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Book of Abstracts

This is the book of abstracts for the 6th International Conference on Material Modelling taking place in Lund, Sweden, 26th-28th June, 2019.

During the past decades, material modelling has become a field of central scientific importance. Although there exist many workshops, meetings, colloquia, etc. on specific materials and particular applications, here a single conference dedicated to material modelling with all its various facets is intended. To this end, the aim of the ICMM conference is to bring together researchers from the various fields of material modelling and material characterization and to cover essentially all aspects of material modelling. This will provide the opportunity for interaction between scientists working in different subareas of material mechanics who otherwise would not come into contact with each other.

This biannual conference is the sixth in the ICMM series. The first ICMM took place in 2009 in Dortmund, Germany. The conference has since then been organized in Paris, France; Warsaw, Poland; Berkeley, USA; Rome, Italy.

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3D analysis of lattice rotation fields in deformed aluminium: 6D-DCT X-ray synchrotron experiments and finite element simulations

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Lattice rotations develop inside grains of polycrystalline materials subjected to plastic deformation, as a function of grain orientation and grain interactions. As the lattice rotations results from restricted crystallographic slip inside grains, they provide some information on the activated slip systems, slip amplitudes and therefore on the local deformation. It is therefore possible to use local lattice rotations inside polycrystals to better understand polycrystal plasticity at large. While 2D observations of lattice orientations and rotations have become standard since the advent of automated EBSD, 3D observations are still much more rare but have become possible, for example, using synchrotron X-ray diffraction imaging techniques.
In this work, the recent 6D diffraction contrast tomography (6D-DCT) technique was used to measure the lattice orientation and rotation fields throughout grains of an aluminium polycrystal subjected to plastic deformation. In its initial state, the material was in a fully-recrystallized state, with uniform orientations inside grains, a nearly-random distribution of the grain orientations (no texture) and an average grain size of 270 micrometers. Before deformation, a volume of 0.5 x 0.5 x 1.65 mm was mapped by 6D-DCT, which contained about 500 grains. The sample was then deformed in situ to 0, 0.5, 0.8, 1.5, 2.8, 3.4 and 4%, and, at each deformation, the same central volume of about 0.5 x 0.5 x 0.68 mm was mapped by 6D-DCT, which contained about 200 grains. The experiment resulted in a series of 3D images of the polycrystal, of 200 x 200 x 240 voxels (voxel size = 3.5 micrometers), where each voxel has its own lattice orientation. Grains are described by 40000 voxels in average, which offers access to fine orientation variations.
The lattice rotations of the individual grains were analysed in detail, in terms of (i) the average rotations and its correlation to the initial grain orientation, (ii) the orientation distributions inside grains and the development of preferential rotation directions, and (iii) the orientation fields and the correlation to the distance to grain boundaries. At the final state of 4%, the grain average rotations were found to vary from 0 to 3.7°, and the maximal average in-grain misorientations was 1.5°.
Finally, the polycrystal deformation was simulated using the crystal-plasticity finite-element method, grains being discretized into several hundreds of elements. A comparison with the experiment, based on the previously-mentioned metrics, is also presented.

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A Coupled Poroviscoelastic Model for Drying Shrinkage-Induced Cracking in Concrete

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Concrete structures, especially at their early ages, may undergo significant deformations due to drying shrinkage accompanied by the time-dependent creep phenomenon. A sound understanding and quantitative prediction of creep and shrinkage-induced deformations, and the associated stress concentrations are of great importance for the accurate estimation of the service life of concrete structures. The latter is greatly affected by durability-related phenomena that start to arise due to initiation of micro-cracks as the principal stresses exceed the current tensile strength of hardening

concrete. The drying shrinkage-induced localization of tensile stresses results from uneven volume changes due to the alteration in relative humidity through the loss of evaporable water from the surface of concrete, in contact with generally less humid air.

In this contribution, we develop a coupled constitutive modeling approach that is furnished by robust computational framework to address the durability problems that arise from drying shrinkage within the three-dimensional framework of poroviscoelasticity. Hence, the proposed approach accounts for the hygro-chemo-mechanical cross coupling effects between the shrinkage-induced strain development due to the pressure evolution through humidity variations and the stress concentrations in hardening or hardened viscoelastic concrete. To this end, we additively decompose the stress expression into the effective stress of viscoelastic concrete skeleton and the pressure developing in pores. The viscoelastic model of the skeleton takes into account short- and long-range creep effects through the well-known micro-prestress theory. The material parameters related with the rigidity and strength of concrete are assumed to evolve with the degree of hydration. In the proposed model, as opposed to the modeling approaches suggested in the literature, the shrinkage strain is not obtained by using an empirical formula involving the hygromechanical expansion coefficient and the change in humidity. Instead, we employ a physically motivated approach where the pore pressure is obtained as a function water content that is determined using sorption-desorption equations for a given value of the local relative humidity. In addition to the conservation of linear momentum equation, the Darcy-type transient continuity equation is used to calculate the temporal and spatial variation of the relative humidity. The coupled model of poro-viscoelasticity is further supplemented by a crack phase-field model to conduct the crack risk analysis of concrete structures subjected to the coupled effects. The results obtained using the proposed model are contrasted with the experimental data involving creep and shrinkage deformations. Additional representative examples of boundary-value problems are analyzed to demonstrate the predictive capabilities of the proposed three-dimensional model.

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A Hashin-Shtrikman type semi-analytical homogenization procedure in multiscale modeling to account for coupled problems

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ABSTRACT

Heterogeneous materials are important for a vast amount of applications e.g. in automotive industry or in aerospace. For instance, when producing components, it can be desired to use materials with a heterogeneous microstructure in order to achieve specific material properties. The resulting properties highly depend on the manufacturing process itself, which can involve mechanical and/or thermal loadings. Therefore, it is necessary to properly depict the microstructural material behavior in order to allow for the calibration of the manufacturing process and for the solution of the inverse problem.

Constitutive models can be used to depict the material response in a simplified manner. These simplifications allow for a more flexible use of the model but restrict it to a certain range of applications. Thus, it is beneficial to take the material's microscopic structure into account and couple its behavior to the macroscopical response. As multiscale methods (e.g. FE^2 , FE-FFT) are computationally expensive, semi-analytical homogenization procedures are investigated to account for the transition between different length scales. There are various well known homogenization techniques discussed in literature such as e.g. the Voigt and Reuss bounds or also the self-consistent method as well as the Mori-Tanaka method. In our presentation, the focus lies on a Hashin-Shtrikman type method in similarity with the one proposed by [Wulfinghoff et al. (2018)]. This homogenization technique will then be applied to a heterogeneous elastoplastic material under mechanical and thermal load. After

presenting the homogenized material model, we will proof its applicability by various numerical calculations.

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A Homogenization Approach for Multiphase Materials with Planar Interfaces

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Microstructural and morphological features strongly influence mechanical properties of materials because they regulate the micro-mechanisms that operate during the deformation. Therefore, morphology is an important factor that should be considered in micromechanics based constitutive models. To this end, we propose a method that could be employed to construct micromechanical models for different morphologies. The method discretizes a geometry representing the microstructure into arbitrary number of regions where each region is in contact with either one or two regions. Two neighboring regions are separated by a planar interface similar to the lamination theory, and deformation gradient field of each region is assumed to be uniform. It is well-known that in rank-1 laminates there exists a single interface where both force equilibrium and deformation continuity are present. In the proposed method, there are multiple interfaces at the same scale, but the force equilibrium and the deformation continuity are not satisfied simultaneously on these interfaces. Instead, we replace one of these physical requirements with an energetically motivated condition that minimizes the free energy expression. However, it is shown that as the orientation of consecutive interfaces approach each other, the neglected condition is better satisfied. Furthermore, if all consecutive interfaces are parallel then the method boils down to the rank-1 laminate. In classical lamination theory, it is well-known that the Hill-Mandel condition is satisfied. In the proposed method, it can be shown by relaxing the force equilibrium or the deformation continuity (or both) that the Hill-Mandel condition is trivially satisfied as well.
Using the proposed method, we first model the disk-like spherulite morphology that is observed in thin film samples of semi-crystalline polymers such as high density polyethylene (HDPE). In a spherulite microstructure crystalline lamellae, which are embedded in a matrix of amorphous material, grow in predominantly radial directions and branch irregularly. The crystal plasticity with orthotropic elasticity and the isotropic 8-chain rubber elasticity constitutive models are employed in the regions that belong to these phases. Then the proposed method is used to model randomly oriented lamellar microstructure of ultra high molecular weight polyethylene (UHMWPE). The model is compared with experimental and numerical results from the literature in terms of both homogenized (elastic and plastic) material properties and the texture evolution.

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A Hybrid Approach to Describe the Elastic-Plastic Deformation Behaviour of Porous Media Including Damage Effects

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The constitutive description of inelastic deformation behaviour of porous media is a challenging task. The complex hardening behaviour (isotropic, kinematic and distortional hardening at the same time) and anisotropic yielding depend strongly on the microstructure and the inelastic behaviour of the bulk material, cf. [1] and [2], respectively.
In a previous work [3] the authors presented a homogenized material model for an elastic-plastic material at the microscopic scale based on an adapted yield function to describe the elastic-plastic deformation behaviour of open-cell structures. The shape of the yield function is not specified completely a priori. The proper shape is found by interpolation between results of cell model simulations using neural networks [4].
Now, this approach is extended towards damage at the microscopic scale. The aim of this contribution is the description of the deformation behaviour at the macroscopic scale while damage occurs at the microscopic scale. The model is fitted to different loading cases in stress space. Thanks to the high adaptability of neural networks, a good agreement is observed. Using this material model, the deformation behaviour of structural components made of porous media can be analyzed under consideration of the coupling of damage and plasticity of
the material.

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A beam theory considering a new class of constitutive relations for elastic bodies

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Recently some new types of constitutive relations have been proposed for elastic bodies considering small strains and rotations, but where the mechanical behaviour is nonlinear. One of such relations corresponds to a constitutive equation wherein the linearized strain is assumed to be a function (in general nonlinear) of the stress. Such constitutive equations can be used to model the behaviour of, for example, concrete, rock, and some metal alloys.

In the present work we present a beam theory considering the above new class of constitutive equation, and we compare the predictions provided by such theory with the case of considering the linearized equations of elasticity, in particular for beams made of rock and concrete.

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A dislocation density tensor-based gradient plasticity framework

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Based on an extended form of the Clausius-Duhem inequality by means of a so-called non-locality residual, a thermodynamic consistent gradient plasticity theory is proposed which relies on the physical interpretation of incompatible plastic deformations in terms of dislocation densities. Taking into account dislocation density tensors as additional arguments of the free energy density function and evaluating the generalised form of the dissipation inequality in accordance with the developments presented in [1], the balance equation of a generalised stress field together with its non-ambiguous constitutive boundary conditions is derived. The latter is found to be additively composed of a classic Mandel-type stress field and of a contribution which can be shown to be closely related to the geometrically necessary dislocation density. Moreover, the generalised stress field is identified as the driving force for the plastic deformation based on energetic dualities. With the evolution equation for the plastic flow being accordingly formulated as a function of the generalised stress field, it is revealed that the stress contribution that is related to the dislocation density tensor takes the interpretation of a back-stress tensor.

After proposing a specific form of the dislocation density tensor-based gradient energy contribution which results into well-interpretable stress contributions, we focus on the solution of the resulting system of coupled partial differential equations by means of a multi-field finite element formulation and study various boundary value problems to show the applicability of the proposed formulation. In particular, the constitutive response at material interfaces where the plastic variables exhibit jump discontinuities, and the shear band formation in softening materials that is induced by geometric imperfections, are subjected to detailed analyses.

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A finite-element framework for the modelling and simulation of phase transforming magnetic solids using energy relaxation concepts

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The macroscopic behavior of ferroic functional materials such as magnetic shape memory alloys is highly affected by microscopic mechanisms such as the formation and further evolution of microstructures. Thus, the modelling of these effects is important for establishing micromechanically well-motivated constitutive frameworks with high physical plausibility. In the present approach, the switching between different crystallographic variants of martensite as well as the propagation of magnetic domains is treated by the evolution of phase volume fractions on the basis of energy relaxation methods. In addition to these mechanisms, possible deviations of the local magnetization vectors with respect to the easy axes also need to be taken into account in order to simulate the material behavior accurately. For homogeneous problems (e.g. elliptic bodies), the influence of the demagnetization field can be captured by demagnetization tensors and the effective quantities such as stresses and the magnetic induction can be calculated in a post-processing step. However for inhomogeneous problems, the demagnetization field has to be treated as an independent

field variable. An intermediate conclusion of the present research project states that a conventional Finite-Element-based implementation, where internal state variables are locally determined at the integration points in a condensed manner, is hardly, if at all, realizable. Thus, the variables describing the microstructure are also treated as global field variables and the related Biot-type evolution equations are solved at the macroscopic level. In this contribution, the theoretical approach as well as the Finite Element implementation will be elaborated along with a comparison between different parametrizations.

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A fresh view on modeling room-temperature martensitic transformations in partially stabilized zirconia using the phasefield approach

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Partially stabilized zirconia (PSZ) based ceramics are well known for their high fracture toughness and have numerous technological and bio-medical applications. The excellent mechanical properties mostly arise from the material's ability to undergo a stress-induced martensitic transformation from the tetragonal to the monoclinic phase accompanied by (pseudo)twin-formation.
These effects have been previously modeled using the phasefield method [1,2]; however, in order to reproduce the expected behavior, the simulations had to be carried out at temperatures close to 1300 K.
We propose a modified Landau potential which allows the simulation of stress-induced tetragonal-to-monoclinic phase transformations in zirconia at room temperature, while still respecting the experimentally obtained M_s temperature. When applied to MgO partially stabilized zirconia, in which the transformation is constrained within lenticular plates embedded in a cubic matrix, the model predicts microstructures that agree very well with available TEM micrographs. The obtained results confirm the assumption of a sequential formation of pseudo twins proposed within the crystallographic (LIS) theory [3].

