasticity are considered. Thereby, efficient time stepping algorithms are derived, where only one scalar equation for one scalar unknown has to be solved within every time step. Some properties of the algorithms will be discussed, numerical test will be presented and examples of the application within the finite element method will be demonstrated.

## References

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# Towards a finite element simulation of coating by means of thermal spraying

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In the automotive industry, metal sheet forming processes like deep drawing are applied in order to produce carriage parts in mass production. Therefore, forming tool surfaces are required that are well protected against wear. This ensures a long tool life cycle with a constant high product quality. Such surfaces are, amongst other techniques, produced by thermal spraying of hard material coatings. These coatings considerably improve the wear resistance of the coated surfaces. The thermal spraying process itself is a highly transient thermo-mechanical process. In order to obtain a better understanding of the heat input and transfer during thermal spraying, a simulation framework for thermal spraying processes is presented.

A finite-element-based software tool for the simulation of heat transfer during thermal spraying was recently proposed, [1]. This continuum thermodynamical framework, based on [2, 3] and references cited therein, is now extended by the application of hot particles on the surface of a workpiece. A time dependent configuration of a rigid heat conductor is considered. The configuration can change from one time step to another by the addition of hot coating particles that model the mass application of a considered thermal spray gun. The heat transfer between the considered workpiece and the environment is captured by Robin type boundary conditions. Several numerical examples of the underlying framework are presented.

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# Modeling the moisture and temperature dependant material behavior of adhesive bonds

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As adhesive bonding becomes more and more relevant in joining technology, a precise description of the mechanical material behavior has to be developed. This work presents a three-dimensional continuum mechanical model to respect environmental influences like changes in temperature or a moist environment that can cause changes in this behavior.

Due to the fact, that adhesive layers are, in the majority of cases, made of cross-linked polymers, the concept of modeling such materials is the starting point of modeling adhesives.

For cross-linked polymers, it is usual to behave viscoelastic close to the glass transition temperature. This rate dependent behavior vanishes if the material is tested at significantly higher or lower temperatures, because intermolecular movement is enhanced or inhibited. In general, this can be assumed to be the case for adhesives as well. For Polymers this effect has been described before [1, 3, 4]. During application, adhesives are subjected to further environmental influences like moisture. Experience has shown, that viscoelastic properties are reduced by increasing moisture inside the specimen. This effect has been taken into account as well [2, 5].

In the past each and every effect that influences the mechanical material behavior of polymers has been investigated separately. In the presented contribution a model taking all of these effects into account is presented. To this the viscoelastic parameters  $\mu_e^i$  are formulated as functions

$$\mu_e^i(\chi, \Theta) = \mu_0^i f^i(\chi) \cdot f^i(\Theta)$$

of the additional moisture  $\chi$  and temperature  $\Theta$  fields. The used interpolation functions  $f^i(\bullet)$  are chosen to fit for interpolation between experimental results and to provide physically reasonable values for extrapolation.

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# Determination of material parameters corresponding to viscoelastic curing polymers

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Two goals characterize the present contribution: First, the development of a numerical approach for determining the properties of the material microstructure, and second, the shift of the focus of the inverse analysis from investigating a purely elastic material toward the parameter identification related to heterogeneous inelastic materials. As a rule, the constitutive laws in this case involve a greater number of material parameters the determination of which requires different kinds of tests.

The numerical approach proposed uses the combination of the Levenberg-Marquardt method and the multiscale FEM [1, 2]. The former is a gradient-based method coupling the advantages of the steepest descent method and of the minimization of the Taylor approximation of a function. On the other hand, the multiscale FEM is a numerical homogenization method such that the coupling of the macroscopic and microscopic scales is realized through the Hill macro-homogeneity condition. Here, the macroscopic scale corresponds to the structural level while the microscale is related to the RVE response. The proposed scenario is advantageous as it is easily applicable for different microheterogeneous materials. For this purpose, the global algorithm has to be retained whereas the material subroutines have to be exchanged at the microlevel.

The application of the method is demonstrated on the basis of an example studying a curing polymer combined with a nonlinear elastic material. The mechanical model related to the curing material includes an equilibrium and a non-equilibrium part and depends on 11 material constants [3]. The potential of the elastic inclusion corresponds to the neo-Hooke material and includes two material parameters. The identification procedure proposed comprises three phases: The final elastic parameters of the curing material and the elastic parameters of the inclusion are determined at the first stage. The second stage deals with the evaluation of the final value of the relaxation time and the elastic parameters related to the curing material. Finally, the last stage determines the constants related to the curing process.

The simulations in the first phase show that the procedure is highly sensitive on the quality of measured values and that their error leads to the inaccuracy and to the non-uniqueness of the solution. This shortcoming opens many interesting issues which can be studied in the future.

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# Towards modelling the curing process in particle-filled electro-active polymers

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In dielectric elastomers, a large actuation voltage is required to produce a desired mechanical deformation. To reduce the amount of the actuation voltage, several mechanisms can be applied and the inclusion of high dielectric permittivity fillers in the matrix material in the uncured stage is one of them. Moreover, to obtain a maximum advantage from the high dielectric permittivity fillers, an electric field is applied during the curing process which helps the particles to align in a preferred direction. The polymer curing process is a complex viscoelastic phenomenon where a liquid polymer gradually transforms into a solid due to cross-linking of the initially short polymer chains. This phase transition comes along with an increase in material stiffness and a volume shrinkage. Such stiffness gaining is modelled by an appropriate constitutive relation where the temporal evolution of the material parameters is considered. We present a phenomenologically-inspired large strain framework for simulating the curing process of polymers that can work under the use of an electro-mechanically coupled load. The application of the proposed approach is demonstrated via some numerical examples. These illustrate that the model can predict common features in particle-filled electro-active polymers undergoing curing processes in the presence of an electro-mechanically coupled load [1,2].

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# FE-simulation of spatially graded gelation during adhesive's curing

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Against the backdrop of increasing demands on energy efficiency and the integration of functions, the Collaborative Research Center/Transregio 39 PT-PIESA of the German Research Foundation (DFG) conducts research on lightweight components with inherent actuator and sensor functionality [1]. One process chain studied within this research project is the manufacturing of layered metal compounds with integrated piezo electric modules by sheet metal forming. Former works present a special layered setup with an adhesive layer on the inside, which protects the piezo from critical loads during the manufacturing process, and demonstrate the fundamental feasibility of this approach [2]. Since the forming is carried out while the adhesive is still in liquid state, spacers surrounding the adhesive's volume are required. The subsequent curing reaction of the already formed compound assures the material closure.

The present work contributes to the further development of this manufacturing process in order to accomplish its series quality. This is to be achieved by employing a different adhesive system as well as a temporally and spatially distinct temperature control which allows for a graded gelation. Thus, the adhesive represents a volume with two different phases and hence fulfills both: protection of the piezo by a liquid core and the fixation as a solid spacer at the outside. In order to evaluate the feasibility of the new process, a simulation based process design is strived. Within this contribution, we focus on processes within the adhesive layer. Several measurement strategies for process dependent mechanical and thermal material properties as well as a material modelling approach based on the work in [2] are shown. Moreover, a finite element based simulation of the partial curing process due to the selected temperature regime and under consideration of the exothermic reaction heat is presented. By the help of this simulation tool, parameter variations as well as the derivation of important information on the process design are enabled.

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# Characterisation of filled rubber with a pronounced nonlinear viscoelasticity

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This contribution presents the characterisation of an incompressible carbon black-filled elastomer as one characteristic example for highly filled rubber. It shows a strongly pronounced nonlinear viscoelastic behaviour and the most important characteristic is the extremely long relaxation time which has to be taken into account. The material model is developed with respect to uniaxial tension data. In this work, a step by step development of a phenomenological model is presented starting with the basic elasticity. For this evaluation the long term relaxation behaviour results in a complex experimental procedure. Therefore, special attention has to be paid according to an optimised experimental process in order to get the necessary reference data in an adequate and reproduceable way [1].

With this model basis further investigations are taken into account concerning the time-dependent viscoelasticity. Therefore, cyclic deformation from zero up to a maximum of deformation are considered for different strain rates. Furthermore, the relaxation behaviour is investigated for multiple strain levels. The phenomena which are observed in the experimental results yield a purely viscoelastic model, based on a rheological analogous model consisting of an equilibrium spring and several Maxwell-elements which contain nonlinear relations for the relaxation times of the dashpot elements [1, 2].

The material model's numerical realisation is accomplished in two ways. Because of its numerical simplicity especially according to the parameter identification the model is restricted only to the simple case of uniaxial tension as the first solution. A second, alternative implementation is executed providing the benefit that more complex deformation conditions can also be taken into account. Therefore, the three-dimensional finite model is implemented in an open-source Finite Element library [3].

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# A study on the influence of mechanical preconditioning on the fatigue behavior of rubber materials

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Rubber is increasingly engaged to many industrial applications like tires, dampers, seals and medical equipment. High demands are set to these technical devices and parts. For instance, the durability in service conditions must be ensured. Hence, it is important to predict the fatigue behavior of technical rubber parts, already during their design phase.

Approaches that assess the lifetime of technical rubber components are intensively elaborated and documented, see e.g. [1, 2]. Most approaches are experimentally motivated by lifetime investigations that base on fatigue tests under uniaxial tension conditions [3]. Usually, these tests are performed with respect to varying stress amplitudes. Any pretreatment of these test samples is generally not considered. Nonetheless, it is well known that diverse preconditioning procedures can lead to markable different degrees of material softening caused by the inelastic behavior of filled elastomers. This means the material softening can be controlled by the preconditioning of the test samples. This leads to the question if the preconditioning influences the lifetime noticeable. In practical applications, it is hard to avoid a preconditioning of the rubber components which is simply triggered by prestretching or -loading these parts during installation. In experimental investigations, the samples are supposed to be barely touched before analyzing the fatigue behavior. It is not clear, if any preconditioning would lead to a reduced or extended lifetime. However, to come closer to a realistic lifetime prediction of filled elastomers, the preconditioning cannot be neglected.

In this contribution we will present a study of investigating the influence of preconditioning on rubber samples. Conventional uniaxial tension tests are extended with different preloading and prestretching conditions. The experimental tests will show that the measured lifetime can depend on the assigned preconditioning. The kind of loading and the type of observed rubber are decisive. Using the Model of Rubber Phenomenology (MORPH) [4], which enables the numerical modelling of softening behavior for large deformed filled elastomers, simulations are performed. The simulations consider the strain-history during loading cycles and allow a more realistic prediction of lifetime. A final comparison of experimental and simulation results with and without preconditioning concludes this study.

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# On the generation of soft magneto-electric effects through Maxwell interactions

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Materials with strong magneto-electric (ME) coupling are of particular interest for the development of new functional materials with multi-field properties. Since in single-phase materials the ME coupling is extremely weak at room temperature, there has been a steady increase in attention to the generation of ME composites. Classically, such ME composites are built from magnetostrictive and piezoelectric phases, whose mechanical interaction gives rise to effective ME coupling [1, 2]. Due to the important notion of the interphase strain, ME composites obtain their optimal performance when built from constituent phases with “giant” magnetostriction and piezoelectric coupling (like, for example, in the case of Barium-Titanate–Cobalt-Ferrite or Lead-Zirconate-Titanate–Terfenol-D composite systems).