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A gradient enhanced damage growth model for ductile fracture

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A gradient enhanced damage model for ductile fracture modeling describing the material response including damage induced degradation is presented. The application in mind is the modeling of impact problems, like split Hopkinson tests and machining process simulations. The continuum damage evolution of Lemaitre type is focusing the degradation of the shear response eventually leading to shear failure, cf. ref [1]. A fundamental formulation is adopted based on continuum thermodynamics to properly describe different components of the energy dissipation induced by the effective material response, thermal effects and damage evolution. A main prototype for the effective material is the Johnson-Cook model, accounting for deformation and strain rate hardening and temperature degrading effects. In the damage modeling we are concerned with:

1. the energy dissipation rate (involving elastic and inelastic components) describing input damage driving dissipation to the damage induced fracture area production process.
2. the description of energy dissipation due to fracture area production. In this development, we consider area production due to "damage convection" and "damage nucleation" in the temporal evolution of the damage field, cf. ref [2]. In addition, a gradient fracture area production effect is obtained due to spatial growth of the damage field.

Thereby, the model facilitates an enhanced control of the damage evolution and fracture energy dissipation. It has been shown that this model, without the additional gradient effect, cf. ref. [3], can partly remove the pathological mesh dependence and have a stable behavior. A major incentive of the present investigation is thus to consider the total model convergence and stability properties in the FE-application. The modeling framework will be verified for FE plane strain/stress tests, showing the convergence properties of the model.

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A gradient-damage model for crack nucleation and propagation in elasto-viscoplastic polycrystalline materials

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In the present work, a gradient damage model is developed to model crack nucleation and propagation in polycrystalline materials. The model uses a scalar damage variable to represent the progressive degradation of mechanical resistance. The spatial gradient of the damage variable, which is treated as an additional external state variable, serves regularization purposes and allows considering the surface energy associated with cracks. Constitutive relations are developed within the thermodynamic framework of generalized standard materials. The coupling of damage with elasticity and/or hardening is considered. Also, the impact of the loading mode on the development of damage is captured by differentiating the influence of spherical and deviatoric stresses and considering closure effects. The proposed formulation satisfies the continuity of the stress-strain relation and is adapted to any class of material symmetry. Numerical implementation is undertaken via the finite

element method, where nodal degrees of freedom are the displacement and the damage variable. The proposed formulation is quite general and allows dealing with different damage mechanisms. To show the capabilities and limits of this formulation, some numerical simulations are carried out. They allow investigating the impact of loading conditions and microstructural heterogeneities on damage development as well as the impact of the damage-elasticity and damage-hardening couplings. Some important aspects of crack nucleation and propagation including kinking and branching and tension/compression asymmetry are discussed.

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A gradient-extended anisotropic brittle damage model

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Due to the renewable energy act, fossil power plants are exposed to complex start and shut down process conditions. This means in turn that special materials are required/have to be designed to meet the extremely high functional and safety requirements. Typical examples include high strength fiber-reinforced composites. Since the effective mechanical properties of such materials is to a large extend determined by physical, topological and statistical details of the underlying microstructure, the development of appropriate constitutive models has been and still represents the subject of intensive research in the material science community.

For the particular problem at hand, the failure prediction of the respective materials is addressed. To account for these phenomena at the mesoscale, an anisotropic damage model [1] is employed in a micromorphic formulation [2]. As a result, the damage growth criterion [3] is fulfilled which ensures the stiffness degradation of the material during a general damage process. Additionally, the micromorphic-based gradient extension yields mesh-independent results.

In order to get a detailed understanding of the influence of microstructural characteristics on the overall mechanical behaviour, representative volume element and unit cell simulations are carried out. Furthermore, voids and pores induced by the manufacturing process at the microstructure scale are also taken into account.

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Nonlinear elasticity / **71**

A micro-macro constitutive model for strain-induced phase transformation in polymers

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This paper deals with molecular ordering in polymers that exhibit strain-induced phase transformation accompanied with plastic yielding. The study is motivated by the anisotropic effects caused by the molecular ordering during the progressive strain-hardening, and thus attempts to contribute to the understanding of the strengthen mechanisms in initially isotropic glassy polymers. The application is performed on initially isotropic amorphous polylactide that exhibits strain-induced mesomorphization and crystallization, whose respective development depends on temperature and strain-rate. A micro-macro constitutive model is presented for the description of the polylactide macro-response along with the transformation phase kinetics. A three-phase representation of the microstructure allows accounting for the effective contribution of the two newly formed phases both to the elastic-viscoplastic intermolecular resistance to small-moderate deformations and to the hyperelastic molecular network resistance to large deformations. The strain-induced phases are distributed on each stretched molecular chain of the network thanks to a transition from the macro-scale to the micro-mechanisms at the chain-scale via the microsphere approach. The model results are compared to experimental data up to very large overall strains and over a wide range of temperatures. The role of the newly formed phases on the strengthen process of polylactide is predicted via our approach.

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A micromechanical approach based on Fourier transforms and continuum dislocation mechanics to simulate grain size effects in polycrystals

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An Elasto-Visco-Plastic (EVP) Fast Fourier Transform (FFT)-based formulation initially developed for conventional crystal plasticity [1] is here coupled with the phenomenological Mesoscale Field Dislocation Mechanics (MFDM) theory [2]. The present numerical approach named "MFDM-EVPFFT" accounts for plastic flow and hardening from densities of geometrically necessary dislocations (or "GND") in addition to statistically stored dislocations ("SSD"). The model also captures GND density evolution through a filtered numerical spectral approach [3], which is coupled with stress equilibrium through the EVPFFT algorithm. The discrete Fourier transform method together with finite difference schemes is applied to solve both lattice incompatibility problem and Lippmann-Schwinger equation, see e.g. [4-6]. Numerical results are first presented for two-phase laminate composites with plastic single crystal channels and elastic precipitates. First, a channel size effect on the overall behavior of laminate composites is obtained due to the pile up of GND densities at interfaces between hard and soft phases [7]. Second, 3D face-centered cubic (FCC) polycrystals using periodic Voronoï tessellations are considered. In comparison with the conventional Crystal Plasticity model (CP-EVPFFT), it is shown that grain size effects occur on the flow stress of polycrystals during monotonic loadings. In addition, GND effects on backstress and plastic strain profiles during reversible loadings are investigated with the present MFDM-EVPFFT numerical approach.

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A micromorphic tissue approach describing non-affine myocardial deformation characteristics

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Computational modelling of cardiac tissue relies on the accurate description of its anisotropic highly non-linear constitutive response. Classical continuum mechanics models have been successfully employed to realistically predict the material response of the heart. In this work, the heterogeneous structure of myocardial tissue is addressed in more detail, focusing on the interplay of cardiac myofibers with the extracellular matrix (ECM). Generally, the hierarchical material composition of the myocardium comprises of muscle cells embedded in a complex fiber network of connective tissue with highly non-uniform fiber orientation, dispersion, thickness, length and relative volume fraction. It has been found that cardiac myocytes exhibit a certain degree of motion flexibility within the constraining cytoskeleton (cf. Spotnitz et al. (1974) and LeGrice et al. (1995)). A micromorphic continuum model is therefore developed which associates the fibrous constituents with additional degrees of freedom being the vector components of so-called micro-directors. The latter provide the means to account for non-affine deformations of myocytes and ECM which is not as straight forward using classical models. Specifically, the proposed micromorphic approach considers three strain and corresponding stress measures describing the deformation of the ECM, the muscle fibers and their interaction, respectively.
Utilising finite elements, the micromorphic cardiac tissue framework is applied to model a patient-specific heart geometry supplied by the Cape Universities Body Imaging Centre (CUBIC) and investigate the influence of non-affine micro-kinematics on the passive and active response of the heart.

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A new Eshelby-type estimator for thermal and thermoelastic characterization of multiply coated ellipsoidal heterogeneities: from analytical development to numerical validation

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In the present work, we address the numerical validation of a new micromechanical estimator, called General Explicit Eshelby-type Estimator (GEEE), primarily developed for evaluating equivalent properties of multicoating inclusions, such as thermoelastic constants and thermal conductivities.
Being formulated from the seminal work of Eshelby (1957), GEEE utilizes Eshelby's tensor, thereby allowing for handling ellipsoidal configurations. In most particulate composite materials, the reinforcing fillers can be satisfactorily approximated with ellipsoidal geometries or limit cases thereof, such as cylinders, platelets and spheres. The distinct advantage of working with Eshelby type estimators, such as GEEE or Hori & Nemat Nasser's Method (1993) (also known as Double Inclusion model) and its modified version by Dinzart et al. (2016), which we use for comparison purposes, is that with a single formulation, the equivalent properties of a large spectrum of multiply coated heterogeneities can be evaluated. Non Eshelby-type estimators, on the contrary, are much less general, as they are developed for specific geometries of heterogeneities with specific material symmetries, and sometimes limited number of phases. Examples of this second class of estimators, which are also implemented here for comparison purpose in elasticity, are Polarization Approximation (PA) method, Maxwell's approach, Hervé & Zaoui's (n+1)-phase model, its more general extension by Chatzigeorgiou, Seidel & Lagoudas (2012), and the Annular Inclusion Coating Model (Wang et al. (2016)).
Initially presented for estimating the equivalent elasticity of n-phase heterogeneities, GEEE is directly extended, in this work, to equivalent thermoelastic and thermal conductivity properties. Examples of already existing estimators for such properties, are found in the works of Levin (1967) and Hervé (2002) for the thermal expansion coefficient, and in Hervé (2002) and Hiroshi & Minoru (1986) for the thermal conductivity. In Hervé (2002), the estimator is of non-Eshelby-type, whereas the estimators proposed in Levin (1967) and Hiroshi & Minoru (1986) are of Eshelby-type. As compared to the non Eshelby-type estimators that are generally expressed by nonlinear, implicit tensor equations, the presented GEEE, for the different properties, has the absolute advantage of possessing a linear and explicit form, which thus makes it more convenient in computer programing.
To assess the efficiency of the developed GEEE by comparison to the above-mentioned mean-field analytical estimators, several multiphase, spherical and cylindrical heterogeneities are investigated. The performance of GEEE is also assessed by comparing full field numerical results from finite element simulations using ABAQUS, and when possible, from XFEM/LevelSet simulations using inhouse code, the XFEM/LevelSet method having the comparative merits of better dealing with interfacial discontinuities. The respect or violation of the Hashin-Shtrikman bounds by GEEE and the other examined estimators is also studied in order to investigate their consistency and efficiency.
The analysis of the various numerical results clearly shows the accuracy, the versatility and the out performance of the proposed new estimator, GEEE, in efficiently estimating the equivalent thermal and thermoelastic properties of multicoating inclusions of different geometrical shapes.

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A new perspective on the J-, M- and L-integrals: from micromechanics of dislocations to body charges and body forces

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A new perspective is given on the J-, M- and L-integrals and their physical interpretation. The J-, M- and L-integrals of straight dislocations are derived in the framework of three-dimensional, incompatible, linear elasticity [1]. The J-integral of dislocations is the well-known Peach-Koehler force. The obtained results reveal the physical interpretation and significance of M- and L-integrals for straight dislocations. The M-integral is half the corresponding interaction energy between the two dislocations plus twice the corresponding pre-logarithmic energy factor. This result gives for the first time to the M-integral the physical interpretation of the interaction energy (depending on the distance and on the angle). The L_3-integral is the z-component of the configurational vector

moment (torque) about the z-axis caused by the interaction of the two dislocations. Moreover, the J- and L_3-integrals are interpreted as translational and rotational energy-release, respectively.
Next, the J-, M- and L-integrals of a single dislocation are derived in isotropic elasticity [2]. The remarkable outcome is that the M-integral represents the total energy of the dislocation which is given by the sum of the self-energy and the dislocation core energy. The latter can be identified with the configurational work produced by the Peach-Koehler force. It is shown that the dislocation core energy is twice the corresponding pre-logarithmic energy factor. This result about the M-integral is valid in isotropic as well as in anisotropic elasticity.
The J-, M- and L-integrals of body charges and point charges in electrostatics, and the J-, M- and L-integrals of body forces and point forces in elasticity are derived and their physical interpretation is investigated [3]. One of the basic quantities appearing in the J-, M- and L-integrals is the electrostatic Maxwell-Minkowski stress tensor in electrostatics and the Eshelby stress tensor in elasticity. It is shown that the J-integral of body charges in electrostatics represents the electrostatic part of the Lorentz force, and the J-integral of body forces in elasticity represents the Cherepanov force. The M-integral between two point sources (charges or forces) equals half the electrostatic interaction energy in electrostatics and half the elastic interaction energy in elasticity between these two point sources. The L-integral represents the configurational vector moment or torque between two body or point sources (charges or forces). The presented results show that the J-, M- and L -integrals are fundamental concepts which can be applied in any field theory.
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Plasticity and viscoplasticity / 127

A non-local damage-plasticity model based on a smooth elastic-plastic transition

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Standard rate-independent elastic-plastic formulations use a yield function to separate elastic response and plastic response. Specifically, the consistency condition, which requires the yield function to vanish during loading, causes a sharp transition between elastic and plastic response with a break in the slope of the stress-strain curve. To eliminate this undesired response, a large deformation model, characterized by a smooth elastic-inelastic transition has been proposed (Hollenstein et al. 2013, Jabareen 2016). Also, their model unifies rate independent as well as rate dependent responses.
Further, it is well-known that classical continuum damage models may not be able to capture the real mechanical behavior of materials due to localization associated with strain softening. In addition, if no adjustments are made, the region of localization will depend on the mesh size of the spatial discretization. The necessity to model damage, which is controlled by the microstructure, has driven the development of the nonlocal and gradient damage formulations. Nonlocal plasticity models incorporate a nonlocal variable defined as the spatial weighted average of a corresponding local field over the entire body. Often, the nonlocal quantity formulation includes an intrinsic length parameter that affects the weight amplitude in the vicinity of a material point.
In the present study, an extension of a smooth inelasticity model to include softening and localization based on a strongly non local gradient-enhanced formulation is presented. A strongly objective integration scheme is developed based on the introduction of the relative deformation gradient – the deformation mapping between the last converged and current configuration. Also, a finite element formulation has been developed, which incorporates three variational fields for the equilibrium equations and an additional field for the Helmholtz type equation for the gradient-enhanced formulation.

The numerical implementation of the proposed model will be presented, and the capabilities of the developed finite element will be demonstrated by a few examples.

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A non-singular continuum theory of point defects using gradient elasticity of bi-Helmholtz type

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We present a non-singular continuum theory of point defects [1] based on a second strain gradient elasticity theory, the so-called gradient elasticity of bi-Helmholtz type [2]. Such a generalized continuum theory possesses a weak nonlocal character with two internal material lengths and provides a mechanics of defects without singularities. Gradient elasticity of bi-Helmholtz type gives a natural and physical regularization of the classical singularities of defects, based on higher order partial differential equations. Point defects embedded in an isotropic solid are considered as eigenstrain problem in gradient elasticity of bi-Helmholtz type. Singularity-free fields of point defects are presented. The displacement field as well as the first, the second and the third gradients of the displacement are derived and it is shown that the classical singularities are regularized in this framework. This model delivers non-singular expressions for the displacement field, the first displacement gradient and the second displacement gradient. Moreover, the plastic distortion (eigendistortion) and the gradient of the plastic distortion of a dilatation centre are also non-singular and are given in terms of a form factor (shape function) of a point defect. Singularity-free expressions for the interaction energy and the interaction force between two dilatation centres and for the interaction energy and the interaction force of a dilatation centre in the stress field of an edge dislocation are given. The results are applied to calculate the finite self-energy of a dilatation centre.

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A simple explicit homogenization solution for the macroscopic elastic response of isotropic porous elastomers

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An approximate homogenization solution is put forth for the effective stored-energy function describing the macroscopic elastic response of isotropic porous elastomers comprised of incompressible non-Gaussian elastomers embedding equiaxed closed-cell vacuous pores. In spite of its generality, the solution — which is constructed in two successive steps by making use first of an iterative technique and then of a nonlinear comparison medium method — is fully explicit and remarkably

simple. Its key theoretical and practical features are discussed in detail and its accuracy is demonstrated by means of direct comparisons with novel computational solutions for porous elastomers with four classes of physically relevant isotropic microstructures wherein the underlying pores are: (i) infinitely polydisperse in size and of abstract shape, (ii) finitely polydisperse in size and spherical in shape, (iii) monodisperse in size and spherical in shape, and (iv) monodisperse in size and of oblate spheroidal shape.

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A simple model of cristal plasticity using pencil glide and kinematic hardening, application in polycristal with the homogenization method

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In various b.c.c crystals (including some titanium alloys), plastic deformation exhibit specific behaviour. We can define the slip directions, but it is very difficult to identify the slip plane beacause the dislocation can glide on many plane containing one of the latter directions possible. We observe that the slip lines are sinuous [1], it can be explained by the cross slip of screw dislocation [2]: Taylor and Elam [3] call this pencil glide or non-crystallographic slip planes. Gilormini [4], Krawietz [5], Becker [6] have been using this theory to explain the behavior of various b.c.c materials.
In a case (new titanium alloys) where the behavior of the slip systems are unknown, the pencil glide slip systems have been introduced to replace the non-identified slip systems in these alloys. The advantage of this model is to reduce the number of parameters to identify still respecting the general behavior. Then, the homogenization method beta-model [7] was implemented in large deformations in the finite element code and used to study the alloy behavior.
In this work, FE computations are performed, using the pencil glide and the classical plasticity models, to evaluate their ability to predict the mechanical behavior of alpha-Iron and the resulting stress distribution of a notched component subjected to an uniaxial loading path.
The work is part of the ANR TiTwip project.

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Ab initio modelling of impurity induced intergranular fracture in tungsten

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Owing to its attractive material properties, tungsten (W) and its alloys are considered to be the leading solid material candidates for plasma-facing components in future fusion devices such as the Tokamak reactors in the international thermonuclear experimental reactor (ITER) as well as the planned future demonstration fusion reactor (DEMO). However, a fundamental concern of using W for such applications is the high ductile to brittle transition temperature (DBTT) and its dependence on the microstructure and impurity concentrations. Experiments have revealed that the DBTT for single-crystalline tungsten can be as low as -196 ℃, whereas poly-crystalline samples can remain brittle up to about 800 ℃. For the application of fusion reactor components, this is a major concern in light of the fact that the temperature at the armour material of the first wall and diverter under operating conditions typically lie in the range 600–900 ℃. This suggests that the first wall armour material is at risk of rupturing because of brittle grain boundary fracture. This situation becomes especially severe when it contains impurities that reduce the grain boundary strength the material.

In the present work we study the impact of embritteling impurities on the grain boundary strength of W by means of first principles quantum mechanical modelling based on density functional theory. The purpose is to model the grain boundary (GB) strength for different impurity concentrations and to investigate how the coverage varies during the gradual separation. In particular, we aim to investigate how the peak stress associated with decohesion and the Griffith work of fracture along with impurity transport influences the cohesive strength during the mode I opening based on a thermodynamic description of the equilibrium impurity coverage. This provides qualitative insight to the influence of impurities on the cohesive strength of grain boundaries and provide traction-separation data that can be used for macroscopic cohesive zone modelling of intergranular fracture in tungsten. As model GB we consider the $\Sigma5(310)[001]$ high angle configuration with varying degrees of phosphorus impurities, which are notorious for having a detrimental effect on the strength of tungsten GB:s.

The results show that by the introduction of a clean (i.e. impurity free) grain boundary in the bulk, the strength and peak stress of the cohesive zone are reduced and they are further reduced by the introduction of impurities. This effect can be attributed to the formation of polar bonds between W and P, which leads to a weakening of the interface. Based on a thermodynamic analysis of the cohesive zone during the straining we find that diffusion of impurities may occur to retain thermodynamic equilibrium for constant chemical potential. This contributes to the gradual reduction of the peak stress related to fracture, which can contribute to diffusion driven delayed cracking, even when subjected to static loads. For further details the reader is referred to [1].

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An FFT based field dislocation mechanics study of discrete dislocations, grain boundaries, and their interactions

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Grain boundary-dislocation interaction plays a crucial role in the mechanics of polycrystalline materials. Most efforts in understanding these interactions often use discrete atomistic based modelling. Continuum scale studies typically suffer from lack of accurate knowledge of local stress fields at the grain boundaries. In this talk, we present preliminary results on using the recently developed continuum scale field dislocation mechanics to study the stress fields of discrete dislocations, grain boundaries, and their interactions. Small strain FFT based approach is used as a numerical method to solve field dislocation mechanics. Local stress and strain fields due to discrete dislocations with both straight and mixed character are calculated. Effect of elastic anisotropy on the local fields is presented and are compared with those obtained from analytical solutions. Further, grain boundaries modeled as a network of dislocations satisfying the Frank-Bilby relationship. Variation in the local stress fields as a function of elastic anisotropy is discussed.

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An assessment of the edge strength of glass

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Float glass is increasingly used as a load-bearing material in structures, e.g. balustrades, wall sections, floors, and roofs. In contrast to a conventional window glass pane, the structure must be designed to resist various actions such as dynamic impact loading from e.g. an object accidentally falling into it or static loading from e.g. snowfall. In such cases, the surface as well as the edge of the glass unit are subjected to significant tensile stress. However, an assessment of the edge strength has not been undertaken to the same extent as for the surface strength. There is a need to explore the strength modelling of the glass edge.

The edge strength is particularly challenging to model because of the range of treatments that are applied in the manufacturing process. These include scribing and cutting, as well as grinding and polishing operations which in turn depend on the choice of cutting fluid and applied pressure, grinding angle and speed, as well as the maintenance level of the machinery in use. This is reflected in the European pre-standard prEN 16612:2017 which adopts a reduction factor for the strength when the failure occurs at the edge as compared to the surface. On the other hand, according to the German structural standard DIN 18001-1:2010 the strength of the edge is the same as the pristine surface.

The strength is governed by material flaws present at the surface. The flaws which magnify the stresses locally become potential failure sites according to linear elastic fracture mechanics. The stress-raising property of a flaw is dependent on its shape and size. The true shape and size distribution of flaws in glass, however, cannot be directly probed by any measuring device at present. Moreover, the initial flaw size is altered during the load history due to stress corrosion which occurs when the glass is subjected to tensile stress in an ambient environment that contains water moisture. The ultimate flaw size, and hence the fracture stress, is a function of the time-dependent stress history.

A large-scale assessment of the edge strength is performed in a comprehensive survey of the experimental results from four-point bending tests which are available in the literature and which pertain to a range of different suppliers and processing methods, glass sheet thicknesses, and edge spans subjected to maximum tensile stress. Using a theory for the effect of load duration, the fracture stress results are converted into an equivalent constant rate of 2 MPa/s within the load span. The statistics of failure are analyzed across the various treatments and inferences about the underlying flaw size distributions are drawn which suggest a practicable representation of the edge flaw condition. A stochastic strength prediction model for the edge is developed based on a weakest-link concept and implemented in a numerical procedure.

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Application of High Order Statistics for Evaluation of Mechanical Characteristics of Porous Heterogeneous Media

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Many modern materials used in various engineering applications have a porous microstructure. The porosity of the material can be determined either by the purpose of application or by the appearance of undesirable defects due to technological features of the production process. It is established that microstructural morphology has a significant influence on the mechanical properties of materials. In addition to the characteristics of the components and interphase boundaries, the properties of such materials are determined by morphological factors, such as volume fraction, size, shape and spatial distribution of inclusions. For successful design and study of such heterogeneous media complex interphase interactions, geometry and the distribution of the properties of the components must be taken into account.
This work is aimed at development of an original technique for analysis of the deformational and mechanical characteristics of porous heterogeneous media using combination of multipoint instruments of mathematical morphology, stochastic analysis and mathematical modeling methods.
The morphology of porous media can be studied as a complex system of many interacting components, for description of which the tools of the mathematical statistics can be introduced. In the present work multi-point statistical descriptors (for example, correlation functions of random variables) are used for establishing a quantitative relationship between the specifics of microstructure, local and effective properties of heterogeneous media. The instruments of mathematical morphology also allow to assess the influence of internal parameters, such as shape, distribution and orientation of inhomogeneities, on the effective mechanical properties.
The analysis of mechanical behavior and properties of porous media, calculation of the characteristics of the local stress and strain fields are be based on stochastic micromechanical models using the integral equations method. This method assumes that the mechanical properties of microstructural components are determined by means of ordinary phenomenological equations and criteria, and the microscopic stress and strain fields are calculated using solutions of stochastic boundary value problems with rapidly oscillating coefficients in displacements. The solution for the displacements field is reduced to an integral equation containing the Green's function.
Modeling of three-dimensional microstructure of porous media is performed taking into account the variation in shape, size, orientation and location of pores. Voxel geometry meshing is used to obtain the values of the statistical descriptors. The obtained methodology is illustrated on some specific examples of analysis of the representative volume elements created based on typical porous heterogeneous media. The interrelation between changes in various parameters of a microstructure with the values of statistical descriptors were investigated and new results were obtained for estimation of the contribution of multipoint statistics to the accuracy of a formalized representation of morphology and geometric features.

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Atomistic phase field chemomechanical modeling of precipitate-solute-defect interaction in metallic alloys

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The interplay between chemistry and defects is important in determining material response in many engineering alloys. Local fluctuations in chemical composition introduces heterogeneity in material properties that affect defect formation and evolution.

On the other hand, the thermodynamics at the defects themselves differ from the bulk causing chemical partitioning between the two regions. Due to its energy-based formulation, the phase field (PF) approach combined with mechanical defect modeling is ideally suited to study this strong two-way coupling between chemistry and defect evolution. A large deformation formulation of mechanical equilibrium is coupled with PF modeling, taking into account elastic anisotropy, concentration dependent stiffness, solute residual distortion, as well as the concentration dependence of dislocation and stacking fault energies. A conservative Cahn-Hilliard model is employed to describe solute concentration, while the non-conservative Allen-Cahn model is employed for defect evolution. The defects considered here are dislocations, precipitates, and low angle grain boundaries. The entire energy model is calibrated using atomistic and / or CALPHAD information (in the latter case, for solute mobility and chemical energy). This ensures for example accurate treatment of core size and dislocation transformation pathways.
A number of example simulations and comparison with results from atom probe tomography and transmission electron microscopy will be given.