As an attractive alternative to that, this talk discusses a new way for the generation of ME coupling based on the construction of *soft* composites. The main idea of these composites is to produce the effective ME coupling through *large-strain Maxwell interactions*, whose key drive is given by electrically and magnetically induced Maxwell stresses [3]. Such soft composites may have several advantages compared to multiferroic composites: Since they are soft, they are less fragile than their crystalline counterparts. Furthermore, they are easy to process, have a long life time, and are cheap. This talk will outline the basic working principle of soft magneto-electric composites as well as possible routes to the generation of maximum coupling coefficients. For the determination and the design of the overall properties, a computational homogenization scheme will be employed [4, 5].

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# Numerical Aspects of Energy Relaxation-Based Magnetostriction Modeling

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Among the broad spectrum of active and multifunctional materials, the subclass of *multiferroic* materials are particularly interesting candidates to potentially enable novel applications in, e.g., actuation, sensing, transducing, and data storage applications, due to their unique response properties triggered by the complex multiscale interplay of ferromagnetic (spontaneous magnetization), ferroelectric (spontaneous polarization), or ferroelastic (spontaneous straining) mechanisms. Magnetic shape memory alloys (MSMA) are *intrinsically multi-ferroic* materials, exhibiting strong magnetomechanical coupling behavior in addition to the conventional shape memory effect. The strain and magnetization response is nonlinear, anisotropic, hysteretic, and highly stress level-dependent. The presented energy relaxation model [1] builds on the foundation of the *constrained theory of magnetoelasticity* by DeSimone and James [2], which combines the Ball and James theory of microstructure formation [3] with classical *micromagnetics* approaches [4] to describe the formation of fine-scale microstructures in magnetostrictive materials. Their approach is based on the relaxation of non-convex energy densities, wherein the state variables are constrained to take values in the energy wells. Although the constrained theory is able to predict many important features of the magnetic shape memory effect, other essential features, e.g. hysteretic behavior and the stress-level dependence of the maximum magnetic field induced strain, are not captured. The presented approach aims to overcome some of its limitations, particularly that (i) elastic strains are omitted, (ii) the magnetizations are rigidly attached to easy axes, and (iii) dissipation is not considered.

In the first step of formulating the extended model we allow for “non-energy-well”-states with respect to elastic deformations, necessitating assumptions about the total strains in each martensitic variant, and magnetization orientations, captured by a finite magnetocrystalline anisotropy energy contribution. Secondly, the hysteretic nature of the response is accounted for by introducing an appropriate dissipation functional in an incremental variational setting. The strains and local magnetization orientations represent additional microstructural degrees of freedom, which are determined via minimization of an incremental potential. In this manner, a relaxed energy density is obtained which serves as an approximation of the mathematically and physically desired *quasiconvex* hull. Two numerical relaxation approaches for the elastic strain energy are considered. The *convexification* approach offers the possibility of accounting for the full spectrum of martensitic phases in a straightforward manner and yields a lower energy bound. The *rank-one relaxation* approach on the other hand enforces interface compatibility requirements and produces an upper energy bound of the quasiconvex hull. The presented MSMA response predictions with the extended model show excellent qualitative and very reasonable quantitative agreement with experiments. We also report on first results in the endeavor of embedding the developed energy relaxation-based magnetostriction models into a *micromagnetics-inspired* finite element framework solving the magnetomechanically coupled field equations. This approach allows response simulations for single crystalline samples and devices of essentially arbitrary geometry as well as meso-scale analyses of polycrystalline aggregates, and will eventually make the discussed models accessible to numerical homogenization based scale-bridging techniques. On-going work is concerned with the extension of the presented approaches to the fully three-dimensional setting and their application to other magnetostrictive material systems.

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# Computational homogenization in micromagnetics

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Ferromagnetic solids are characterized by a complex microstructure that consists of magnetic domains separated by domain walls. The evolution of the microstructure can be driven by external magnetic and mechanical stimuli and gives rise to the overall hysteretic response of the material. In order to directly link the microstructure evolution with the macroscopic response we propose a computational homogenization framework for dissipative magnetostriction. The formulation is based on a rigorous exploitation of *rate-type* and *incremental* variational principles bridging the two scales. These principles serve as canonical ingredients for the micro-to-macro transition and determine *macroscopic variables* in terms of their *microscopic* counterparts. The scale transition is performed between a gradient-extended dissipative micromagnetic model and a standard Boltzmann continuum on the macroscale. On the microscale, we use a phase field model of *micromagnetics* coupled with *projection based methods* in order to satisfy the unity constraint on the magnetization. An important aspect for the design of such a computational homogenization method is the definition of suitable *boundary conditions at the micro-level*. These are derived from an extension of a *Hill-Mandel-type micro-macro compatibility condition* to the micromagnetic scenario. In order to incorporate these boundary conditions into the proposed variational homogenization principles we use Lagrange multiplier and penalty methods conceptually similar to the purely mechanical treatments. Two- and three-dimensional numerical simulations will analyze the micromagnetic domain evolution as well as the associated overall hysteretic response of ferromagnetic materials for macroscopic strain- and magnetic-field-driven scenarios.

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# An atomistic scale analysis of ferroelectric nanodomain interfaces

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Ferroelectric functional materials are of gaining importance for modern sensing and actuation applications. Today it is possible to fabricate ferroelectric components on length scales of only several nanometers [1]. Therefore, atomistic simulations are indispensable to predict and understand material behaviour of ferroelectric nanocomponents. Especially nanodomain interfaces are of great interest. Atomistic simulations help to understand the physical properties of domainwalls and interfaces. Furthermore, atomistic simulations also increase the accuracy of constitutive models, e.g. phase field modelling by providing model parameters such as domain wall energies and thicknesses.

The aim of this talk is to present the latest numerical results of nanodomain interfaces using a new extended molecular statics algorithm for ferroelectric materials [2]. The new algorithm is able to not only calculate the change of the polarization behaviour caused by strain but also the influence on the polarization behaviour due to mechanical stress. The size effects of 180° head to head and tail to tail nanodomains have already been investigated [3]. This study also considers 90° domain walls and discusses the impact of mechanical stress on polarization patterns and system energies of nanodomain interfaces.

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# Analysis of Micro- and Macro-Instability Phenomena in Computational Homogenization of Finite Electro-Statics

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Dielectric materials such as electro-active polymers (EAPs) belong to the class of functional materials which are used in advanced industrial environments as sensors or actuators and in other innovative fields of research. Driven by Coulomb-type electrostatic forces EAPs are theoretically able to withstand deformations of several hundred percents. These devices become practical as soon as the material is robust, reliable and long lived. However, large actuation fields and different types of instabilities prohibit the ascend of these materials. One distinguishes between *global structural instabilities* such as buckling and wrinkling of EAP devices, and *local material instabilities* such as limit- and bifurcation-points in the constitutive response. Numerically predicting global and local instabilities is a necessary, however demanding task for designing optimal devices.

We outline variational-based stability criteria in finite electro-elastostatics and design algorithms for accompanying stability checks in typical finite element computations. We start from a *canonical energy minimization principle* which is then shifted to an *enthalpy-based saddle-point principle* for convenience of numerical treatment. Here, global structural stability is based on a *perturbation of the total electro-mechanical energy* and related to statements of positive definiteness of incremental finite element tangent arrays. Local material stability is based on an incremental *quasi-convexity condition* inducing the positive definiteness of both the incremental electro-mechanical moduli as well as a generalized acoustic tensor. It is shown that the incremental arrays to be analysed in the stability criteria appear within the enthalpy-based setting in a *distinct diagonal form*, with pure mechanical and pure electrical partitions.

These accompanying stability checks are embedded into a *computational homogenization framework* to predict the macroscopic overall response and onset of local material instability of particle filled composite materials. Application and validation of the suggested method is demonstrated by representative model problems.

# Modeling of Carbon Fiber Reinforced Plastics for Wave Propagation Analysis in Plates

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The increasing use of carbon fiber reinforced plastic, e.g. in aerospace structures, requires advanced techniques for the monitoring of components from this material. Actually, guided waves (LAMB-waves), cf. [1], are considered as an appropriate means for the detection of structural defects like delaminations. After the excitation of guided waves, e.g. by a thin adhered piezoelectric actuator, at least two wave modes are propagating, i.e. the symmetric  $S_0$ -mode and the antisymmetric  $A_0$ -mode. Due to the higher group velocity, the  $S_0$ -mode is faster than the  $A_0$ -mode and thus these wave modes separate with time.

In non-damaged plates the optical observation of propagating waves through a scanning laser vibrometer shows a regular pattern, which, however, is disturbed by structural defects. At defect localizations, mode conversions take place which become clearly visible by optical measurements. Moreover, a detailed experimental observation of the wave propagation shows an additional effect between the moving  $S_0$ - and  $A_0$ -waves which has the appearance of an  $A_0$ -wave. At this location, the occurrence of an  $A_0$ -wave cannot be explained by the originally excited  $A_0$ -wave, since the group velocity is too low. For this reason, a "quasi-continuous" mode conversion is assumed, cf. [3].

First, this work presents mode conversion effects in carbon fiber reinforced plastic plates. A single layer has to be considered as transversely isotropic. Furthermore, the material is inhomogeneous by nature since it consists of stiff carbon fibers in a comparatively weak epoxy matrix. The optically observed pattern of wave propagation, which include these effects and which contain additionally the information of eventually existing defects, will be discussed.

Secondly, the modeling of the carbon fiber reinforced plastic for subsequent finite element analysis of wave propagation in plates from this material will be presented. Microscopic observations show, that the distribution of the fibers in the matrix material is not periodical, but clusters of fibers and matrix material occur. Therefore, a random distribution of stiffness and mass is present. This local inhomogeneity has to be considered in a microscale model if the above mentioned quasi-continuous mode conversion shall be captured properly, cf. [2]. Finally, a numerical example will show the influence of the material model on the developing wave modes.

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# Strain determination in full-field measurements using DIC

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Digital image correlation (DIC) provides the experimental possibility to obtain the distributed deformation at the surface of a specimen or an entire mechanical part, see, for example, [1]. Similar to commercial finite elements, the concrete implementation is not known to users. Moreover, different approaches to determine the strain distribution are proposed in the literature. In view of the concept of verification and validation, see [2], these codes must be verified. Thus, verification examples must be provided.

In this contribution the strain determination at the surface of a material body is discussed leading to strains in a manifold. In this respect, the surface description is one essential ingredient in the geometrical representation. Moreover, verification examples are developed which make clear that there might be large errors, in particular, in metal forming processes, where large curvatures occur. These are simple shear, bending of a thin plate, torsion and a deep drawing problem. Finally, it is shown that the strain determination procedure is also applicable for comparison purposes with finite elements.

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# Inverse Parameter Identification for Orthotropic Elasto-Plastic Sheet-Steel

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Reducing the need for experimental testing and therewith development time and costs, simulating manufacturing processes and real world usage has established itself as a standard. The obtained predictions of simulation however can only be as good as the modelling. This includes the choice of an appropriate material model, as well as suitable input parameters.

In this contribution the Finite Element Model Updating (FEMU) approach is utilized to determine the material parameters of sheet-steel. From experimental testing it is observed that the considered cold-rolled steel exhibits orthotropic behaviour. To regard this in the simulation, a user-implemented material model based on Hill's yield function [1] is used. Via the method of digital image correlation (DIC), the displacement field of a biaxially loaded specimen is measured from images taken at different stages of loading. Using full-field optical methods, the obtained resolution is very high and the measurement has the advantage of being contactless. The experimentally determined displacements are interpolated to the according nodes of the FEM mesh and compared to those obtained by simulation. This way an error measure is defined which can be minimized by optimization algorithms. Starting with initial values for the orthotropic elasto-plastic material parameters, the FEM model is thus updated consecutively until a specified error margin is reached.

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# The Inversion of Hutchinson's Flow Rule

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An important problem in the application of crystal plasticity is the inversion of Hutchinson's flow rule [1], i. e., determining the stress deviator  $\mathbf{T}'$  for a given strain rate deviator  $\mathbf{D}'$

$$\frac{1}{\dot{\gamma}_0} \mathbf{D}' = \sum_{\alpha} \text{sign} x_{\alpha} |x_{\alpha}|^p \mathbf{S}_{\alpha} \quad x_{\alpha} := \frac{1}{\tau_C} \mathbf{T}' \cdot \mathbf{S}_{\alpha}$$

where  $\dot{\gamma}_0$ ,  $\tau_C$  and  $p$  are material parameters (shear rate, critical resolved shear stress, and strain-rate sensitivity, respectively) and  $\mathbf{S}_{\alpha}$  is the symmetric part of the Schmid tensor of slip system  $\alpha$ .

While this flow rule is bijective and has been suggested in order to circumvent the problem of selecting active slip systems [2], it still proves numerically challenging due to the highly nonlinear ( $p \gg 1$ ) function involved. This function maps quite different stress states to very similar strain rates. Though in principle this problem can be overcome by means of a sufficiently large data base [3], even browsing that data base can prove prohibitive in terms of computing time.

We start with the analysis of the mathematical problem and establish a representation of the inverse flow rule. This is followed different strategies for the numerical solution. For moderate strain-rate sensitivity  $p \sim 25$ , a newly designed algorithm requires on average 5-6 Newton iterations to reduce the relative error to  $10^{-8}$ . Key to this algorithm is the selection of an appropriate starting point for the subsequent iterative procedure. Some two-dimensional examples are used to elucidate the problem, but the results refer to the three-dimensional case.

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# Parameter Identification by Inverse Modelling of Biaxial Tensile Tests of Discontinuous Fiber Reinforced Polymers

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Due to their high lightweight potential, economical mass-production, and excellent formability long fiber reinforced polymers are used in nonstructural components in the automotive sector. However, the application of this class of materials is hindered by a lack of a understanding for robust modeling the whole process chain as well the process related thmero-mechanical properties. The material classes under consideration are LFT-D (long fiber reinforced thermoplastics manufactured in a direct in-line process) and SMC (sheet molding compounds). The fiber orientation and length distribution of both material types is highly heterogenous and determined by the moldfilling flow of the plastificate. As a result the material behavior is spatially heterogeneous and anisotropic in a process sensitive way.

To gain a better insight into the material behavior, biaxial tensile tests on cruciform specimen are performed. The electro-mechanical biaxial testing machine used for the experiments allows for a maximum load of 150 kN on each axis and is equipped with an integrated strain measurement system, which is also used for adaptive midpoint control. The full 3D strain field is measured via gray scale correlation.

The observed results including inelastic effects are discussed in detail for uniaxial and biaxial loading paths. The anisotropic material properties are identified through inverse modeling and digital image correlation (DIC) by comparison of the heterogeneous experimental and simulated strain fields. A Gauss-Newton type algorithm is used to identify the optimal parameter set [1].

The identified material parameters are compared to homogenized material properties based on fiber orientation distribution obtained by micro-computer-tomography and fiber orientation analysis of moldfilling simulations. Meanfield approaches such as the three phase model interaction direct derivative estimate [2] and a Mori-Tanaka scheme are used to determine the macroscopic material properties.

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# Shape control of piezolaminated thin-walled composite structures using nonlinear piezoelectric actuators

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Smart piezolaminated thin-walled composite structures gained significant research interest in recent decades. Many of the available nonlinear models deal with geometrically nonlinear strain-displacement relations with linear electromechanical coupling. A very few authors considered the material nonlinearities by considering the rate-independent hysteresis in ferroelectricity. However, the literature on the behavior of piezolaminated structures under strong electric fields using nonlinear constitutive relations is very scarce. Nevertheless, all the numerical models available in literature except [1] neglect the two-way electromechanical coupling which results in inaccurate solutions. Furthermore the literature [1, 3] is restricted to beam or plate finite elements only.

Therefore, the present study is focused on the nonlinear FE-simulation of smart piezolaminated composite shells using nonlinear constitutive relations in piezo-mechanical coupling. The present shell element is based on the assumptions of small strains and large electric fields. The large electric field characteristic is considered by applying rotationally invariant nonlinear constitutive relations of Tiersten [2]. A numerical model is developed and validated with the available experimental and numerical results in literature. Additionally, static behavior of the piezolaminated composite structures under strong applied electric fields is demonstrated by deploying developed numerical FE-model in some numerical examples.

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# On the sonic composites with scatterers made from auxetic material

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A finite size periodic array of resonators made from auxetic material, embedded into an epoxy matrix is analyzed in this paper. By definition, an auxetic material (with negative Poisson's ratio) expands in all directions when pulled in only one, giving an opposite deformation to that of conventional foams. The classical mechanics fail in describing the mechanical behavior of the auxetic material under deformation. The Cosserat, the micropolar and classical theories of elasticity are continuum theories, which make no reference to atoms or other structural features of the material. Elasticity theory represents more than an analytical description of the phenomenological behavior since it can be derived as a first approximation of the interaction between atoms in the solid [1], [2]. According to the Bragg's theory, the sound attenuation band is due to the superposition of multiple reflected waves inverse proportional to the central distance between resonators. The sound attenuation in such composites is studied using a new method that combines the features of the cnoidal method and the genetic algorithm [3], [4]. The sound transmission through a single finite panel of this composite is characterized with the transfer matrix method coupled with the spatial window technique. The finite size of the panel is taken into account by applying a double spatial window to the incident waves and the vibration velocities of the infinite panel before calculating the radiated field. The method seems to give a correct description of the sound transmission through the acoustic panel and the transmission factor is calculated for every incidence angle with high accuracy.

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# The influence of a damping coefficient on a non-invasive strategy for inverse form-finding

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Inverse form finding aims in finding the optimal blank design (material configuration) of a workpiece, whereby the desired spatial configuration, that is obtaining after a forming process, is known. Inputting the optimal material configuration, a subsequent finite element computation results in exactly the nodal (spatial) coordinates of the desired deformed workpiece.

To determine the optimal blank design, [1] recently proposed an iterative algorithm, which is purely based on geometrical considerations. As a benefit this geometrical approach is not depend on a constitutive model and can be easily coupled non-invasively via subroutines to an arbitrary finite element programm. The applicability of this strategy to metal forming problems with friction, contact and large plastic strains is exemplified by [2] and [3] for the case of coupling the form finding algorithm, which is implemented in Matlab, with the commercial simulation software MSC.MarcMentat.

Applying a damping coefficient within the update step of the material coordinates avoids mesh distortions and also improves the convergency rate for finding the optimal blank design. The damping coefficient is herein automatically controlled by analyzing the mesh quality.

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# Modeling of imperfect contact interfaces in sonic composites

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A sonic composite is a finite size periodic array composed of scatterers embedded in a homogeneous material. It exhibits the full band-gaps, where the sound is not allowed to propagate due to complete reflections. The band-gaps or the well-known Bragg reflections occur at different frequencies inverse proportional to the central distance between two scatterers. If the band-gaps are not wide enough, their frequency ranges do not overlap. These band-gaps can overlap due to reflections on the surface of thick scatterers, as well as due to wave propagation inside them. Then, any wave is reflected completely from this periodic array of acoustic scatterers in the frequency range where all the band-gaps for the different periodical directions overlap [1], [2]. Sonic composites are characterized by imperfect interface conditions defined in terms of linear relations between interface tractions and displacement jumps. These kinds of interfaces can be evaluated on the basis of the Eshelby's [3] and the Hashin models [4], [5]. In this paper, the tangential and normal discontinuities at the interface between the scatterer and the matrix are independently modeled, and these relative displacements are directly proportional to the corresponding components of tractions at the interface. The effective elastic moduli are obtained on the basis of the derived imperfect interface conditions for a sonic plate with an array of acoustic piezoceramic hollow spheres scatterers embedded in an epoxy matrix. The scatterers are made from functionally graded materials with radial polarization (the Reddy and cosine laws). Numerical evaluation has shown that imperfect interface may have a significant effect on the generation of full band-gaps.

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# Direct and Inverse Identification of Composites with Microstructure

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The study treats two level modeling of composites, namely: (i) micromodeling considering a multi-component microstructure, and (ii) macromodeling considering a homogeneous macrostructure. The direct identification supposes knowing the mechanical characteristics of the microstructure components. An approximate method of finding the characteristics of the homogeneous macromaterial can be proposed on that basis. The approach is applied to thin plates undergoing plain stress. A rectangular representative element is considered for the purpose of study, applying various combinations of uniform macroloads at its boundaries. Load combinations are selected following a cubic plan of the numerical experiments. Regarding specific conditions, one can find the macrostrains, performing an averaging procedure along the macroelement boundaries. As a result, an approximate homogenization is realized. On the other hand, the inverse identification is performed applying an iterative procedure which involves direct solutions. Linear elastic materials are objects of study, most of all, but nonlinear materials can also be modeled via a step-wise linearization. The procedure developed is applied to real composite materials.

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# Optimal bounds from below of the critical load for elastic solids subject to uniaxial compression

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Bifurcation and stability issues are of considerable importance in the framework of the non-linear theory of elasticity, since they provide a setting for studying various phenomena relevant for engineering applications.

Bifurcation and stability theories deal with different general issues at the fundamental level: bifurcation theory basically concerns the non-uniqueness of solutions, while stability theory regards the behaviour of deformed bodies under disturbances. Nevertheless, it is possible to find examples which show a close relationship between bifurcation and stability, for instance when studying small on large problems through the classical method of adjacent equilibria, i.e., when one checks if there exist other equilibrium solutions close to a given primary equilibrium state through the analysis of the equilibrium equations linearized around the deformed configuration.

In this vein, the Hadamard energetic criterion of infinitesimal stability (cf. [1]) is a classical and widely used tool for testing the stability of an equilibrium state, since the violation of the so-called Hadamard stability condition plays the role of an indicator of possible bifurcations from the primary equilibrium configuration. Indeed, in a monotonic loading process governed by a loading parameter it is usually assumed that the body remains in the fundamental equilibrium state (no bifurcation allowed) until the Hadamard stability condition ceases to hold. Then, possible bifurcation modes may arise at the critical load, defined as the value of the load parameter which first renders the Hadamard functional zero.