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Automated identification of material models at large strains

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A concept by Ihlemann (2014) enables the formulation of material models at large strains based on directly connected rheological elements. With respect to this concept and the work by Kießling et al. (2016), the choice of an appropriate rheological model can be considered as the main step within the formulation of a material model. This contribution aims for the automated identification of this rheological model and, thus, of the automated generation of material models at large strains based on a set of experimental data.

At first, the basics of the concept of directly connected rheological elements are introduced and extended. This comprises the formulation of the kinematic and kinetic relations of a parallel and series connection of an arbitrary number of rheological elements. Here, the multiplicative decomposition of the deformation gradient as well as the additive decomposition of the stress power are assumed. Furthermore, some rheological elements are defined. Each rheological element represents an individual material law at large strains modelling a basic phenomenological property, like elasticity, viscosity or plasticity. With respect to these individual material models, a complex material model at large strains can be formulated by evaluating the connection relations of the rheological model. Consequently, a computer routine can be developed which numerically evaluates these connection relations and, thus, an arbitrary material model at large strains.

Based on this implementation, an automated identification of a rheological model can be realized. Here, a genetic algorithm, belonging to the group of stochastic optimization procedures, is particularly applicable. To this end, the rheological models have to be represented by a numerical code. Thereby, the utilization of tree structures is beneficial. Additionally to the clear representation of the hierarchical structure, operations can be defined enabling the generation of further rheological models. In accordance with the basic idea of genetic algorithms, these operations are based on

mutation, which corresponds to the modification of a single rheological model, and on crossover, which corresponds to the exchange of the structure between two rheological models. Within the genetic algorithm, several rheological models are generated and rated. To this end, the parameters of the corresponding material models are identified from a set of experimental data and the resulting residuum is calculated. Besides some further criteria, like the complexity of the model, the considered rheological model is assessed on the residuum. Based on this assessment, the genetic algorithm is further executed or the rheological model, meeting the abort criterion, is indicated as the result of the identification procedure.

The developed algorithm is tested using synthetic data. Because the genetic algorithm identifies the rheological model, which was applied to generate the synthetic data, the presented approach seems to be appropriate. To finally demonstrate the potential of the concept as well as of the according implementation, a rheological model and, thus, a material model at large strains is identified using a set of real experimental data.

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Boundary value problems in the linear coupled theory of poroelasticity

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The prediction of the mechanical properties of porous materials has been one of hot topics of continuum mechanics for more than 100 years. The construction of mathematical models of fluid flow through porous media and the intensive investigation of the problems of porous continua arise by extensive use of porous materials into civil and geotechnical engineering, technology, hydrology, and recent years, medicine and biology.

There are a number of theories which describe mechanical properties of single porosity materials, and the most well known of them are: i) Biot (1941) consolidation theory based on Darcy's law and ii) Nunziato-Cowin (1979) theory based on the concept of volume fraction.

In the present talk the coupled mathematical model of poroelasticity based on the combination of Darcy's law and the concept of volume fraction is introduced and the non-classical problems of steady vibrations of this model are completely investigated. Indeed, the basic properties of the plane harmonic waves are established. The fundamental solution of the system of steady vibrations equations in the considered theory is constructed by elementary functions. Green's formulas and Somigliana-type integral representation of regular vector and classical solution of the system of equations of steady vibrations are obtained. The uniqueness theorems for classical solutions of the boundary value problems (BVPs) are proved. The basic properties of surface and volume potentials are established. The BVPs are reduced to the singular integral equations and the corresponding singular integral operators are studied. Finally, the existence of classical solutions of the BVPs by means of the potential method and the theory of singular integral equations are proved.

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Callus remodeling model for mandible fracture healing – finite element analysis

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Introduction
Mandible fractures are among the most common bone injuries in maxillofacial trauma, accounting for 20%-60% of all facial traumas [1]. The medical goals in treatment of this kind of fractures depend on the arrangement of bone fragments and aim at restoration of callus functionality in order to re-establish the dental occlusion, masticatory function and preinjury bone anatomy. According to Champy [2] fixation plates should be placed to specific lines to get the best results. When placed along these lines, identified along the physiological tension lines, plates produce stable fixation.

Material and method
A new mathematical model of callus remodeling was used to investigate the healing process of the mandible. The local bone density changed as a function of the mechanical stimulus. The model was described in the previously published paper [3]. In this study two models of the fractured mandible were constructed using Mimics software (V20.0, Materialise, Leuven, Belgium). Two different fixation designs were simulated: model 1 with only one plate and model 2 with two plates. The plates, elongated in the middle part, had six holes, four screws and 1,7 mm thickness. All screws were of 7 mm length. It is noted that there are various relations between density and bone Young's modulus E available in the literature. The properties of the bone were assumed to be linear, elastic and isotropic. The behavior of the bone was described by two constants (the Young modulus E and the Poisson ratio ν). In most papers mandible is modeled as a homogenous material or rarely consisting of two tissue types: outer cortical bone and inner trabecular bone. In reality, mandible is highly heterogeneous tissue with various modulus of elasticity due to the wide range of calcification. In our study, the mechanical properties of the mandible were calculated based on the Hounsfield units from CT images. The relations between HU units, bone mass density ρ [g/cm3] and the Young modulus E [MPa] were established. Fifteen groups of material properties were described for the mandible. The bone density ranged from 0,01 to 2,82 [g/cm3] and the corresponding Young's modulus ranged from 0,00379 [MPa] to 85 [GPa].

Conclusions
Our results confirm reports of other authors that two-plate stabilization of the bone fragments ensures the proper stabilization and create the favorable environment for appropriate osteosynthesis. Presented results confirm that mathematical model of callus remodeling is a useful tool for predicting the tissue healing and might be helpful in assessing the quality of mandible fixation. It is particularly useful for describing regions of tissue growth and resorption mainly due to underload.

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Characteristic Nonlocal Elastic Properties of Homogenized Framework Structures with Micromorphic and Micropolar Beams

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The micromorphic body with the additional microscopic deformation gradient tensor can diversely extend the deformability by modeling the deformable material point instead of the classical rigid

one. It contains nine degrees of freedom (DOFs) at any point in addition to the macroscopic three DOFs while the micropolar has three additional DOFs. Based on totally 12 DOFs, three kinds of strain tensors, which total number of components reaches 42, are defined and the conjugate dual stress and double stress tensors are identified via the constitutive laws. Relationship between the deformability and rigidity of the body is an inevitable issue when applying such a microcontinuum theory. In order to make clear of the characteristic nonlocal elastic properties of micromorphic and micropolar bodies, two-scale homogenization method based on such microcontinuum theories has been formulated in the finite element method. The orthogonal and oblique lattice framework structures consisting of micromorphic and micropolar beams are analyzed to summarize the difference between the two theories and the size dependence of unit cell. The framework structure has such a high porosity that the node at which some beams are linked is strongly affected by the surrounding deformation state. Therefore, the beam has been recognized as a typical model of nonlocality.
The results point out some noticeable facts. First, even if the microscopic framework structure doesn't have any nonlocality, that is, it just contains the conventional local elastic constants, the nonlocal elastic constants of the homogenized macroscopic body exit because the rotation DOF in the microcontinuum is the same dimension to the conventional deflection angle of the beam. Both bodies clearly illustrate the size effect for the different sizes of unit cells. Comparing the two microcontinuum bodies, the approximated Young's modulus of the homogenized framework structure in the micromorphic becomes much softer than that in the micropolar. This suggests the typical trade-off relationship between the diverse deformability and the rigidity of the structures.

Nonlinear elasticity / 17

Characterization of the multi-axial behavior of a hyperelastic Mooney-Rivlin material using a novel test: Results of finite element simulations

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The modeling of hyperelastic behavior of elastomeric materials is well established in framework of continuum mechanics. Due to the complex behavior of elastomers, the model parameter calibration requires complex experimental protocols, from experimental setup and sample (e.g., complex multi-axial loadings, optimized geometry). Moreover, the identification of the material parameters is still a difficult task [1]. Classically, material parameters can be determined either at homogeneous deformations (uni-axial tensile, pure shear and equi-bi-axial tensile) [2] or at inhomogeneous deformations [3]. In this short communication, we propose an alternative test for the parameter identification (or validation). Indeed, we present a novel test protocol that consists of deforming a sample by coupling both the deformations of pure shear and of simple shear. One main characteristic of this test is that, the stress-strain relations are depending on the direction of the stretching, i.e. $\Theta \in \left]0, \frac{\pi}{2}\right[$(orientation of the sample in a special device attached to a single column universal tensile testing machine) and the displacement U (or γ). We have calculated by FE the Cauchy stress field in core region of the sample for γ=1, 2 and 4 and different values of Θ. Then, we assumed that the strain field is homogeneous in central region of the sample, so that the deformation gradient is as follows: $(F) = e_1 \otimes E_1 + \kappa\lambda e_1 \otimes E_2 + \lambda\, e_2 \otimes E_2 + \lambda^{-1} e_3 \otimes E_3$ in which $\lambda = 1 + \gamma \sin\Theta$ and $\kappa\,\lambda = \gamma\, \cos\Theta$ are respectively, the macroscopic or global stretch ratio along the X_2-axis and amount of shear. Thereby, we are able to compute analytically the Cauchy stresses, which are almost equal to results of FE simulations. Consequently, the Cauchy stresses in core region of the sample could be related to the applied forces via the macroscopic deformation gradient and under condition that the boundary value problems are well controlled (uniform stresses). So, the experimental data arising from this test should be suitable for identification or/and validation of hyperelastic models.

Keywords: Hyperelasticity . Multi-axial behavior . Finite element simulations.

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Optimization and inverse problems in multiscale modelling / 48

Clustering Multiscale Optimization of Thermoelastic Lattice Materials

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The clustering multiscale topology optimization of thermoelastic lattice materials and structures based on Extended Multiscale Finite Element Method is studied. The strain energy of thermoelastic lattice materials that is an effective measure of the average stress is chosen as the objective function. The microstructural configuration of the thermoelastic lattice materials and their distribution on the macrostructure are designed through topology optimization. The two-scale design with multiple materials is implemented through clustering optimization. The K-means clustering methods is proposed to group the microstructure, and the average clustering method is adopted as a reference. Microstructures are grouped based on their strain energy to enable reasonable distribution of the base material at the macrostructural and microstructural scales. Results show that the clustering multiscale-optimization design is superior to the classical multiscale-optimization design of the lattice material from the numerical examples. The clustering multiscale optimization is implemented with a microstructure characterized a square configuration composed of 20 bars. The square microstructural configuration can help to solve the disconnectivity issue when we want to produce the multiscale materials and structures with the advances of manufacturing techniques, such as additive manufacturing. Taking a two-end clamped beam as an example, we discuss the effects of the number of clusters (groups), amplitude of thermal loads, size factor of the microstructure, and material volume fraction on the optimization results. Numerical examples demonstrate that the proposed method can substantially improve the structural performance with reasonable computation and manufacturing costs.

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Comparison of different implicit integration procedures for an elasto-viscoplastic model

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Numerical integration of non-linear elasto-viscoplastic models is a critical point in the design of industrial parts. The main objective of this study is to compare different implicit time integration schemes for a particular model (1). We present here integration procedures based on a fully implicit integration scheme associated with a radial return, which has been proved unconditionally stable and faster for temperature dependent yield limit and viscous flow (2). In order to obtain a quadratic rate of convergence, a consistent tangent operator (2) is used. Four different stress-prediction algorithms are compared in this study.

The first integration scheme presented is based on a classical Newton-Raphson procedure: the state variables increments are calculated with the inversion of a Jacobian matrix representing the couplings between all the variables. Each state variable is described through an evolution law and contribute to a complete residual vector. The calculation of the terms of the Jacobian is the most difficult point of the implicit method, and several alternatives are tested in the following methods.
In the second integration scheme studied, the terms of the Jacobian matrix are evaluated with a perturbation within second-order finite difference. Although this greatly reduces development times, it may also increase significantly the computational costs.
Then we present a third solution to avoid the expensive numerical step of Jacobian calculation and consequently to shorten the integration time by expressing all the integration variables according to one variable and finally by solving a unique implicit equation thanks to a Newton algorithm. However, convergence problem may arise with such a scalar equation.
Then, in order to assure the convergence of the Newton-Raphson algorithm, a coupled-method based on Newton-Raphson procedure and Brent method can be tested (3).

All these integration procedures are implemented with the open-source MFront code generator (4,5). MFront is co-developped by CEA and EDF in the framework of the PLEIADES plateform (6). Implementations are first compared on a single integration point with a tool called MTest, delivered with MFront. Calculations on industrial structures are then performed in ABAQUS/Standard implicit finite element solver (7) and then compared the current methodology of Groupe PSA.

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Experimental identification and material characterization / 166

Comparison of different model formulations for the optimisation of material parameters in thermomechanics

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The Finite Element (FE) based parameter identification is well-established for the identification of material parameters of mechanical material models, but can also be used for the optimisation of calorical quantities within a thermo-mechanically coupled model. This requires the use of full field temperature data together with displacement field data. In a first step, a parameter identification for a rather simple thermo-mechanically coupled material model is performed, demonstrating the underlying framework and especially the handling of thermal boundary conditions. In a second step the influence of the chosen model on the obtained thermal material parameters is analysed. The influence of the dissipated energy is examined more closely, since several model formulations may represent a similar or even the same mechanical material response, but predict different amounts of dissipated energy. For each of these models, a different set of optimal calorical parameters is to be expected and the question arises which model to choose. Hence, different model formulations are subjected to the parameter identification process and the results are compared.