These considerations show that stability in the Hadamard sense requires the determination of the sign of the Hadamard functional but, unfortunately, this is not a simple task. A strategy for avoiding the direct study of the sign of the Hadamard functional may be represented by the evaluation of lower bound estimates of the Hadamard functional, with the aim of seeking a lower bound estimate of the critical load, below which the Hadamard stability condition is definitely satisfied.

In the literature, one may find lower bound estimates for the critical load both for compressible or incompressible elastic bodies (see, e.g., [2-4]). In particular, we proposed in [5] a new procedure (based on the Korn inequality) for determining a lower bound estimate of the critical load for compressible elastic solids which improves other proposals in literature.

Here, on the basis of [6], we first determine new sufficient conditions for the Hadamard stability, and then apply our method to the determination of an optimal lower bound estimate of the critical load for incompressible elastic solids. The effectiveness of our procedure, which is expandable to general cases of hyperelastic materials subject to inhomogeneous deformations, is here discussed with reference to the homogeneous uniaxial compression of a homogeneous, incompressible, isotropic Mooney-Rivlin circular cylinder. In particular, we show that our approach improves the estimate proposed in [4] and it is also advantageous for applications, since it yields a very simple method for numerical applications.

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# Constitutive modeling of fiber-reinforced aerogels

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Aerogels are open-cell highly porous solids having exclusive properties such as lowest bulk density, lowest thermal conductivity and lowest acoustic velocity. These properties make them useful over a large spectrum of applications. However, their brittle and hydrophilic natures result in a road block which is overcome by polymer or fiber reinforcement [1]. In this study, we are focussing on fiber-reinforced aerogels which retain the exclusive properties of aerogels mentioned above while giving them a good load bearing strength at the same time. These fiber-reinforced aerogels show many complex phenomena under loading such as, a strong nonlinearity, cyclic stress softening, and permanent set. However, there have been very few studies on fiber-reinforced aerogels oriented towards their mechanical characterization [2, 3]. To the best of our knowledge, there also is no micromechanical model that can capture the constitutive response of these fiber-reinforced aerogels.

In this contribution, we propose a micro-mechanically motivated constitutive model of fiber reinforced aerogels. The prime source of elasticity and damage in these aerogels is the effect of bending and breakage of fibers in the material network. Accordingly, we consider non-linear bending of fibers supported by an elastic foundation of particles. Based on this concept, the strain energy function is analytically derived for a single fiber in a particular direction. The strain energy of the whole network is then obtained by integration over an unit sphere. The model shows good agreement with experimental data.

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# Characterization of short fiber reinforced polymers

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This contribution presents ideas, how composite materials can be characterized with respect to experimental testing. Composite materials, like short fiber reinforced polymers, are of great interest because of their good properties for industrial applications. In this work a polybutylene terephthalate (PBT) reinforced by short glass fibers is characterized. The matrix material PBT is chosen due to its heat stability over a large range and the high resistance against outer influences as water. The stiffness and the geometrical stability of the polymer are increased by adding short fibers during injection molding process. The benefit in comparison to metals, like alumina or other metal-composites for applications in automotive industries, is its lightweight.

In this work the material properties of the investigated material are obtained by providing results from the experiment in order to separate different material effects such as elasticity, plasticity, damage, viscoelasticity, compressibility and anisotropy. The material under study shows a pronounced strain rate dependency, which has to be taken into account. Therefore, cyclic uniaxial tensile tests with different rates are accomplished. The application of the material in this work is the machining by a three-dimensional forming process. Hence, multiaxial loadings have to be additionally taken into account matching these conditions. At first, bending experiments are added. In order to provide more information, biaxial tensile tests are realized using a testing device supplying the additional necessary experimental data [1, 2]. The difference according to the uniaxial tensile test is, that the multiaxial deformation information is not provided directly by the device output. In order to examine the complete strain information, an optical areal analysis with a digital image correlation (DIC) software is applied. For the biaxial tensile test, the testing force and the deformation field cannot be correlated directly. Therefore, an inverse method comparing the information of the complete deformation field as well as the force data of the experiment and the model is executed [3].

A final aim of this work is to realize a verification experiment representing the three-dimensional forming process as realistically as possible, e.g. a Nakajima test [4]. For this case, a three-dimensional optical analysis in order to get the necessary measurement data, is indispensable.

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## Formation of microstructure in the plates under compression

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Deformation of the plates under compression is investigated by the theory of formation of grain boundaries in ductile single crystals within the nonlinear continuum dislocation theory (CDT) that leads to the minimization problem of a non-convex energy functional. By constructing an energy minimizing sequence having piecewise constant plastic slip it is shown that the formation of shear bands in these plates under compression is energetically more preferable. The number of shear bands is estimated by comparing the energy of shear banding plates including low angle tilt boundaries with that of the uniformly compressed plates.

# On fast and accurate modelling of distributed fibre directions in composites

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Composites like connective tissues with collagen fibres or short fibre reinforced thermoplastics contain fibres whose arrangement deviates from unidirectionality. There are several approaches to describe the mechanical behaviour of such materials. All of them employ a distribution function, which describes the probability of every possible fibre direction. The integration of the stress combined with the distribution function over the unit sphere, i.e. the solution of angular integrals (AI), is supposed to yield the exact solution. However, those integrals require numerous calculations as they usually cannot be solved analytically. In order to shorten the calculation time, the concept of generalised structural tensors (GST) makes use of averaged tensor representations of the fibre distribution. Thus, only a one-time integration is necessary. Recently this concept was extended to higher order tensors (cf. [1]). However, a known disadvantage of the GST is their tendency to respond softer to strain than the AI.

This contribution presents an alternative approach, which is almost as accurate as the AI method but considerably faster. It makes use of representative directions according to an Angular Central Gaussian distribution function and does not require the solution of angular integrals. As the choice of the representative directions bears a significant impact on the accuracy of the method, a study on the integration error is presented. Furthermore, the results of homogeneous deformations using the AI, the GST as well as the new approach are compared to each other, pointing out the advantages and disadvantages of each method.

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# Meso-macro modelling of fiber-reinforced composites exhibiting elastoplastic deformation

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Fiber composite materials such as carbon fiber-reinforced composites are typically characterized by their high Young's modulus and low density making them particularly attractive in lightweight constructions. In addition, the architecture of these materials means that the correct modelling of their orthotropy is very important.

Anisotropic elastoplasticity has been investigated by various authors over the years, especially in the context of crystal plasticity where the structural tensors in the intermediate configuration are fixed and the yield condition is formulated in terms of the Schmidt stress. In the present work, the situation is different in that the fiber orientations represent so called material line elements. This kind of material is described in the framework of phenomenological anisotropic modelling. Such a model has been proposed in [1] and [2] for the large deformation behaviour of pneumatic membranes with the former restricted to purely elastic behaviour and the latter taking into account the inelastic behaviour of the fibers. In recent times, the model in [1] restricted to purely elastic behaviour has been adopted in [3, 4] through a slight modification to model carbon fiber-reinforced composites.

The present model is also meso-mechanically motivated and it is an extension to the model proposed in [3]. It is based on structural tensors as well as the linearized strain energy function proposed in [1]. Additionally, the inelastic nature of the matrix material is taken into account whilst still preserving the linear elastic nature of the fibers. The model is divided into two main sections. The first section deals with virtual experiments to generate stress-strain curves upon which the phenomenological model is fitted. The reason for this is to mainly understand the effect of the material inhomogeneities on the overall material response. The second step deals with implementation of the derived model into a finite element software as a user material subroutine.

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# A micromechanical model for the transformation induced plasticity in poly-crystalline steels

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The effect of transformation induced plasticity (TRIP) results in an improvement of the steels' ductility [1]. Therefore, TRIP-steels are very promising materials, e.g. for the automobile industry. The material behavior is characterized by very complex inner processes, namely phase transformation coupled with plastic deformation and kinematic hardening. To describe the change in microstructure, we will use the volume fractions of the single phases, the plastic strain and the hardening parameter in every grain of the poly-crystalline material as internal variables. Furthermore, we will use the Principle of the Minimum of the Dissipation Potential to model the material behavior. The use of a coupled dissipation functional and a combined Voigt/Reuss bound will directly result in coupled evolution equations for the internal variables and in one combined yield function. Additionally, we will show some numerical results that prove our model's ability to give a first prediction of the TRIP-steels' complex material behavior.

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# A novel contribution to the relaxation of non-convex energy density functionals in the context of martensitic phase transformations

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Energy relaxation methods are known to yield reliable frameworks in the context of material modelling providing both physical and mathematical plausibility. The most frequently applied relaxation scheme is *rank-one convexification* with respect to laminates of different order. This concept has successfully been utilised for, e.g., the modelling of large strain crystal plasticity and solid-to-solid phase transformations in shape memory alloys. In the latter case, energy relaxation based on laminated microstructures in particular allows the micromechanically well-motivated modelling of single crystalline behavior in terms of explicitly taking into account a parent phase (austenite) and several crystallographic variants (of martensite). While standard lamination approaches facilitate to consider exactly  $2^n$  different phases, where  $n$  indicates the order of the laminates, the ansatz established in [1] allows the modelling of a parent phase together with an arbitrary number of martensite variants, the crystallographic orientations of which are kept static. However, experimental observations reveal that rather mixtures of austenite and *twinned martensite*, i.e. two martensite variants with a compatible interface, occur in reality. In this regard, this contribution focusses on the derivation of a laminate-based material model which takes into account only two martensite phases. In order to avoid cumbersome and inefficient combinatorial treatments for the determination of the energetically favourable composition of phases, rotational degrees of freedom for the martensite crystal structures are introduced. These serve as additional minimisers and improve the relaxation of the underlying non-convex energy landscape with regard to the approximation of the *quasiconvex hull*. The proposed framework thus provides a continuous modelling and simulation of *twin formation*.

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# A simplified approach to calculate adhesive joints in multi-material structures

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With the requirement of reducing energy consumption of mobile applications, lightweight design significantly gained in importance. One way to develop lightweight vehicles is the utilisation of multi-material structures. In such components like hybrid car bodies dissimilar materials are applied which require a reliable junction. For most material combinations, adhesive joints are particularly suited and widely used. Another opportunity of lightweight design is the application of topology optimization to reduce the material requirement. Our current development is the combination of both aspects. To get realistic results, the adhesive joints should be taken into account during the topology optimization process. The optimization process requires a mesh consisting of equilateral hexaeder elements and modifies the structure based on stress components. Hence, the stress states of the adhesive joints are crucial for the optimization process.

The challenge is to calculate the maximum normal and shear stresses in the adhesive layer, since dissimilar materials lead to stress singularities at boundaries. Therefore, a non-linear material model and geometrically non-linear, special finite elements are commonly required. This conflicts with the requirement of a minimum of computational costs for the topology optimization. In order to solve this problem and obtain an optimized structure including adhesive joints in reasonable time, the modelling of the adhesive layer should not exceed the minimal necessary complexity.

In this paper, the possibility of a simplified modelling approach using linear continuum elements with virtual zero thickness is examined. The in-house finite element code elPaSo is used as a numerical tool. The first step is to calculate the relevant stress components of simple structures such as a single lap joint. The stress state is compared to complex calculations in academic literature. Finally, the usability of the simplified approach for the multi-material topology optimization and the transferability to complex structures are evaluated.