Creep, damage and fatigue / 45

Competing mechanisms of particle fracture and decohesion in fatigue initiation of a disk superalloy

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Superalloys produced via powder metallurgy have a tendency to contain non-metallic inclusions. Inclusions have different mechanical properties than the metallic medium they are suspended in which causes stress localisations to produce cracks when the material becomes subjected to cyclic loading [1].
Crack nucleation around inclusions is known to occur by three initiation modes: particle fracture, particle decohesion and slip-driven initiation [2]. In the material system presented, the two former modes are observed in a mixed-manner. Decohesion of the particle interface has been determined unambiguously by a strong normal stress component in a previous study [3]. The nature of particle fracture however, was not determined.
To investigate the competing mechanisms between particle fracture and particle decohesion, an experimentally validated crystal plasticity finite element model which incorporates cohesive surface interactions was used.
In an initial study, we found that the maximum principal stress within a particle is often coincident with the location of cracking in experiment. By comparing the stress at the interface and the peak maximum principle stresses within the particle over time we extracted estimates of oxide cleavage strength. Proceeding this, cohesive surfaces were applied to metal-oxide and oxide-oxide interfaces, representing decohesion and fracture zones respectively. The nucleation of a microcrack in experimentally obtained DIC map was found to coincide with the location of highest effective plastic strain within the model. We also investigate the case for which slip-driven cracks occur rather than particle fracture and decohesion. Slip-driven cracks have been successfully predicted by a stored energy criterion previously [2]. With criteria for all three modes available we have the foundations for building a fatigue initiation map. The results highlight the importance of considering interfaces when modelling metal-oxide systems and allow us to interpret the strength of decohesion and particle fracture by modelling means.

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Constitutive modelling of anisotropic rate-dependent Ti-6Al-4V titanium alloy for aircraft fan blade design

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During the design stage of an aircraft engine fan blade development, the behavior of the materials involved must be fully understood. In the present case we are interested in the design of fan blades regarding impact loading resulting mostly from bird strike or engine fan blade loss and involving high strain rate, non-proportional loading paths, plastic dissipation induced self-heating and potential damage and fracture. Due to its high strength-to-weight ratio and good tenacity, the Ti-6Al-4V titanium alloy is considered as a promising candidate for the fan blade leading edge. A good knowledge and description of the material's response under the above mentioned conditions are necessary for a reliable prediction of the resistance of the overall engine structure. For that purpose, an extensive experimental campaign has been carried out and a constitutive model has been developed.
The thermo-mechanical characterization carried out on specimens made of a grade of Ti-6Al-4V titanium alloy provided in the form of cold rolled plates has evidenced a strong orthotropic behavior with a significant strength dissymmetry between tension and compression. This behavior is frequently observed in materials with a hexagonal close packed crystallography due to the activation of different slipping and twinning mechanisms. In addition, viscous and thermal effects on both tension and compression specimens have been quantified performing low strain rate tests at various temperatures and high strain rate tests using Split-Hopkinson pressure bar set-ups. The experimental campaign also allowed for distinguishing the isotropic and kinematic contributions of the strain hardening.
Relying upon the analysis of the experimental campaign results, a constitutive model has been developed accounting for the combined effect of nonlinear, isotropic and kinematic strain hardening, strain rate hardening, tension/compression dissymmetry and machining direction. Indeed, the orthotropic plasticity model developed by Cazacu and coworkers, see [1], has been extended within a rate-dependent and isotropic vs. kinematic hardening formulation. The identification of the constitutive model constants has been conducted by means of the commercial software Zset. The constitutive model has been implemented as a user material subroutine in the commercial finite element computation code LSDYNA. Numerical simulations have been conducted considering some basic cases involving representative volume elements as well as structures such as the specimens used for the experimental campaign.
The incorporation of void growth induced damage and self-heating in the constitutive model is in progress.

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Constitutive models for stainless steels exposed to temperature and complex cyclic loadings

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The design of high-temperature components usually relies on viscoplastic constitutive models. Most macroscopic models were established years ago by various research groups [1] and rely on phenomenological equations. This often leads to difficulties to cope with complex loading conditions and to reproduce the behaviour over wide loading ranges. Recent propositions [2] use a physically-based modified flow equation to reliably predict the behaviour of cast-iron under thermal-mechanical loading and introduce dislocation densities as internal variables to describe static recovery effects in stainless steels. This formalism provides a good agreement between the experiments and model prediction under various thermal mechanical loading path. It, however, fails to precisely describe, with a unique parameter set, both small (just beyond the elastic limit) and large strain loadings (several percents of viscoplastic strain).

Stainless steels often have particular microstructures related to rolling processes that must be considered to propose a better description of small strain states. Grain crystallographic orientation and applied stresses, by piloting the progressive activation of slip systems, can indeed master the transition between the elastic (all grains are elastic) and the viscoplastic regime (all grains present plastic strains). EBSD analyses for the studied stainless-steel show furthermore the existence of preferential crystallographic orientations [3]. The material could then be treated in terms of a polyphase alloy; each group of equivalently-oriented grains is then considered as a phase with its own behaviour. The polycrystalline alloy behaviour is then dependent on the characteristics of each phase and its volume fraction. Homogenization techniques can be used to propose a macroscopic model capable of describing mean behaviour. Here, self-consistent approaches [4,5] enable to build a complete constitutive model, following the principles proposed by [2] and by only adding two material parameters.

The model is tested on a specific experimental test, consisting of a succession of loading cycles with an increasing strain amplitude (from 5.10^{-4} to 8.10^{-3}) for a constant strain ratio equal to zero. A very good agreement with the experiments is observed for the whole strain range while the same material parameters set also give very predictive results for a tensile test up to a strain of 5.10^{-2}. Materials parameters identification and plasticity activation in the different phases are finally discussed.

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Continuous-time fatigue model: Acceleration for cyclic load

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Continuous-time models for high-cycle fatigue are useful for arbitrary load histories with nonproportional or aperiodic load. In this work, we consider a previously published model (Ottosen et al. 2008, Ottosen et al. 2018), which is based on an endurance surface controlled by the current stress state and a load history-dependent back-stress, where the latter controls the center of the endurance surface. Damage develops when this endurance surface moves, but only during the loading phases. The versatility of the model comes at a computational cost; it is necessary to integrate the back-stress evolution and damage across the full load history. We seek a method for accelerating the computations in the special case of cyclic load.

We fit the continuous-time fatigue model to the material data of AISI 4340 alloy steel by considering the Haigh diagram and the Wöhler curve. There is compelling experimental evidence that rotary stress states are more detrimental to materials than proportional states (Anes et al. 2014). To capture this effect, a nonproportional load case must be included in the fitting procedure. Due to the lack of experimental work on nonproportional load for AISI 4340, we fit the model parameters to a qualitatively proper model behavior.

We investigate the development of a steady-state in the incremental damage per cycle for proportional and nonproportional cyclic load, respectively. The existence of a steady-state would enable extrapolation of the damage at the end of the transient, thus reducing the number of cycles necessary for integration. We demonstrate that proportional stress states lead to a brief transient of less than ten cycles, whereas some cases of nonproportional stress states lead to a prolonged transient that persists over several hundred cycles.

Having established the existence of a steady-state, we formulate a method of extrapolation. The damage D_i at the end of each cycle i is obtained by integration, producing a sequence $S_n = \{D_i\}_{i=0}^n$ with $D_0 = 0$, and n the total number of integrated cycles. Linear extrapolation is employed for each pair (D_{i-1}, D_i) to find the extrapolated damage $\tilde{D}_i^N$ at cycle $N \gg n$. Thus, we obtain a new sequence $\tilde{S}_n = \{\tilde{D}_i^N\}_{i=1}^n$ of extrapolated values. Finally, an approximation of the damage D_N is obtained by applying the sequence acceleration method known as Wynn's epsilon algorithm (Wynn 1956) to $\tilde{S}_n$. We show that this procedure efficiently reduces the computational cost for the continuous-time fatigue model for general cyclic load.

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Cosserat crystal plasticity with dislocation driven grain boundary migration

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Thermomechanical processing of metallic polycrystals may lead to significant microstructural rearrangements due to the viscoplastic deformation and subsequent or concurrent grain nucleation and growth.

In order to describe the microstructural evolution directly related to viscoplastic deformation, single crystal plasticity theories are useful. In particular, when strong size and gradient effects are present, non-local theories such as Cosserat or strain gradient approaches are called for. Plastic slip processes induced by the deformation results in local reorientation of the crystal lattice, possibly resulting in the creation of new subgrains with associated grain boundaries. On the atomistic level, the incompatibilities associated with lattice gradients are resolved by insertion of so called geometrically necessary dislocations (GNDs). Furthermore, during deformation so called statistically stored dislocations (SSDs) accumulate in the grains due to random trapping processes.

Energy is stored in the structure due to the accumulation of dislocation densities. This stored energy is an important driving force for subsequent grain boundary migration as dislocation free grains nucleate and expand to replace the old grains. Nucleation is favored at locations of high dislocation content, such as grain boundaries.

It is thus clear that grain nucleation and grain growth is strongly linked to viscoplastic deformation. Non-local single crystal plasticity theories can predict the evolution of both GNDs and SSDs but it cannot handle by itself grain nucleation and grain boundary migration. In this work, a Cosserat crystal plasticity model has therefore been enhanced with a phase-field variable. The evolution of the phase-field variable is coupled to the lattice curvature which makes for a formulation where grain boundaries are defined as areas of high density of GNDs and are mobile thanks to the associated phase-field dynamics.

The model has been implemented as a coupled system of partial differential equations and solved monolithically by the Finite Element Method (FEM). Numerical investigations on bi- and polycrystal systems show that the coupled model is capable of predicting coupled microstructure evolution due to deformation and grain boundary migration, i.e. the orientation of a material point may change due to deformation or when it is being swept by a moving grain boundary. The model predicts grain boundary migration due to capillary forces as well as energy stored due to accumulated dislocations.

A particular point is the discussion regarding the interplay in the model between lattice curvature induced by deformation and the formation of stable subgrain boundaries.

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Coupling void growth and coalescence criteria for porous single crystals

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Ductile failure and related micromechanical phenomena have been thoroughly investigated from experimental and numerical point of views in the last decades. In metallic materials, void nucleation, growth and coalescence of intragranular voids have been identified as one of the main mechanisms

taking place during the ductile fracture process. Limit analysis, thermodynamical and variational approaches have led to yield potentials for homogenized porous media. The first models were developed for perfect, isotropic plastic matrix materials containing either spherical or cylindrical voids. Recently great efforts have been put into extending these models to anisotropic plasticity and more general void shapes and orientations. In addition evolution laws governing internal variables have been proposed, and in particular an heuristic law is often adopted to take into account strain hardening. Recently homogenized void growth and coalescence yield criteria have been developed for a crystal matrix material. These models are suited for materials for which the most detrimental void population (regarding the mechanical properties) is sub-crystalline. For void growth in a single crystal single- and multi-criteria yield surfaces were proposed in the literature. Extensions to finite deformations were also developed. Only a few works investigated void coalescence in single crystals. Hure (2019) proposed and assessed a coalescence single-criterion for perfectly plastic porous single crystals using FFT-based numerical limit analysis. In the present work we propose an extension of this coalescence criterion for a strain hardening crystal matrix. In contrast to isotropic plasticity all material directions are not equivalent in single crystals, thus hardening varies upon crystal orientation. Therefore a mean critical resolved shear stress is defined and predicted coalescence stresses are validated from reference periodic unit-cell simulations involving several crystal orientations. An estimate of the fracture strain defined as the coalescence onset in these simulations is also obtained. Predictions of this criterion are compared to another extension proposed in the literature (Yerra et al., 2010). The criterion is then applied as a threshold above which an effective porosity has to be used in a void growth model in order to simulate the coalescence phase. This threshold is implemented in a single crystal void growth model at finite deformation (Ling et al., 2016) and is shown to lead to a good agreement with unit-cell results. Finally a reformulation of the coalescence criterion into a yield criterion is investigated as well as its coupling with the growth criterion.

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Critical thickness and misfit dislocations in rocksalt ZnMgO layers grown on MgO (100)

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Zinc oxide has wurtzite structure (wz-ZnO) at ambient conditions. Due to the promising bandgap (4.0-7.8eV) we consider the misfit stress for the growth of rock salt rs-$Zn_xMg_{1-x}O$ layers on rock salt MgO. At the ambient conditions, a solid solution of ZnO in MgO is stable only up to 13% of ZnO. Nevertheless, due to the compression induced by misfit stress the range of chemical composition of thermodynamically stable layers can be extended.

We consider a mechanism of the dislocation network formation at the interface $Zn_xMg_{1-x}O$/MgO. Based on the dislocation theory, many different analytic formulas for critical layer thickness have been derived, cf. Hu (1991), Brown (2002). The formulas concern the critical thickness of the layers

which retain thermodynamically stable at atmospheric pressure. On the other hand, for thin layers which lose the stability earlier, before the stress relaxation, we can expect a lower critical thickness. We present a derivation of an analytic formula for the critical thickness of rs-$Zn_xMg_{1-x}O$ layers which lose the stability due to the rocksalt-wurtzite phase transition, cf. Lu et al. (2016). In the new formula the dependency of the onset elastic energy $E(\sigma, x)$ of the rs→wz phase transition is taken into account. In the general case this energy depends on the misfit stress and chemical composition.