## On the natural Fiber (Maize) Composite material

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This work is presented the properties of a composite material made of stalk-based fiber of maize and unsaturated polyester resin polymer as matrix with methyl ethyl ketone peroxide as a catalyst and Cobalt Octoate as a promoter [1]. The potential of this material for noise enclosures is investigated by using a coupled method cnoidal - Extended Finite Element Method (XFEM). XFEM enables the accurate approximation of solutions with jumps, discontinuities or general high gradients across interfaces [2], [3]. The dissipation of the sound power into a plate/cavity system shows the efficiency of this composite to achieve noise reduction better to that obtained at low and higher frequencies with traditional foams. The interesting features of the natural fiber composite combine both sound absorption and enhanced insulation. At low frequencies up to 200Hz, the power radiated by system is governed by the in vacuo plate modes, and in this case the composite is laid against the cavity rigid wall. At higher frequencies up to 500 Hz, the noise radiation is driven by the rigid walled cavity modes, and in this case the composite is applied in front of the plate. In both cases, the composite material increases the sound absorption and reduces the sound transmitted by the plate outside the system.

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# Numerical Modeling of Functional Fatigue in NiTi Wires

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Shape memory alloys (SMA) have a high potential for a wide variety of industrial applications due to their remarkable ability to recover their original shape at certain characteristic temperatures under large applied strains. One of the challenging problems connected to such a process is the so called functional fatigue, which describes the deterioration of the beneficial features of SMA under cyclic loading. This phenomenon is strongly related to the phase transformation which mainly governs the distinguished SMA effect. A numerical treatment of such challenging problems is therefore necessary in order to improve the characteristic features of SMA. In this work, we introduce a thermodynamically consistent model describing martensitic phase transformations in SMA. It is based on an explicit geometrical resolution of phase fronts obtained by an extended Ritz-type ansatz within a one-dimensional setting. To be more precise, the position of the phase front—which is treated as a global variable—coincides with the position of a weak discontinuity captured by a  $C^0$ -smooth displacement field. The associated global variables are determined by incremental minimization of the total energy potential. Functional fatigue is introduced via a phenomenological model which incorporates the decreasing stress plateau during cyclic loading and the occurrence of the "characteristic point" in the stress-strain diagram, together with increasing loading amplitudes and accumulating irreversible strains showing up even under pseudoelastic conditions. Diverse numerical examples are provided to clarify the theory and underline the key conclusions.

# On the variational formulation and implementation of Allen-Cahn- and Cahn-Hilliard-type phase field theories

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Phase field theory is a promising framework for analyzing evolving microstructures in existing materials and for designing new materials. Phenomena like those related to microstructures in Ni-based superalloys, twin structures in martensites or precipitation in Al-alloys can be predicted by phase field theory. Due to different elastic properties in the phases, interfacial energies, crystallographic eigen strains and chemical diffusion processes, the constitutive modeling is indeed very challenging. Typically, phase transformations such as those characterizing twinning are captured by an Allen-Cahn-type approach, while a Cahn-Hilliard-type formulation is used, if the respective interface motion is driven by the concentration of the species. Although the Allen-Cahn and the Cahn-Hilliard formulation are indeed different, they do share some similarities. To be more precise, a Cahn-Hilliard model is obtained by enforcing balance of mass in the Allen-Cahn approach. Within an energy-based formulation this can be implemented by adding additional energy terms to the underlying Cahn-Hilliard energy. Such a universal energy-based framework is elaborated in this presentation. Furthermore, implementation aspects concerning the enforcement of natural constraints are also discussed within this work.

# A coupled phase-field – Cahn-Hilliard model for lower bainitic transformation

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The phase-field method is a widely used tool to model the material behavior on a mesoscale [1]. Especially for steel there are many approaches describing the different transformations using this method [2]. Yet there are few phase-field models for the bainitic transformation [3], because it is one of the most complex transformations in steel. Bainite consists of carbides, bainitic ferrite and may have residual austenite. In recent reports the formation of carbides has not been considered.

A phase field model to simulate the transformation of lower bainite including carbon diffusion und carbide formation has been developed. To model the evolution of the carbides it is necessary to simulate the diffusion of the carbon. Therefore the model which is based on a classical phase-field approach is coupled with a viscous Cahn-Hilliard equation to simulate the typical coarsening of the carbon. During the isothermal process a sheaf of bainitic ferrite grows. The carbon starts coarsening because the bainitic ferrite can only contain a fraction of the carbon which was stored in the austenite. At the peaks of the carbon concentration carbides are formed. The simulations successfully show the described growth characteristics of the lower bainite transformation including carbide formation.

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# Martensitic Transformations and Damage: A Combined Phase Field Approach

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There are different structures with various mechanical properties on the microlevel of metastable austenitic steels. During the martensitic transformation the crystal lattice changes from the  $\gamma$ -austenitic to the  $\alpha'$ -martensitic phase which is accompanied by a volume change plus a lattice shear, leading to an eigenstrain within the martensitic phase. The focus of this investigation is on the complex interactions of the phase transformation with propagating microcracks. A phase field model for martensitic transformations which considers the transformation induced eigenstrain is combined with a phase field model for fracture. Since the eigenstrain leads to both tensile and compressive loads, the model accounts for the sign of the local volume change. With aid of this model the interactions between microcrack propagation and the formation of the martensitic phase are studied in two dimensions. Within the phase field approach an order parameter indicates the present phase while a damage variable is related to the fracture field. The evolutions of both, order parameter and crack field, are governed by time dependent Ginzburg-Landau type equations. The coupled field equations are solved using finite elements together with an implicit time integration scheme. Illustrative numerical examples demonstrate the interactions of microcrack propagation and formation of martensitic phase.

# Phase-field modeling of martensitic phase transformations in polycrystals coupled with crystal plasticity

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The purpose of this work is the modeling of fcc to bcc martensitic phase transformations in polycrystals, the coupling with crystal plasticity and the incorporation of inheritance of plastic deformation during the phase transformation. Assuming periodic fields (e.g. stress, strain), Green function and fast Fourier transform (FFT) methods (e.g. [1], [2],[3]) are used to compute the micromechanical fields of heterogeneous microstructures. Following [3], an elasto-viscoplastic model of crystal plasticity is coupled to the phase-field modeling of martensitic phase transformations (e.g. [4]) in polycrystals. The non-conserved order parameters are updated by using a semi-implicit time integration scheme in Fourier space [5]. Two dimensional results of fcc to bcc martensitic phase transformations are presented and the interplay between phase-field evolution and plastic slip is discussed at different stages of the deformation.

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# Phase Field Modeling of Ductile Fracture

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Most metals fail in a ductile fashion, i.e., fracture is preceded by significant plastic deformation. The modeling of failure in ductile metals must account for complex phenomena at micro-scale, such as nucleation, growth and coalescence of micro-voids, as rooted in the work of GURSON [1]. In this work, we start with a simple model based on standard von-Mises plasticity without considering void generation. The modeling of macroscopic cracks can be achieved in a convenient way by recently developed continuum phase field approaches to fracture, which are based on the regularization of sharp crack discontinuities [2]. This avoids the use of complex discretization methods for crack discontinuities, and can account for complex crack patterns. The key aspect of this work is the extension of the energetic and the stress-based phase field driving force function in brittle fracture to account for a coupled elasto-plastic response in line with our recent work [3]. We develop a new theoretical and computational framework for the phase field modeling of ductile fracture in elastic-plastic solids. To account for large strains, the constitutive model is constructed in the logarithmic strain space, which simplifies the model equations and results in a formulation similar to small strains. We start our investigation from a homogeneous one dimensional model problem to illustrate the response of the coupled elasto-plastic phase field driving force. Later we advance the model to account for multi-dimensional cases. We demonstrate the modeling capabilities and algorithmic performance of the proposed formulation by representative simulations of ductile failure mechanisms in metals.

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# Simulation of micro cutting considering crystal plastic deformations

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In micro machining processes the heterogeneous microstructure influences the cutting forces as well as the surface properties. As the characteristic size of the grain structure of the material is comparable to the size of the micro cutting tool a crystal plastic material model for cp-titanium is employed. It considers basal and prismatic slip systems of a hcp crystal and latent hardening. In a small strain setting the interaction of a crack tip with a grain boundary is studied by means of configurational forces, which can be interpreted as driving forces on material inhomogeneities such as crack tips [1]. Assuming a standard dissipative medium the calculation of the elastic contribution of the configurational force is straightforward. The part due to the dissipative processes in the material, is more complex, because the gradients, treated as internal history variables, are to be computed [2]. This analysis gives some basic understanding of the deformation mechanisms encountered in machining situations. This model is then extended to large deformations according to the method proposed in [3] in order to simulate cutting processes. The examples demonstrate the dependency of surface properties on the crystal orientation.

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# Finite Gradient Elastoplasticity with Internal Constraints

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The intention of this contribution is to give a mechanical framework for the modelling of gradient effects in elasticity and plasticity. It is an extension of the approaches in Refs. [1] and [2] to finite deformations. The theory fulfils Euclidean invariance and is based on the concept of material isomorphisms to describe the thermoelastic behaviour in all elastic ranges. This concept has been used in Ref. [3] in the context of classical finite plasticity.

Presently, the general form of a finite constitutive gradient theory is given, including the notion of symmetry transformations, anisotropy and isotropy, etc. This is then extended to materials with non-classical internal constraints. Such constraints not only restrict the deformations of the material, but also the distribution of the deformations within the body. It turns out that a natural introduction of internal constraints can be given in the same way for simple materials (see [4]) and for second gradient materials. This opens the door for interesting applications in continuum mechanics.

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# A link between the molecular statistical theory and Ogden's model of rubber elasticity

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It has been shown in the past by several authors that many phenomenological non-linear constitutive models that are formulated in terms of the principal strain invariants can be reconciled with the molecular statistical theory of rubber elasticity, see e.g. [1, 2, 3]. In the present contribution, this discussion is extended to strain-energy functions which are given in terms of the principal stretches. In particular, a link is established between Ogden's model [5], in a general form with an arbitrary number of terms, and the non-Gaussian statistical theory.

The reconciliation uses similar steps as those applied for invariant-based strain-energy functions before, however, accomplished in an alternative manner. Particularly three representative chains are considered that undergo non-affine deformations and whose motion is subjected to topological constraints. Together with an alternative approximation of the inverse Langevin function in terms of a generalised power series, this leads to a representation of Ogden's material in terms of physical constants that characterise the polymer chain and network, and a few additional parameters that account for the non-affine deformation of topologically constrained polymer chains [4].

The reformulated model provides good agreement with different sets of experimental data at a reduced number of fitting constants. Moreover, the parameters of the statistical and the usual phenomenological representations are connected and it is shown that the parameter set obtained by Ogden [5] for Treloar's data [6] entails a good approximation of the inverse Langevin function in the statistical model. The results of this work suggest that the success and excellent performance of Ogden's model is due to a strong link with the physical basis of rubber elasticity [4].