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Experimental identification and material characterization / **117**

Crystal Plasticity Finite Element study of the impact of texture/architecture on the mechanical behavior of Ni micro-wires

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Warthi et al. [1] have reported a significant increase of the tensile strength of Ni micro-wires with a reduction of diameter from 120µm down to 20µm obtained by electropolishing. Thorough characterization of the microstructure and the tensile behavior of wires [2] has revealed the presence of a duplex fiber texture (<100>, <111>) with core/shell-like architecture. Core is mainly composed of <111> oriented grains while shell exhibits <100> and <111> oriented-grains. Diameter reduction of the micro-wires using electropolishing results in the removal - at least partly - of the shell which was found to participate significantly in the evolution of the mechanical properties leading to an apparent extrinsic size effect. In addition, in-situ tensile tests under synchrotron radiation have been carried out to get insight into the local deformation modes, especially during the elastic-plastic transition. Crystal plasticity Finite Element (FE) simulations have been carried out to assess the role of the crystallographic texture of micro-wires, as well as the core-shell structure, on the observed behavior. Virtual polycrystalline microstructures have been generated based on large EBSD maps (characterizing grain size/shape and crystallographic orientation distribution within the differing micro-wires) and on global texture measurements obtained by high-energy X-ray diffraction pole figures. Elongated grains of the micro-wires have been modeled by prolate ellipsoids combined to a close-packing algorithm. Crystallographic orientations from EBSD maps have been sampled and assigned to grains in order to achieve virtual polycrystalline aggregates whose texture and core-shell structure is representative of the differing studied micro-wires. Small strains FE computations have been carried out using Z-set. Meric-Cailletaud elasto-visco-plastic crystalline constitutive equations have been used with a grain-size independent formulation in order to isolate and assess the sole effect of crystallographic macro- and micro-texture. A special attention has been paid on the influence of the anisotropic elasticity on the stress-strain heterogeneities and on the elastic-plastic transition. Simulation results are analyzed and compared qualitatively and quantitatively to experiments.

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Plasticity and viscoplasticity / **105**

Crystal plasticity modeling of thin aluminum foil

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For thin aluminum foils, such as used e.g. in food packages, the thickness is of the same order of magnitude at the typical grain size. EBSD imaging of the cross section of the foil reveals that the foil typically has one or a few grains through the thickness. This causes the mechanical properties to depend heavily on the grain structure of the material. Furthermore, the material has an crystallographic orientation texture induced by the rolling process, resulting in anisotropic properties. In order to be able to predict and model the mechanical behavior of the foil, it is therefore necessary to utilize a model taking the microstructure of the material into account.

In the present work, a model has been developed which extracts data on the microstructure from EBSD-images to generate a statistically representative virtual microstructure in terms of grain sizes and orientation texture. EBSD analysis has been performed on both the surface of the foil and its cross section, and the information is used to create a three dimnesional model of the foil. Utilizing a Crystal Plasticity Finite Element model it is possible, using the obtained grain structure, to reproduce the anisotropic behaviour of the foil observed during tensile testing. Thus this model can be used as a tool to predict the mechanical behavior of the foil based on the observed microstructure.

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Data-driven mechanics - an alternative to constitutive modeling?

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Data analysis and data science have become fundamental domains in the past decade. Data science has not only a big impact on financial markets but also in engineering areas. Experimental measurements get increasingly reliable and data-rich. To find a description of the usually strongly non-linear material behaviour, complex constitutive laws have to be developed and fitted to the experimental measurements. An interesting alternative idea is the use of the data directly.
In our work we intend to use data from experiments to extract pairs of stress and strain to execute computations by evaluating them without constitutive model. Hereby, we bypass any kind of modelling error as well as any problem concerning parameter fitting.
Recently, in [1] a new technique for data-driven modelling for elastic materials was proposed. This effective reformulation of the initial boundary value problem divides the problem into a constraint set E and a material data set D. As the latter is no longer a continuous function the solution is obtained by minimizing the distance d between both sets.

Obviously, an extension to inelasticity must be also incorporated. The authors met this challenging problem by an extension being able to describe any kind of inelasticity in principal [2]. Material behavior which shows path-dependence can be described by a function of previous deformations. Further, many materials show fading memory properties. This extended data set can be used by a

history-matching technique which adds further components to the distance measure introduced in [1] and [2]. An important goal is that the data-driven formulation for inelasticity must be able to deal with extracted data from experiments e.g. by digital image correlation (DIC) [3].

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Optimization and inverse problems in multiscale modelling / 148

Design of bi-stable devices using topology optimization

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n this talk we discuss computational methods which is intended to be used to design structures that are expected to snap. One example of such structures are multi-stable micro-flexures that buckle to perform digital computations. Since such structures inevitably function under finite strains we model the material by general finite strain hyper-elasticity. The balance equations are solved using the finite element method in a total Lagrangian setting along with Newton-Raphson iterations. To trace the load paths and to be able to pass singular points we make use of path following technique.

To find the optimal material layout we associate one design variable with each element such that material and void can be represented. The optimization problem is then to find a material distribution such that the objective is minimized while fulfilling the constraints. In our application the objective is to find a layout that gives a stable state in terms of energy level while having distinct states, i.e. the difference in deformation between the stable states should exceed a given threshold. We also impose a constrains on the availibe mass of the device.

To solve the optimization problem we use mathemetical programming and in particular we use the Method of Moving Asymptotes (MMA). The gradients required to form the convex approximations are established via the adjoint sensitivity approach. To form a well-posed problem we reguralize the optimization problem via the use of a PDE filter.

Creep, damage and fatigue / 53

Development of a cohesive zone model for thermomechanical fatigue

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Engineering components in many high temperature applications undergo cyclic mechanical and cyclic thermal loading resulting in thermomechanical fatigue (TMF). In this study, a temperature dependent elastic-viscoplastic cohesive zone model is developed to predict the TMF behaviour of high performance metallic materials. The theory is based on rheological models and enhanced with two damage variables. The micro-mechanically motivated damage variables represent material degradation due to creep and fatigue [1] effects. The activation and evolution of the damage variables depend on strain rate and temperature. The material law captures monotonous, cyclic, dwell, thermomechanical, and time dependent loads. Damage variables interact and evolve until their sum reaches unity indicating complete damage.

The material model is used to simulate the deformation behaviour and lifetime. The lifetime predictions of total strain controlled in-phase (IP) and out-of-phase (OP) TMF simulations are compared with that of isothermal low cycle fatigue (LCF) simulations at the maximum TMF temperature. It is seen that the material under IP and OP tests can have a lower lifetime than isothermal LCF simulations. It is also observed that IP simulations at high mechanical strain amplitude have a lower lifetime than OP [2]. The OP simulations at a low mechanical strain amplitude have a lower lifetime than IP.

The developed cohesive law is implemented as a user-material subroutine in cohesive zone elements and applied to crack analysis. Creep and fatigue damage behaviour dominates the IP- and OP-TMF simulations, respectively which is in agreement with the experiments [3]. Crack growth studies are performed to understand the influence of material parameters on crack growth rate.

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Development of a novel thermomechanically coupled damage approach for modeling woven ceramic matrix composites

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Ceramic matrix composites (CMCs) as an enhancement of classical technical ceramics overcome limitations such as low fracture toughness and brittle failure under mechanical or thermomechanical loading (e.g., Chawla, 2013). Their low weight and high temperature stability makes them attractive for use in various fields, especially aerospace industry, where they improve engine efficiency as substitutions for metal components. Despite their positive attributes current CMCs lack well established material property design databases for a reliable use in critical aerospace structures. Demonstrating the durability and lifespan of this relatively new class of materials is the present task. Therefore their failure mechanisms need to be investigated further, taking into account the extensive range of temperatures the components are subjected to. This contribution deals with the successive development of a woven representative volume element (RVE) for arbitrary CMCs. In contrast to previously developed approaches, the introduced model combines various damage formulations. The fiber bridging effect is governed using a cohesive zone (CZ) (e.g., Rezaei et al., 2017) formulation to adress the debonding mechanism in the weak interface between matrix and reinforcement and a continuum

mechanical approach to account for matrix damage (e.g., Brepols et al., 2017).
To cover the temperature dependency of the material parameters, thermal coupling is included in both element formulations.

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Disclination effects on the multislip flow rule in finite crystal plasticity

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The paper proposes a new elasto-plastic constitutive model to describe the behaviour of crystalline materials with microstructural defects such as dislocations and disclinations, which is compatible with the multislip plastic flow rule, and formulates the appropriate initial and boundary value problem. Concerning the kinematics: the deformation gradient is multiplicatively decomposed into elastic and plastic components, and the so-called plastic connection with non-zero torsion and metric property is considered. The dislocation density is related to the incompatibility of the plastic distortion. The plastic connection is expressed in terms of a Bilby-type compatible connection and a disclination (second order) tensor. Concerning the energetic aspects: the macro and micro forces, as pairs of stresses and momenta, are introduced to be conjugated with the appropriate rate tensors and their gradients. They satisfy the specific balance equations. The defects are introduced in the expression of the free energy function: disclinations via the disclination tensor and its gradient, and the dislocation density tensor via Cartan's torsion associated with the plastic connection. Based on the formulated free energy imbalance principle, the appropriate viscoplastic (diffusion-like) evolution equations are derived for shear plastic rates (in slip systems) and for the disclination tensor. We mention that the multislip flow rule for plastic deformation is assumed as in classical crystal plasticity. The specific form of the microforces is computed based on the virtual power dissipated during the virtual rate plastic flow compatible with the multislip flow rule. The scalar micro-stresses related to the slip systems are expressed in terms of the Mandel plastic stress tensor, projected on the slip systems. The micro momentum vectors related to the slip systems are given by Bilby-type plastic connection (or the gradients of plastic distortion), applied to specific tensors characterizing geometrically slip systems. The slip systems are activated if and only if the appropriate yield (activated) conditions are satisfied, i.e. generalized Schmid's laws are applied. The effective reduced shear stresses in slip systems are also dependent on the dislocation density tensor and the disclination tensor. The dissipative power is reduced to the contributions due to: the power generated by the effective reduced shear stresses in slip systems on the plastic shear rates, and the viscoplastic type power generated by the driving forces associated with the disclination mechanism. The initial and boundary value problem accounts for the equilibrium equation in terms of Piola-Kirchhoff stress tensor together with the complete set of evolution equations concerning the plastic distortion tensor, the disclination tensor, the components of Bilby's type plastic connection and the shear rates. To exemplify the material behaviour we restrict to the small elastic and plastic distortions in a simple tensile problem, under the supposition that only two pairs of slip systems are active. The edge and screw dislocations are generated by the active slip systems and they are coupled with the appropriate wedge and twist disclinations. The proposed model is based on the following papers Cleja-Tigoiu Int.J.Fract.(2010), Cleja-Tigoiu MMS (2013), Cleja-Tigoiu and Pascan MMS (2013), Cleja-Tigoiu et al. (2016, 2019).

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Discontinuous Plastic Flow In The Low-Temperature Superconductors

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Low-temperature superconductors (LTS) consisting of a copper matrix and filaments (e.g. Cu/NbTi, Cu/Nb3Sn) are used in elements which work at near to 0K temperatures. The thermomechanical effect, the so-called the discontinuous plastic flow (DPF) is observed independently in a matrix and in filaments during a plastic deformation at extremely low temperatures. DPF is attributed to the mechanism of local catastrophic failure of lattice barriers (including Lomer–Cottrell locks), under the stress fields related to the accumulating edge dislocations. Failure of lattice locks leads to massive motion of released dislocations, accompanied by step-wise increase of the strain rate, and a drastic drop of stress (serrations). Moreover, the plastic power dissipated in the slip band is partially converted to heat, which results in a drastic increase of temperature promoted by the thermodynamic instability [1]. Thus, DPF is a potential factor leading to the loss of superconductivity in the magnet.

In order to investigate the behaviour of LT superconductors during plastic deformation at cryogenic temperatures, a custom built experimental set-up was used [2]. A cryostat equipped with tested specimen and the relevant transducers was mounted between traction machine grips. The kinematically controlled tests were carried out. During each test, the time responses of extensometers, force transducer and thermistor were recorded. Based on the experimental results, the physically based model of DPF in the superconducting multifilament composite was proposed. The response of stress was defined in terms of three stages within each serration cycle: elastic loading (1), smooth plastic flow (2), abrupt drop of stress (3) (Skoczeń et al., 2010). Effective stiffness modulus for each stages were estimated based on the Mori-Tanaka homogenization scheme. The model allows us to reproduce the observed serrations in the LTS, which can be crucial for its application in the design of components operating at extremely low temperatures.

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Biomechanics and biomaterials / 86

Discrete and continuum models to capture extreme kinematics of fibre network materials

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Fibre networks at various length-scales are a typical microstructure found in both biological tissues and man-made materials. The properties of the fibres, their orientation and interaction with each other and with interstitial substances in the network largely predefine the macroscopic behaviour of the network material, and furnish it with particular mechanical properties. As an example, extreme lateral contractions with large positive tangent Poisson's ratios >5 and drastic volume reductions were reported in previous work for soft collagenous tissues under tensile loads [1]. Discrete computational models of the collagen networks revealed that the strong asymmetry between the tension and compression responses of the string-like fibres with negligible resistance to compression was

key to this counter-intuitive behaviour [2]. Notwithstanding, it was shown that the seemingly unusual volume loss under tensile load is allowed for by hyperelasticity theory in agreement with thermodynamics [2].

After revisiting these results, we show in the present contribution that the particular micro-kinematics of fibre networks can, vice versa, also cause extremely pronounced auxetic behaviour with strikingly negative Poisson's ratios and enormous volumetric expansion under tensile loads. In particular, a set of experiments is presented that illustrate the auxetic behaviour of nanofibrous electrospun membranes. Based on dedicated multi-scale finite element simulations of the discrete beam-like fibre network [3], the behaviour is rationalised in terms of buckling fibre segments that undergo large sudden changes of geometry when the instability sets in. Finally, an affine and continuum structural modelling approach [4] equipped with the response of post-buckling fibres is shown to capture the main features of this striking kinematics.