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# Equivalent Plastic Strain Gradient Theory with a Grain Boundary Yield Condition

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In the context of microstructured materials it is essential to discuss non-local mechanical behavior of micro specimens. Strain gradient plasticity theories introduce an internal length scale and thus can be used to investigate size-dependent effects, e.g. the Hall-Petch effect, cf. e.g. [1]. One major influence on the non-local behavior of crystals with a few grains is the presence of grain boundaries and their resistance against the transmission of dislocations through the grain boundary. This resistance, in general, may depend on a broad variety of micro-material properties like, e.g., the crystallographic orientation of the adjacent grains.

An equivalent plastic strain gradient plasticity model for small deformations, cf. [2], is extended by the dependency of the grain boundary resistance against plastic flow on the geometric mismatch between grains. For this purpose, the grain boundary dislocation density (GBD), cf. [3], is used as a geometrical criterion to express the total mismatch between all glide systems of two adjacent grains. The applicability of the GBD for tilt grain boundaries is investigated by numerical calculations of a bicrystal. Twist grain boundaries are discussed by analytical means. Finite-Element simulations are performed under different loading conditions. An application of the continuum model regarding discrete dislocation dynamics is discussed, cf. [4]. Further possibilities of a refinement of the theory with respect to the incorporated defect energy are outlined.

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# Primary and secondary instabilities in soft bilayered systems

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Wrinkling phenomena emerging from mechanical instabilities in inhomogeneously compressed soft bilayered systems can evoke a wide variety of surface morphologies. The cause of compression can be of different nature: external impacts like pressure but also internal effects like constrained growth can evoke surface wrinkling. Applications range from undesired instabilities in engineering structures such as sandwich panels, via fabricating surfaces with controlled buckling patterns of unique properties, to wrinkling phenomena in biological systems such as lungs, mucosas, and brain convolutions [1]. While moderate compression generates a regular pattern of sinusoidal wrinkles with a relatively homogeneous energy distribution, higher compression induces secondary instabilities - the surface bifurcates into increasingly complex morphologies. Weakly nonlinear theoretical approaches have provided first insights into secondary instabilities [2], but the highly nonlinear post-buckling regime remains underinvestigated. Here, we establish a computational model of differential growth to explore the evolving buckling pattern beyond the first instability point [3]. With continuing growth, the energy progressively localizes and new complex morphologies emerge. Our model provides a mechanistic understanding of growth-induced primary and secondary instabilities and reveals the effect of layer thickness, stiffness, and growth on the evolving buckling pattern. We show that amongst all possible secondary bifurcations, the mode of period-doubling is energetically favorable. Yet, we can numerically suppress the emergence of period-doubling, by choosing the simulation domain such that periodicity favors alternative modes, e.g., period-tripling. We experimentally validate our simulation results by examining buckling of a mechanically compressed polymer film on a soft foundation. The polymer experiments qualitatively and quantitatively confirm the numerical predictions. Our computational studies not only open new paths in the microfabrication design of unique multiperiodic patterns but have broad applications in the morphogenesis of living systems, where growth is progressive and the formation of structural instabilities is critical to biological function.

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# A physically motivated model for filled elastomers including strain rate and amplitude dependency in finite viscoelasticity

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A microstructure-based model of rubber reinforcement, the so-called dynamic flocculation model (DFM), is presented describing filler-induced stress softening and hysteresis by the breakdown and reaggregation of strained filler clusters [1]. An extension of this model allows to consider incomplete deformation cycles that occur in the simulation of arbitrary deformation histories [2]. Good agreement between measurement and the model is obtained for CB-filled elastomers like NR, SBR or EPDM, loaded along various deformation histories. One very important aspect is that the model parameters can be directly referred to the physical properties.

This benefit is used to extend the model to further essential effects like time- and rate-dependent material behavior. In the limit range above the glass transition temperature these viscoelastic effects originate mainly from the filler-filler interactions. In the material model these interactions are characterized by two material parameters  $s_v$  and  $s_d$ , respectively. The parameter  $s_v$  defines the strength of the virgin filler cluster, whereas  $s_d$  represents the strength according to the broken or damaged filler clusters. Both parameters can be defined as functions of time  $s_{v,d} = \hat{s}_{v,d}(t)$ , which can be motivated by physical meaning [3]. Due to this extension it is possible to capture the very complex strain rate and amplitude dependency during loading and relaxation.

The implementation of the model into the finite element method is realized by using the concept of representative directions [4]. In this framework we are able to validate the model also for arbitrary loading histories on complex structures.

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# A Hardening Model based on a Finite-Deformation Gradient Crystal Plasticity Description: Formulation and Numerical Implementation

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Intrinsic size-dependence response of materials along with inhomogeneous plastic flow on the micro-scale level are widely observed in the experimental results [1]. Prediction of such a size-dependence response requires incorporation of atomistic slip systems, gradient description and length scale parameters into the conventional plasticity models. In this study, a well-defined finite-deformation gradient crystal plasticity is employed to study size-dependence strengthening behavior of a single crystal under simple shear loading [2-5]. The constitutive description is an extended crystal plasticity model based on the microscopic force balance combined with consistency of thermodynamic laws. Free energy comprises two parts: a hyperelastic description for large-deformation compressible material and a function of dislocation densities via Peach-Koehler forces conjugate to corresponding glide directions. A non-local plastic flow rule in the form of partial differential equation is introduced, while incorporates energetic and dissipative gradient strengthening as well as latent hardening in a multi slip-system crystal.

In terms of numerical solution, an implementation method which has been recently introduced in [6] is adopted. In this method, the proposed constitutive model is implemented in the FEM software ABAQUS via a user-defined element subroutine (UEL). A plain-strain quadratic-element (8-node element with 9 integration points) in which displacement components and dislocation densities were treated as nodal degrees of freedom is defined (Global variable). The flow rule is applied to the integration points and solved to obtain the plastic flow in each slip system via Newton-Raphson scheme (Local variable).

As examples, effect of gradient strengthening, latent hardening and scale-variation in mechanically plastic response of a single crystal subjected to isothermal quasi-static loading is studied and discussed.

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# Phenomenological modelling for viscohyperelasticity: How to find suitable evolution laws in order to extend hyperelastic models?

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The expansion of the utilization of modern adhesive tapes, for example to install glass windows into building structures, calls for long-term prediction of the material behaviour of the tapes itself. The used polymers to produce those adhesive tapes undergo large deformations during application, and additionally, show time-dependent and strain-rate-dependent effects in their stress-strain-time response in experimental testing.

In order to predict the long-term behaviour suitable material models are required. For our reference polymer the quasi-static experimental testing suggests a material behaviour which can be modelled via models for hyperelasticity. Deformation at different strain rates and recording stress relaxation at high hold strains indicate that the use of viscohyperelastic material models is needed to cover the observed effects. A possibility to extend existing hyperelastic models for viscous effects is via the Prony series approach, see [1].

In this paper we present an alternative modelling approach for viscohyperelasticity based on pure phenomenological results directly derived by the experiments. Separating in the loading and relaxation parts, we are able to develop a suitable evolution law for the shear modulus of a classic hyperelastic Arruda-Boyce model to capture the viscous effect during the relaxation. Identifying the parameter sets for different loadings during tension, we suggest an extension of the model using the response surface methodology.

Based on the ideal shear modulus, the Arruda-Boyce model, see [2], is extended by stating an evolution equation for the shear modulus. Capturing phenomenological dependencies on equivalent strain rate and additional dependency on the first strain invariant, this differential equation approach in its simplicity allows us to cover and to predict the visco-hyperelastic material behaviour of the reference material for a variety of tension tests with different strain rates, and influences to the relaxation behaviour.

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# Comparison of micromorphic, micropolar and microstrain continua

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Micromorphic continua are equipped with additional degrees of freedom in comparison to the classical continuum, representing micro deformations of the material points of a body, see [1]. Secondary they are provided with a higher order gradient. Therefore, they are able to account for material size-effects and to regularize the boundary value problem, when localization phenomena arise. Arbitrary micro deformations are allowed for in the micromorphic continuum, while the special cases micropolar continuum and microstrain continuum merely allow for micro rotation and micro strain respectively. Only the micropolar case has been covered extensively in the literature, e.g. [2]. The microstrain continuum was introduced in [3].

One goal of this presentation is to make the transition from a full micromorphic continuum, as presented in [4], to a micropolar or microstrain continuum, by varying the constitutive equations. Another goal is to present a constitutive model encompassing the micromorphic, micropolar and microstrain continuum as special cases and arbitrary mixtures of micropolar and microstrain parts, enabling the representation of versatile material behaviour. The results are illustrated by numerical examples.

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# A variational viscosity-limit approach to the evolution of microstructures in finite crystal plasticity

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Kochmann and Hackl introduced in [1] a micromechanical model for finite single crystal plasticity. Based on thermodynamic variational principles this model leads to a non-convex variational problem. Employing the Lagrange functional, an incremental strategy was outlined to model the time-continuous evolution of a first order laminate microstructure. Although this model provides interesting results on the material point level, due to the global minimization in the evolution equations, the calculation time and numerical instabilities may cause problems when applying this model to macroscopic specimens.

In order to avoid these problems, a smooth transition zone between the laminates is introduced to avoid global minimization, which makes the numerical calculations cumbersome compared to the model in [1]. By introducing a smooth viscous transition zone, the dissipation potential and its numerical treatment have to be adapted. We outline rate-dependent time-evolution equations for the internal variables based on variational techniques and show as first examples single slip shear and tension/compression tests.

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# Thermoplastics under Long-Term Loading: Experiments and Viscoelastic-Viscoplastic Modeling

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Thermoplastics subjected to long-term quasi-static loading generally show increasing deformation over time, so-called creep. During periods of partial or complete unloading, the deformation recovers at least partially. To further analyze this phenomenon and more accurately describe the long-term time-dependent deformation behavior of a semicrystalline thermoplastic, uniaxial tensile experiments are carried out and a suitable material model is formulated.

For the initial experiments, the load applied is held constant to determine creep deformations without recovery. During following experiments, the specimens are unloaded periodically such that distinct alternating creep and recovery phases are observed. The recovery phases allow for a distinction between recoverable and irrecoverable deformation during creep.

Based on identified characteristic features of the deformation behavior, a viscoelastic-viscoplastic model using an additive split of deformations is formulated. The viscoelastic part is represented by a generalized Maxwell model whereas the viscoplastic part derives from typical nonlinear creep evolution equations without incorporating a yield surface. An additional damage model interacts with both parts to represent further degradation of the material.

Numerical uniaxial simulations based on the experimental loading profiles are carried out and compared with the experimental results. The overall fit of the model towards the experimental results is demonstrated.

# Formation of grain boundaries in ductile single crystals at simple shear

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This presentation is concerned with the formation of grain boundaries in single crystals. From experiments producing large deformations, like equal-channel angular pressing (ECAP) the formation of grain boundaries in crystals can be observed [1]. Our aim is to propose a model, which is capable of predicting this phenomenon.