Altogether, this contribution exemplifies for two particular cases of extreme kinematic effects in fibre network materials that computational discrete models help disclosing the key mechanisms, whose consideration in continuum constitutive models enables numerically efficient simulations.

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Discrete material optimization of vibrating composite structure

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The layout design of vibrating composite structure is studied by the discrete material optimization method for realizing the vibration control. The vibration of composite structure is excited by an external mechanical loading with given amplitude and frequency. The design optimization of stacking sequence, fiber angles and selection of material of the composite structure is performed simultaneously by the discrete material optimization method. Furthermore, the piezoelectric macro fiber composite is introduced as an attached layer to the vibrating structure in order to realize the active vibration control. By using the Discrete Material Optimization method, the layout design of the piezoelectric composite patches and design optimization of the stacking sequence, fiber angles and selection of fiber reinforced composite material can be performed simultaneously. Numerical examples are presented to demonstrate the effectiveness of the simultaneous design of the structure and attached piezoelectric patches.

Cosserat, micromorphic and gradient materials / 49

Dislocation Transport within a Gradient Crystal Plasticity Theory

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In this talk a finite gradient crystal plasticity theory is presented that accounts for the evolution of dislocation densities, introduced in [1], and interactions of dislocations with and their transfer through grain boundaries. For the simulation of a grain boundary behavior in between the limits of full transparency and impenetrability on the continuum scale (see, e.g., [2]) a grain boundary yield condition is introduced. As introduced in [3], a grain boundary flow rule is evaluated at sharp interfaces using discontinuous trial functions in the finite element implementation, thereby allowing for a discontinuous distribution of the plastic slip.

Taking the plastic slip on each slip system into account, an additional degree of freedom for each slip system is required. In order to reduce the degrees of freedom in crystal simulations, a simplified gradient crystal plasticity theory based on an accumulated plastic slip was introduced in [4]. For each slip system of the face-centered cubic crystal one gradient-stress associated with the in-plane gradient of the accumulated plastic slip is introduced. An approach is formulated in order to regain the computational benefit of accumulated field variables within a physically motivated framework.

Further investigations for the special case of single-slip are presented in order to discuss details of the framework. By three-dimensional finite element simulations the influence of model parameters on the mechanical response of a laminate grain structure under monotone and cyclic loading is investigated. A particular emphasis is placed on the dislocation self energy, the dislocation curvature energy and the energy which is stored on the grain boundaries.

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Dislocation based strain gradient plasticity model for prediction of length scale dependent initial yield strength

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Many experimental studies have shown a plastic strengthening effect for structural length scales approaching microstructural dimensions. Both increases in initial yield strength and strain hardening have been observed. Over the last 30 years different strain gradient plasticity (SGP) theories have been developed in order to capture these length scale dependences. However, up to now no generally accepted theory has emerged. In the present presentation, focus is directed into a physically based SGP model for initiation of plastic deformation.

The plastic behavior is governed by a dissipative part that primarily controls the hardening at moderate plastic strains and an energetic part that is of importance for the initiation of plastic flow. It is shown that a model based on the self-energies of dislocations can be translated into an internal free energy in terms of plastic strain gradients. Similarly, the dissipative part of the model is based on the Taylor model, which also gives a direct connection to dislocation theory.

In this way, a physical connection is made between the SGP framework and dislocation mechanics. It is shown that the same length scale emerges for both the energetic and the dissipative part of the model. Apart from a non-dimensional factor of the order of unity, the length scale can be defined as the Burgers vector divided by the strain for initiation of plastic deformation.

When the structural length scale approaches this microstructural length scale, strengthening effects result. The three-dimensional SGP model is specialized to the simple load cases of tensile tension with a passivation layer that prohibits plastic deformation on the surfaces as well as pure bending with free and fixed boundary conditions for plastic strain. Simulations of initial yield stress for varying thicknesses are compared to experimental observations reported in the literature. It is shown that the model in a good way can capture the length scale dependences. Also upper bound solutions are presented for a spherical void in an infinite volume as well as torsion of a cylindrical rod. The model is as well applied to derive a prediction for the Hall-Petch effect.

Atomistic/continuum transition on nanoscale / 126

Ductile deformation of core-shell architectured Si-SiC nanoparticles controlled by shell thickness

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The present study is part of a bigger project that aims to get a better description of nanomaterials mechanical behavior thanks to a better understanding, and an enriched description of the nanophase behavior [1]. We here focus on nanophase exhibiting complex architecture, like core-shell systems. Architectured nanophases are interesting in a broad range of applications as they exhibit the great interest of allowing to combine both effects of the nanophase and the one of complex architecture, either to reinforce properties or to combine multi-physics one. But, though the literature on nanostructures is quite extensive, the one dedicated to mechanical behavior is less developed [2-7] – mainly because experiments on such small systems remain a formidable task, and the one on core-shell nanoparticles is even less.
The present study is thus dedicated to the mechanical behavior of Si-SiC spherical core-shell nanoparticles at room temperature. In these systems, one could genuinely assume that the softest part, be it the core or the shell, will first yield when submitted to compression. To test this view, we have carried out large scale molecular dynamics simulations of uniaxially compressed core-shell Si-SiC nanoparticles, exhibiting different geometries.
Our first conclusion is that for the investigated size range (diameters equal or below 50 nm), the nanoparticles yield plastically with no signs of fracture, in agreement with experiments on single material systems. Furthermore, our investigations also reveal that depending on the shell thickness, plastic deformation is confined either in the core or in the shell [8]. We propose a model, based on the theory of contact mechanics and geometrical arguments, to explain this surprising result [8]. Furthermore, we find that for a specific shell to diameter ratio, corresponding to the transition between core and shell, the stress concentration in the nanoparticles is apparently hindered, leading to a delayed plastic deformation.

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Ductile failure of fiber-reinforced composites: variational model and numerical results

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Composite materials made of strengthening fibers embedded in brittle matrices (e.g., fiber-reinforced concretes) usually exhibit failure mechanisms characterized by an initial stress-hardening phase, associated to micro- and multi-cracking within the matrix, and a following softening stage, associated to the development of macro-cracks. The bridging effect of fibres plays a key role in this process, conferring improved ductility to the composite.

In the present communication, a variational model is proposed, which schematizes the composite as a mixture of two phases coupled by elastic bonds: a brittle phase and a plastic phase, accounting for matrix and fibers contributions. The model is able to capture the progressive opening of micro-cracks in regime of stress-hardening, as observed in real composites, and the subsequent stress-softening process of plastic strain localization, that leads to the final failure.

The variational procedure followed to deduce balance and evolution equations is illustrated. Attention is drawn on the role that three different internal lengths play in the description of the composite failure. Finally, results of numerical simulations are shown and discussed.

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Effect of anisotropic elasticity on dislocation pile-ups and stress-induced slip transmission at grain boundaries

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This study deals with an analytical approach based on the Stroh formalism (1,2,3) which provides the elastic fields of single straight dislocations and different dislocation pile-ups in anisotropic homogeneous media, half-spaces, bi- and tri-materials (4) while considering (or not) free surface effects (5). The tri-material configuration allows considering a non-zero thickness in the nanometer range and a specific stiffness for the grain boundary (GB) region. The configuration with two free surfaces could be used to study size effects. The effects of anisotropic elasticity, crystallographic orientation, GB stiffness and free surfaces are first studied in the case of a single dislocation in a Ni bicrystal. Image forces may arise because of both dissimilar grain orientations, the presence of a finite grain boundary region and the presence of free surfaces. In particular, it is shown that the Peach-Koehler force projected along the dislocation glide direction can exhibit a change of sign with the dislocation position (6). For pile-ups, the dislocation positions are calculated by an iterative relaxation scheme minimizing the Peach-Koehler force on each dislocation. Both GB stiffness and grains misorientation influence pile-up length and induced resolved shear stress, but the effect of misorientation is clearly seen to be predominant (6). In parallel, in-situ micromechanical tests of micron-sized bi-crystals and observations coupling SEM, AFM and EBSD are performed. Different FCC bi-crystals are obtained from FIB (focused ion beam) machining. Step height spatial variations due to localized slip bands terminating at GB are measured by AFM (Atomic Force Microscopy) to determine the Burgers vector distribution in the dislocation pile-up. Furthermore, the local misorientation along slip bands is measured by high resolution EBSD in order to determine the deformation caused by dislocation pile-up. Hence, the driving force for slip activation in the neighboring grain can be computed and compared to the observed GB resistance to slip transmission.

Key Words:
Dislocation pile-up, Anisotropic elasticity, Micromechanical testing, Grain boundary

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Atomistic/continuum transition on nanoscale / 51

Effect of chemical heterogeneity on the mechanical and structural response of CoCrFeMnNi high-entropy alloy during deformation

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The features of the chemical element redistribution near the interfaces in CoCrFeMnNi high-entropy alloy are investigated on the basis of molecular dynamics simulation. The effect of element segregation on the behavior of the alloy under uniaxial tension is studied. For comparison, systems of two types are considered: samples with 1) a random distribution of elements and 2) thermodynamically equilibrium distribution after atom swaps according to the Metropolis Monte Carlo algorithm.
The strongest segregation on free surfaces is found for Mn and slightly weaker for Ni. The fraction of Fe decreases substantially, the content of Co also decreases, and the concentration of Cr does not change. Twins nucleate and grow in samples under tension. Cr segregates on symmetric tilt grain boundaries more intensely than others, and the Mn content also increases. The remaining elements partially leave the region of a grain boundary. Stacking faults are generated in grain boundaries and then occupy all grains under tension.
Defect structures of samples with the segregation and the random distribution of elements do not differ qualitatively. However, chemical element segregation can reduce or increase stresses and strains at the elastic limit depending on the stoichiometric composition of HEA. Moreover, the difference

between these values increases as the loading rate decreases.
The work was carried out with the financial support of the Russian Science Foundation (project No.17-79-10108).

Heterogeneous materials / 99

Effective response of elastic-viscoplastic metals of strong viscous anisotropy - validation of estimates by sequential linearization method

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Macroscopic response of the polycrystalline material in the viscoplastic regime is significantly affected by the anisotropy of the single crystal. Anisotropic behaviour originates from the presence of easy- and hard-to-initiate mechanisms of plastic deformation. As demonstrated in the literature on the subject, estimation of the effective properties of such materials is a challenging task. In the frame of the mean-field methodology either the schemes based on the Laplace-transform technique or the approaches that employ the approximate linearization in a real time space are used. Validation of such approaches is usually performed by means of computational homogenization based on the FEM or FFT simulations. In the paper the verification of predictions offered by mean-field schemes based on the approximate linearization and finite element RVE analyses will be presented for crystals of strong viscoplastic anisotropy and varying strain rate sensitivity. Polycrystalline samples will be subjected to non-proportional deformation paths under the assumption of the small strain regime.

Approximate linearization of elastic-viscoplastic response offered by the sequential linearization method will be applied. According to the method the response of the Maxwell-type elastic-viscoplastic polycrystal is established by solving at each strain increment two sub-problems: creep-type one and instantaneous one. Two Hill interaction equations corresponding to two mentioned sub-problems are then formulated, in which viscoplastic incremental and elastic moduli are used, correspondingly. In the case of non-linear viscoplastic polycrystals tangent or secant linearization of the local response is performed at each deformation increment.

The standard rate-dependent crystal plasticity with the Norton-type power law is assumed as a constitutive model of the single grain. Hardening phenomenon is neglected. Viscoplastic flow is realized by the movement of dislocations on the crystallographic slip systems defined by the lattice geometry. It relates the slip rate and the resolved shear stress at a single slip system. The ratio of critical values of the resolved shear stress for easy and hard slip systems can be treated as an anisotropy indicator. The anisotropic Hooke's law is used to describe elastic response.

FE calculations are performed using AceFEM environment. The checker-board space distribution of grains is assumed in the volume element of polycrystal. They have randomly selected grain orientations which results in approximately isotropic averaged response. Each grain is divided into the specified number of elements. The non-proportional deformation path is imposed on the analyzed sample using microperiodic boundary conditions.

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Biomechanics and biomaterials / 64

Effects of aging on crack propagation in cortical bone modelled with the extended finite element method

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Healthy cortical bone tissue is both tough and strong but mechanical properties are deteriorated by age or diseases, which results in a higher risk for fracture. Bone tissue is reinforced by cylindrical osteons and crack deflection along the osteonal interfaces is an important toughening mechanism in healthy bone. This ability to deflect cracks is impaired in old bone tissue where cracks instead penetrate osteons, which results in straighter and shorter crack paths and lower fracture toughness compared to healthy bone [1]. The underlying changes that cause this behavior are not fully known and the aim of this project was to study how the fracture energy of the tissue affected the trajectory of a propagating crack.

A scanning acoustic microscopy (SAM) image of human cortical bone was used to create model geometries including bone matrix, osteons and cement line interfaces. Crack propagation was simulated with the extended finite element method (Abaqus v2017) using the modelling framework proposed in [2]. The quadratic nominal strain criterion was used to model damage in the interface and the maximum principal strain criterion was used in all other tissue components. All components were modelled as linear isotropic elastic materials. Tensile tests with high and low fracture energies (G=0.4 and G=0.05 kJ/m^2) were simulated while keeping all other parameters constant.