Plastic deformation of crystals is possible due to the movement and generation of dislocations in the material's crystal lattice. The kinematics related to these deformations is based on the nonlinear continuum dislocation theory (CDT) [2]. To model the formation of sub-grain boundaries all necessary equilibrium conditions are derived for a single crystal containing a surface of discontinuity, which is interpreted as a grain boundary, using the variational principle of minimum of the energy. Two novel equations are presented, namely

$$w_{\nabla\beta} \cdot \mathbf{n} = 0,$$

where  $w_{\nabla\beta}$  is the partial derivative of the free energy per unit volume of the single crystal with respect to the gradient of plastic slip  $\beta$  and  $\mathbf{n}$  is the unit normal vector of the surface of discontinuity. This equation can be interpreted as the equilibrium of micro-forces acting on dislocations. The second equation represents a thermodynamic condition that ensures that the driving force  $f$  acting on grain boundaries vanishes

$$f = -\mathbf{q} \cdot \mathbf{P} \cdot \mathbf{n} + \llbracket w \rrbracket + 2\zeta\eta = 0,$$

preventing movement of grain boundaries in the crystal. Here  $\mathbf{q}$  is a constant vector taken from Hadamard's compatibility condition for the total deformation,  $\mathbf{P}$  is the first Piola-Kirchhoff stress tensor,  $\llbracket w \rrbracket$  denotes the jump of the free energy density at the surface of discontinuity and  $\zeta$  and  $\eta$  are the energy per unit area of the surface of discontinuity and its mean curvature, respectively.

To illustrate how the derived set of equations can be used to model the formation of grain boundaries, the case of plane-strain simple shear deformation of a single crystal is investigated. It is shown that the proposed energy density function of the material exhibits non-convex behavior, indicating that there are states that allow for a laminate structure formation in the material in order to lower the energy of the crystal. This is accomplished by constructing an energy minimizing sequence mixing two energy states [3].

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# Modeling Dynamic Recrystallization in Polycrystalline Materials via Probability Distribution Functions

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A model of dynamic recrystallization in polycrystalline materials is investigated in this work. Within this model a probability distribution function representing a polycrystalline aggregate is introduced. This function characterizes the state of individual grains by grain size and dislocation density. By specifying free energy and dissipation within the polycrystalline aggregate an evolution equation for the probability density function is derived via a thermodynamic extremum principle. For distribution functions describing a state of dynamic equilibrium we obtain a partial differential equation in parameter space. To facilitate numerical treatment of this equation, the equation is further modified by introducing an appropriately rescaled variable. In this the source term is considered to account for nucleation of grains. Then the differential equation is solved by an implicit time-integration scheme based on a marching algorithm [3]. From the obtained distribution function macroscopic quantities like average strain and stress can be calculated. Numerical results of the theory are subsequently presented. The model is compared to an existing implementation in Abaqus as well.

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# Chiral acoustic metamaterials: dispersive waves and low frequency band-gaps

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Periodic acoustic metamaterials designed to get complete sound attenuation for a certain frequency range, namely acoustic wave spectral gap, pose interesting issues concerning their mechanical modelling [1], [2], [3]. The present analysis is focused on chiral lattices made up of an array of circular rings connected by ligaments and is devoted to understand the influence of resonators located inside the rings on the band gap structure. To get the essential aspects of the system some simplifying assumptions are put forward. The ligaments are assumed massless, while both the rings and the internal resonators are modelled as rigid. A discrete Lagrangian model having six dofs per node is derived and by a Hamiltonian approach the equations of motion are obtained. Dispersive waves in the periodic micro-structure are analysed in terms of dispersive functions and polarization vectors. The exact acoustic and optical branches are derived for harmonic waves in the discrete model. A further simplified description to obtain a synthetic representation of waves propagation is obtained by assuming an expansion of the generalized displacement field around the node of interest. This allows to get an enriched micropolar equivalent continuum whose equations of motion (partially relies on that obtained in [4], [5]) involves six degree of freedom. To assess the validity limits of the enriched micropolar continuum model the dispersive functions in terms of the fundamental parameters of the mass-in-mass dynamic system are compared with those obtained from the discrete Lagrangian model.

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# Finite Element Simulation of the creep behavior of directionally solidified NiAl-9Mo

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For high temperature structural applications, the B2-ordered intermetallic phase NiAl has promising material properties, such as high oxidation resistance, high melting temperature, high thermal conductivity and relatively low density [1]. However, the use of NiAl for structural applications suffers from its low creep resistance and its weak room temperature fracture toughness [2]. To improve these two material properties at the same time, directional solidification of eutectic alloys leads to a formation of stoichiometric NiAl and a reinforcing phase of a refractory metal e.g. Cr, Mo, W, Re [1]. A directional solidified NiAl-9Mo (at. %) eutectic consists of well-aligned single-crystal molybdenum-rich fibers embedded in a Ni-50Al matrix. The steady-state creep rate of the directional solidified NiAl-9Mo can be more than five orders of magnitude lower compared to the intermetallic NiAl [3]. It has been shown that these as-grown molybdenum-rich fibers are dislocation free and plastic flow begins, when the fibers' stress approaches the theoretical strength [4]. After start of yielding, the flow stress reduces due to strain softening of the fibers [4]. An additional advantage of using the directional solidification of eutectic alloys is that the phases are thermodynamically stable even up to the melting point [1]. To be able to predict the directional solidified NiAl-9Mo material behavior under several conditions, material models describing each phase are necessary. Our single crystal plasticity model for large deformation is based on a phenomenological approach with a state variable describing the average dislocation density of the glide systems. We use an overstress type power law flow rule to model the slip in each slip system and to consider the elastic range of the fibers. The two phases are modeled by an elasto-viscoplastic approach with a softening behavior for the fibers and a perfect plasticity behavior for the matrix. The softening behavior is motivated by the observation of the strain softening of the fibers [4]. This elasto-viscoplastic approach shows for a one-dimensional model reasonable agreement with experimental results. A creep curve simulation of a NiAl-9Mo representative volume element with periodic boundary conditions is compared to experimental results. The simulation results show that the molybdenum-rich fibers carry the load and reduce the stress in the NiAl matrix. This load partitioning leads to a reduction of the steady-state creep rate compared to the NiAl intermetallic phase.

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# Direct connection of rheological elements at large strains: Application to multiplicative viscoplasticity

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In the field of nonlinear continuum mechanics, rheological models are often used to exemplify the structure of complex material models at large strains. For this purpose, different rheological elements are combined in series and parallel connections. One approach to deduce the according constitutive equations consists of a multiplicative decomposition of the deformation gradient, a formulation of a free energy function and the evaluation of the Clausius-Duhem inequality. Subsequently, inelastic material behaviour is defined by appropriate evolution equations. Contrary to this, Ihlemann [1] developed an innovative concept, which enables material modelling at large strains based on the direct connection of rheological elements. In this contribution, we present the application of this approach to multiplicative viscoplasticity.

Starting from the additive decomposition of the stress power and demanding the stress power equivalence of the rheological connections, we first formulate constitutive equations within the framework of the multiplicative decomposition of the deformation gradient. These relations were already applied in the development of nonlinear viscoelasticity of Maxwell type by Landgraf and Ihlemann [2]. Next, we modify the derived connection relations with respect to the limitation on near-incompressibility. Then, individual material models, i.e. the rheological elements, are introduced. Among others, we define elements of hyperelasticity, Newtonian and non-Newtonian viscous flow as well as deformation rate independent plastic flow.

The regarded concept is employed to a model of multiplicative viscoplasticity. On the one hand, the connection relations are analytically evaluated to derive the constitutive equations typically used in the literature. On the other hand, we propose a numerical procedure, which evaluates the connection relations rather than solving the evolution equations for inelastic strains. Thereby, a predictor-corrector strategy is applied to consider the element of plastic flow. This alternative numerical procedure is tested and compared to the commonly used numerical algorithms. Due to a demonstrable accordance with the analytical and numerical solutions from the literature, the potential of the examined concept in the context of material modelling at large strains is shown.

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# Modelling Thermoplastic Material Behaviour of Dual-Phase Steels on a Microscopic Length Scale

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To support and physically motivate the development of a thermomechanical material model for the macroscopic material behaviour, the polycrystalline microstructure of the material is considered necessitating the development of a material model for the single crystal behaviour. In this work focus is especially placed on the behaviour of the ferritic matrix of dual-phase steels. Since the driving mechanisms for plastic deformation here are the formation, movement and pile-up of dislocations on preferred planes in preferred directions, many crystal plasticity models for the purely mechanical single crystal behaviour motivated by these mechanisms were proposed in the past. In this work these ideas are extended to thermomechanical material behaviour and a thermomechanical crystal plasticity model is developed for the single crystal behaviour. Attention is paid to the description of the evolution of the microstructure and its dependence on the history of the temperature of the processes under consideration. Elementary processes of multiplication and annihilation of dislocations are analysed in terms of temperature and deformation rate dependence. Thermal activation is used to describe these dependences and evolution equations are postulated for the state variables describing the current dislocation structure and by this the influence of the deformation and temperature history on current material behaviour. As the underlying dislocation structure determines the yield stress and the energy stored in the material, these evolution equations and their temperature and rate dependence are crucial for the formulation of the model. Estimations of the critical resolved shear stress necessary to move dislocations through the crystal resulting from the interaction of dislocations on different slip systems and the resistance of the atomic lattice and the energy associated with a line element of a dislocation allow to formulate a thermoplastic constitutive material model for the single crystal behaviour of the ferritic phase.

The developed ideas and the resulting model are transferred to the macroscopic behaviour of sheet metal wrought material consisting of dual-phase steels. Focus is placed on the consistency between experimental observations on a macroscopic length scale, the belonging constitutive thermoplastic material model on a macroscopic length scale and the developed material model for the single crystal behaviour. Possible forms and dependences on temperature and state variables for the macroscopic thermomechanical material model are deduced. Especially a thermodynamically consistent form for the energy stored in the material is presented.

# On the thermodynamics of pseudo-elastic material models which reproduce stress softening effects

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The mechanical material behavior of rubber is primarily affected by a stress softening effect called the Mullins-effect. Due to this effect, the stress depends strongly on the maximum load which occurred in the history of the material. Especially in inhomogeneously loaded components this effect has to be considered, as different regions with varying stiffness evolve. Due to this resulting inhomogeneous distribution of the material properties the overall behavior of the component is affected considerably. Therefore the Mullins-effect has to be taken into account to simulate the behavior of elastomeric components.

A very popular material model which allows for the Mullins-effect was proposed by Ogden and Roxburgh [1]. They introduced so-called pseudo-elastic material models, which are based on an arbitrary hyperelastic stress. After reaching a maximum load which is measured by the free energy of the basic hyperelastic model, the stress on unloading and successive reloading is decreased by a so-called softening function. A similar approach was used by Elías-Zúñiga and Beatty [2]. There, the norm of the right Cauchy-Green tensor is used as a measure for the load in the material.

In [1] and [2] only a few thermodynamical considerations are incorporated. Thus, the two mentioned models are analyzed theoretically and their thermomechanical properties are derived. These findings are used to deduce an alternative approach to deviate pseudo-elasticity. This is achieved by defining a suitable free energy which yields conditional equations for the stress tensor and the dissipation after exploiting the Clausius-Duhem inequality. It is shown, that under weak demands on the properties of the softening function the dissipation is always non-negative.

The concept of pseudo-elasticity is then generalized to extend arbitrary thermomechanical, even inelastic, material models to allow for softening effects. Under weak assumptions on the softening function the thermomechanical consistency is shown [3].

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# Experimental and numerical characterization of the mechanical properties of Ni/Al hybrid metal foams from the atomic to the microscale

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The increasing demand for lightweight and energy absorbing materials leads to popular design of foams and other cellular materials which combine many interesting physical and mechanical properties [1]. In this contribution, nano-Ni/Al hybrid foams were investigated. This hybrid foams consist of an open-cell aluminum alloy (AlSi<sub>7</sub>Mg<sub>0.3</sub>) foam strengthened with a nanocrystalline nickel coating [2]. The enhanced mechanical properties are characterized by experiments and numerical modeling at different scales. Nanoindentation is a well-known technique to measure the mechanical behavior of thin coatings with an extremely high resolution at nano-scale. Hence, the local mechanical properties of both the nanocrystalline nickel coating and the aluminum alloy strut are measured from nanoindentation with a very sharp Berkovich tip. The hardness and elastic modulus are determined through the Oliver & Pharr method. An elastic-plastic model without hardening is considered to describe the force-displacement behavior in nanoindentation. The local values of the elastic modulus and the yield stress are identified with an inverse computation based on the FEM simulation and the experimental measurements [3]. The local properties obtained from nanoindentation strongly depend on the distance of the indentation position to the Ni/Al interface, which is believed to be related with the microstructure [4]. Therefore, nanoindentation is coupled with EBSD to reliably explain the local measurement and to identify the relationship between the local microstructure and local properties.

Besides, the results obtained above are verified with molecular dynamic simulation of nanoindentation on different structured nickel atoms. The determined hardness and elastic modulus at the atomic scale will be compared with the values obtained at the nano-scale.

Furthermore, micro-tensile tests are performed on a wire made of the same matrix material and coating as the nano-Ni/Al hybrid foams. These were done to get a more homogeneous elastic-plastic behavior of this Ni/Al composite. So it is able to compare the local properties of Ni coating and Al strut at nano-scale with the global stress-strain behavior of the Ni/Al composite at micro-scale.

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# An Intrinsic Geometric Formulation of the Equilibrium Equations in Continuum Mechanics

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In this paper an intrinsic differential geometric formulation of the equilibrium equations in continuum mechanics is presented in its weak and strong variational form. Invariant continuum mechanics as proposed by Segev [1], considers the body  $\mathcal{B}$  and the physical space  $\mathcal{S}$  to be three-dimensional smooth manifolds with and without boundary, respectively. Furthermore the physical space is equipped with an affine connection. To respect the impenetrability condition the configuration  $\kappa : \mathcal{B} \rightarrow \mathcal{S}$  has to be a  $C^1$ -continuous embedding. Thus, the set of all  $C^1$ -continuous embeddings constitutes the infinite dimensional configuration manifold  $\mathcal{Q} := \text{Emb}(\mathcal{B}, \mathcal{S})$ . As in analytical mechanics, the virtual displacement field  $\delta\kappa$  is an element of the tangent space at the current configuration  $T_\kappa\mathcal{Q}$  which is isomorphic to the space of  $C^1$ -continuous sections of the pull-back bundle  $C^1(\kappa^*T\mathcal{S})$ . By duality, the forces of the continuum can be represented in the domain of the body  $\mathcal{B}$  by smooth covector- and tensor-valued volume forms. On the boundary, the forces are represented by covector-valued surface forms. For the classical theory, [2] postulates the principle of virtual work in the sense of Germain [3] as the fundamental principle of invariant continuum mechanics, stating that

$$\delta W(\delta\kappa) = - \int_{\mathcal{B}} \nabla \delta\kappa : \pi + \int_{\mathcal{B}} \delta\kappa \cdot \beta + \int_{\partial\mathcal{B}} \delta\kappa \cdot \tau = 0 \quad \forall \delta\kappa \in C^1(\kappa^*T\mathcal{S}).$$

Herein, the covector-valued volume form  $\beta \in \Gamma(\kappa^*T^*\mathcal{S} \otimes \Lambda^3T^*\mathcal{B})$  describes the external body forces, the covector-valued surface form  $\tau \in \Gamma(\kappa^*T^*\mathcal{S} \otimes \Lambda^2T^*\partial\mathcal{B})$  the external traction forces and the tensor-valued volume form  $\pi \in \Gamma(\kappa^*T^*\mathcal{S} \otimes T\mathcal{B} \otimes \Lambda^3T^*\mathcal{B})$  is called the variational stress describing the internal forces. The dot and the colon denote the contraction and double contraction of the adjacent tensor slots. The covariant derivative of a pull-back section of  $C^1(\kappa^*T\mathcal{S})$  is denoted by  $\nabla$ . The principle of virtual work as the weak variational form of the equilibrium equations defines insofar the interaction between internal and external forces independent of any constitutive laws.

With the definition of a contraction map  $p_\sigma : \Gamma(\kappa^*T^*\mathcal{S} \otimes T\mathcal{B} \otimes \Lambda^3T^*\mathcal{B}) \rightarrow \Gamma(\kappa^*T^*\mathcal{S} \otimes \Lambda^2T^*\mathcal{B})$  a new object, a covector-valued area form  $\sigma = p_\sigma(\pi)$ , called traction stress [4], is introduced. Using a telescopic expansion and defining the divergence of the variational stress by the relation  $\delta\kappa \cdot \text{Div}\pi = -\nabla \delta\kappa : \pi + d(\delta\kappa \cdot p_\sigma(\pi))$ , where  $d$  denotes the exterior derivative, the strong variational form

$$\delta W(\delta\kappa) = \int_{\mathcal{B}} \delta\kappa \cdot (\text{Div}\pi + \beta) + \int_{\partial\mathcal{B}} \delta\kappa \cdot (\tau - \iota^*\sigma) = 0 \quad \forall \delta\kappa \in C^1(\kappa^*T\mathcal{S})$$

is obtained by Stokes' Theorem. The pullback  $\iota^*$  by the inclusion map  $\iota : \mathcal{B} \rightarrow \partial\mathcal{B}$  restricts the covector-valued area form  $\sigma$  to the oriented boundary  $\partial\mathcal{B}$  and induces a traction force. By the arguments of the Fundamental Lemma of Calculus of Variations, the local equilibrium equations and the traction boundary conditions follow directly.

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# Numerical analysis of Ni/Al hybrid metal foams using the finite cell method

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Light-weight structures are used more and more in many engineering disciplines in order to save weight and to preserve natural resources. Metal foams represent one important class of materials that are used to manufacture such structures. Beside their low density they also have a good acoustic absorption and mechanical damping behavior which also make them attractive for many other applications. A new method to further improve the properties of aluminum metal foams is to coat them by electrodeposition with a thin nickel layer [3]. In order to find a macro-mechanical material law for such hybrid metal foams a lot of mechanical experiments are necessary. These experiments can be supported or replaced to some extent by a numerical homogenization procedure [2] which allows for a precise and systematic variation of the quantities of interest and help to understand the complex deformation mechanism. One of the main obstacles for such simulations is the immense labor effort to generate the mesh for a suitable discretization. In case of aluminum foams coated by nickel this problem becomes even more severe due to the thin nickel layer. In order to avoid this problem we employ the finite cell method (FCM) [1]. The FCM is a combination of a fictitious domain method and a high order finite element method. Due to the fictitious domain approach the surface of the foam and the material interface between the aluminum and the nickel do not need to be taken into account during meshing. This simplifies the meshing process and allows to automatically generate a simple Cartesian grid using the voxel model which comes out of a computed tomography scan. Due to the high order shape functions each element - or cell as referred to in terms of the FCM - can represent a set of voxel. As a consequence the number of degrees of freedom can be reduced a lot as compared to a voxel FEM simulation. Different issues of the finite cell method and of the numerical homogenization procedure will be discussed in order to carry out an efficient computation of the elastic properties of nickel coated aluminum foams.

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# The perturbation method applied to tube drawing with floating plug

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The determination of the load on the machine tool is crucial in the mechanics of metal forming processes as it has a critical influence over the deformation of the material into a new shape and the optimal conditions for the process. The problems of strip, wire, tube drawing without plug, tube drawing with floating plug [1]-[4] viscoplastic deformation has no exact solutions, but this paper addresses them using an approximate method. The influence of speed given by Bingham parameter and the influence of acceleration given by Reynolds parameter in the tube drawing with floating plug, is considered. The problem is solved using a viscoplastic constitutive equation of Bingham type. The friction between the rigid tool and the sliding viscoplastic continuum was considered in a local form,  $t_{r\theta} = m\sqrt{II_{I'}}$ , where  $II_{I'}$  is the second invariant of the deviatoric part of the stress tensor and  $m \in [0, 1]$  is the friction factor. An exact functional relationship between friction and variables such as: normal stress, lubrication, sliding speed etc. cannot be easily formulated, even though the description of the friction resistance between die and material in plastic forming of metals has been much studied. The shape of the floating plug, the drawing force are determined involving various parameters of the problem (the plug angle, the die angle, friction coefficients, the Bingham and Reynolds numbers), which allow the optimization of the drawing process.

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# Mathematical problems in the theory of elasticity for materials with double porosity

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The theories of elasticity and thermoelasticity of double porosity media, as originally developed for the mechanics of naturally fractured reservoirs, has found applications in civil engineering, geotechnical engineering, technology and biomechanics. Indeed, the double porosity model would consider the bone fluid pressure in the vascular porosity and the bone fluid pressure in the lacunar-canalicular porosity [18].

The theory of consolidation for elastic materials with double porosity was presented in [19]. This theory unifies the earlier proposed models of Barenblatt for porous media with double porosity [3] and Biot for porous media with single porosity [4]. The theory of elasticity for double porosity materials [19] is constructed with the help of Darcy's law and the basic equations involve the displacement vector field, a pressure associated with the pores, and a pressure associated with the fissures.

The double porosity concept was extended to media with multiple porosity in [1], [11]. A great attention has been paid to the theories of poroelasticity taking into account the thermal effects. The basic equations of the one and two-temperatures thermo-hydro-mechanical coupling theories for elastic materials with double porosity are presented in [2], [7], [9], [10]. The basis properties of the plane harmonic waves and the boundary value problems (BVPs) of the theories of elasticity and thermoelasticity for double porosity materials are investigated by using the potential method (boundary integral method) and the theory of singular integral equations in [5], [12]–[18].

Recently, the theories of elasticity and thermoelasticity for materials with a double porosity structure are presented in [8]. In this paper the theory of materials with voids [6] is generalized to derive a theory of thermoelastic solids, which have a double porosity structure. The new theory is not based on Darcy's law. The basic equations for elastic materials with a double porosity structure involve the displacement vector field and the volume fraction fields associated with the pores and the fissures.

In the first part of this talk, a review of the basic results in the theories of elasticity and thermoelasticity for materials with double porosity are presented. In the second part, the linear theory of elasticity for materials with a double porosity structure [8] is considered and a wide class of the internal and external BVPs of steady vibrations are investigated. Indeed, the Green's formulas and Somigliana-type integral representation of regular vector and classical solution of equations of steady vibrations are obtained. The radiation conditions for regular vector are established. The uniqueness theorems of the internal and external BVPs of steady vibrations are proved. The basic properties of surface (single-layer and double-layer) and volume potentials are established. The singular integral operators of the linear theory of elasticity for materials with a double porosity structure are studied. The existence of regular (classical) solutions of the internal and external BVPs by means of the potential method and the theory of singular integral equations are proved.

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