The results showed that the fracture energy in the tissue affected the crack trajectory. The model with low fracture energy predicted a straighter crack that penetrated the osteons, while the model with high fracture energy predicted a crack that was deflected to follow the interfaces around the osteons. The simulated crack patterns agree with what is reported from experiments [1]. However, alterations in fracture energy is not the only effect of aging and future work will, for example, also include the effect of increased porosity, to give a more comprehensive description of the effect of aging in bone.

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Optimization and inverse problems in multiscale modelling / 150

Eigenfrequency Optimization of Nonlinear Hyperelastic Structures using Element Removal

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Whereas topology optimization of linear structures is well established, topology optimization of nonlinear structures is relatively immature. For example topology optimization with respect to eigenfrequencies has been studied extensively for small deformations, whereas few have investigated this

type of optimization for structures undergoing finite deformations. In this work, we thus expand this topology optimization application to nonlinear hyperelastic bodies.

We perform the eigenfrequency topology optimization for structures that undergoes large deformations and small oscillations. This assumption allows us to linearize the system about a given load level which results in a system that is very similar to the usual linear case. The difference is that the stiffness matrix depends on the displacement field. This complicates the adjoint sensitivity analysis.

One issue often encountered when performing eigenfrequency optimization is the presence of spurious localized eigenmodes in low density regions. These localized eigenmodes are a consequence of the SIMP-penalization scheme which is applied to the material stiffness, but not on the density. A common mean for eliminating this issue has been to introduce a non-linear interpolation to the density such that the mass in low density elements rapidly tends to zero. In this work we compare this approach to an element removal method technique, whereby low density elements are entirely removed from the finite element discretization.

In the numerical examples, we minimize the displacement of the structure subject to a maximum volume constraint and a lower bound constrain on the minimum eigenfrequency. A well-posed problem is formulated by using restriction in which a minimum length-scale is imposed on the design via the Helmholtz PDE-filter. From the numerical examples we conclude that the element removal method successfully eliminates spurious localized eigenmodes. We also conclude that constraints on the smallest eigenfrequencies significantly change the structural response.

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Elastodynamic transformation cloaking

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We formulate the problems of nonlinear and linear elastodynamic transformation cloaking in a geometric framework. In particular, it is noted that a cloaking transformation is neither a spatial nor a referential change of frame (coordinates); a cloaking transformation maps the boundary-value problemof an isotropic and homogeneous elastic body (virtual problem) to that of an anisotropic and inhomogeneous elastic body with a hole surrounded by a cloak that is to be designed (physical problem). The virtual body has a desired mechanical response while the physical body is designed to mimic the same response outside the cloak using a cloaking transformation.
We show that nonlinear elastodynamic transformation cloaking is not possible while nonlinear elastostatic transformation cloaking may be possible for special deformations, e.g., radial deformations in a body with either a cylindrical or a spherical cavity. In the case of classical linear elastodynamics, in agreement with the previous observations in the literature, we show that the elastic constants in the cloak are not fully symmetric; they do not possess the minor symmetries. We prove that elastodynamic transformation cloaking is not possible regardless of the shape of the hole and the cloak. It is shown that the small-on-large theory, i.e., linearized elasticity with respect to a pre-stressed configuration, does not allow for transformation cloaking either. However, elastodynamic cloaking of a cylindrical hole is possible for in-plane deformations while it is not possible for anti-plane deformations.
We next show that for a cavity of any shape elastodynamic transformation cloaking cannot be achieved for linear gradient elastic solids; similar to classical linear elasticity the balance of angular momentum is the obstruction to transformation cloaking. We finally prove that transformation cloaking is not possible for linear elastic generalized Cosserat solids in dimension two for any shape of the hole and the cloak. In particular, in dimension two transformation cloaking cannot be achieved in linear Cosserat elasticity. We show that transformation cloaking for a spherical cavity covered

by a spherical cloak is not possible in the setting of linear elastic generalized Cosserat elasticity. We conjecture that this result is true for a cavity of any shape

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Elastostatic field distributions in cracked polycrystals

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This work is devoted to the reconstruction of the local fields distribution occuring in linear elastic polycrystals with a strong crystalline anisotropy.

Full-field FFT computations have been performed on Johnson-Mehl polycrystalline microstructures for the sound material and including various crack populations. The results indicate that the field histograms present pronounced van Hove singularities in the intergranular case, and appear somewhat smoother in the transgranular one.

Self-consistent estimates of the elastic field distributions are derived by assuming a multivariate normal (Gaussian) distributions at the phase scale (i.e. for each crystalline orientation). This is done either with the classical self-consistent model for the sound polycrystalline material, or by using a two-step homogenization scheme for the cracked polycrystal (transgranular case only). The agreement with the FFT computation is almost perfect for the uncracked polycrystal and quite good for the cracked case.

Experimental identification and material characterization / 93

Evolution of anisotropic material behavior in a pearlitic steel subjected to large shear deformations

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Rolling contact fatigue typically initiates in the highly shear deformed surface layer of railway rails. However, the material behavior of this layer is not well known. In order to investigate this material behavior, we have predeformed a pearlitic rail steel by twisting solid test bars under compressive axial loads. Thereafter, the test bars have been re-machined into tubular specimens that are used to characterize the changes of the material behavior. Changes in both the elastic and plastic properties are observed, quantified and discussed.

In the first part we evaluate the ability of different yield criteria to model the observed experimental behavior. Three anisotropic yield criteria from the literature have been evaluated: Hill (1948), yld2004-18p from Barlat et. al. (2005) and Karafillis and Boyce (1993). Their fitting abilities are compared with the estimated experimental uncertainties. The predictive abilities are evaluated by investigating how well they can predict data points not included in the calibration set, using exhaustive cross-validation.

In the second part we consider the modeling of the evolution of the microstructure using crystal plasticity simulations. The modeling is conducted in a framework specialized for modeling of biaxial loading.

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FEM-Cluster Analysis method (FCA) for Efficient Numerical Prediction of Effective Nonlinear Properties of Heterogeneous Material

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The present study introduces the theory and implementation of FCA method (FEM-Cluster Analysis Method). The computation of FCA consists of two phases. At the offline phase the reduced order model is built up by clustering algorithm in [1] and construction of the interaction matrix under the assumption of the linear elasticity. The nonlinear incremental analysis of RUC is carried out on the reduced order model, which makes the method very efficient.
For efficient numerical prediction of effective nonlinear properties of heterogeneous material, we apply the RUC method based on the well-known Hill-Mandel theory. The basic RUC model is subjected to given periodic homogeneous boundary condition and the properly distributed eigen-strain, which plays the role of the external load. In the clustering process, the RUC is divided into a number of the clusters according to the elemental strain concentration factors, which are obtained from full FEM analysis of the high-fidelity RUC subject to a set of uniform orthogonal eigenstrains over the entire RUC. The cluster interaction matrix is constructed with numerical results of the DNS subjected to uniform eigen-strain for each cluster in turn. It represents the interactions between each two arbitrary clusters in the RUC in terms of the uniformly distributed eigen-strain over one cluster and the average stress over another cluster. Its mathematical structures and physical properties are discussed. The online elasto-plastic phase of the reduced order model is performed by the incremental non-linear FE analysis using the constant cluster-interaction matrix, which plays a role in the present work conceptually similar to the initial elastic modular matrix used in the "initial stiffness method" for the traditional incremental elasto-plastic analysis. By doing so, accurate and efficient numerical prediction of effective properties of heterogeneous material in nonlinear range are fulfilled in a consistent way. The performances of the proposed reduced order model and its numerical implementation are studied and demonstrated by several numerical examples.
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Features of defect propagation in nanocrystalline nickel under shear loading

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The behavior of nickel nanocrystallites with grain boundaries under different types of shear loading was investigated. The study was carried out on the basis of the molecular dynamics method using many-body interatomic potentials.
It was found that localized nanobands with elastic lattice distortion are formed in nickel crystallites by adjacent regions which impose tensile and compressive stresses on the free surface. The collective vortex movement of atoms occurs in the region of the nanoband propagation. Grain boundaries of different types do not change the angle of lattice reorientation in the nanoband. The change in the direction of nanoband propagation is determined by the crystallographic orientations of the grains. The mechanisms of structural rearrangements in nickel crystallites with the symmetric tilt grain boundary $\Sigma 5$ (310)[001] under shear loading parallel to its plane were studied. It was shown that the grain boundary can migrate in the process of loading. The velocity of its migration can reach several hundred meters per second. Grain boundary migration begins when the shear stress reaches a critical value. The movement of the grain boundary is stick-slip in nature and is realized by a specific sequence of rearrangements of atomic planes adjacent to the grain boundary. Firstly these planes are rearranged into the structure of the grain boundary planes, and then into the structure of the growing grain. Periodic boundary conditions excluded the grain rotation. The grains of the crystallite had the same shear moduli in the direction of the applied loading due to the symmetry of the simulated grain boundary. As a result, there were no driving forces in the bulk of the material. The grain boundary migration was caused by the coupling effect. Defects of structure were not formed during the grain boundary migration in the simulated crystallite. The grain boundary migration was accompanied by a change in excess atomic volume in planes which were transformed from the lattice of one grain into the lattice of the another grain.
The work was carried out with the financial support of the Russian Science Foundation (Project No. 17-19-01374).

Coupled field problems / 161

Finite element analysis of the properties of porous PZT ceramics with metallized pore surfaces and the effectiveness of its use in piezoelectric devices

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Investigation of porous materials has gained considerable interest in the last years. These materials have been applied as active elements in hydroacoustic transducers, medical ultrasound devices, in piezoelectric generators of renewable energy, etc. Compared to dense piezoceramics, an acoustic impedance of porous piezoceramic differ less to the impedance of liquid or gas. The generated acoustic waves propagate more effectively through the boundary between the transducer and external medium. The thickness piezoelectric moduli for some types of porous piezoceramics almost do not depend on porosity, which gives higher effectiveness of the transformation of electric energy into mechanical energy. However, porous piezoceramics have one significant disadvantage related to the decrease of its strength with the porosity growth.
This paper is devoted to the investigation of materials with pore surface covered by metal or other

durable material. In the first part of the paper, the homogenization problems for microporous piezoceramics with pores fully or partly covered with a thin layer of metal are considered. To solve this problem, we use the effective moduli method and the finite element method. The representative volume is generated as a cubic array of finite elements with closed porosity. Then the pore surfaces get covered with elastic shell finite elements with the properties of metal. These surfaces were also subjected to the condition of equipotentiality for electric field, usual for the problems of electroelasticity with free electrodes.
As a result of computational experiments, we have calculated full sets of the effective moduli for porous piezoceramic with various porosity and degree of the pore surface metallization. The obtained results have shown that microporous piezoceramics with metallized pore surfaces had a range of unusual properties perspective for practical applications. For example, the effective moduli of dielectric permittivities of porous piezoceramics with metallized pore surface grow with the porosity increase, whereas for ordinary porous piezoceramics the effective moduli of dielectric permittivities decrease with the porosity growth. The most interesting fact is the growth of the absolute values of the transverse piezomoduli when the porosity increase, which is not the case for ordinary porous piezoceramics.
In order to check the effectiveness of the applications of porous piezoceramics with metallized pore surfaces, in the second part of the paper we have considered some models of piezoelectric transducers working at the thickness, transverse and shear oscillation modes. Here for the steady-state oscillations problems we have analyzed the frequency responses of the considered transducers in the vicinity of working resonance frequencies. For the modes of excitation of oscillations by the electric potential difference, the amplitude-frequency responses were obtained in the vicinity of the electric resonances, and for the modes of excitation of oscillations by the electric current, the amplitude-frequency responses were obtained in the vicinity of the electric antiresonances. Thus, the transducers made of porous piezoceramics with metallized pore surfaces have high effectiveness, especially when exciting the oscillations by electric current.

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Finite element simulations of local heterogeneous stress field in framework of hyperelastic Mooney-Rivlin materials and equi-biaxial tensile test

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The parameters identification (and/or validation) of hyperelastic models are crucial issues for mechanical design. Standard tests related with this purpose require sample geometries that can lead to homogeneous deformations. However, the parameter identification requires multi-axial biaxial test in order to ensure predictive ability of a model [1]. The material parameters of Mooney-Rivlin model can be determined using the so-called virtual field method [2]. The determination of stress state in core region of the specimen represents very critical issues for biaxial testing [3]. In fact, the biaxial test gives rise to heterogeneous displacement and stress fields. In this work, we show that the heterogeneity turns out to be an advantage. We consider a circular zone (of radius ρ) of a cruciform sample, in which the full-field displacement is assumed provide by a DIC system and the corresponding stress fields i.e. $(\sigma_{rr}(r,\ \theta)\ ,\ \sigma_{r\theta}(r,\ \theta)\ ,\ \sigma_{\theta\theta}(r,\ \theta))$ were computed by FE in the context of two cases: i) with a small hole in the center of the sample $(a \leq r \leq \rho)$ and ii) without hole in the

center of the sample $(0 \leq r \leq \rho)$. In polar coordinates, the Cauchy stresses are computed as follows:
$$\begin{pmatrix} \sigma_{rr}(r,\ \theta) & \sigma_{r\theta}(r,\ \theta) \\ \sigma_{r\theta}(r,\ \theta) & \sigma_{\theta\theta}(r,\ \theta) \end{pmatrix} = \begin{pmatrix} cos\theta & sin\theta \\ -sin\theta & cos\theta \end{pmatrix} \begin{pmatrix} \sigma_{xx}(x,\ y) & \sigma_{xy}(x,\ y) \\ \sigma_{xy}(x,\ y) & \sigma_{yy}(x,\ y) \end{pmatrix} \begin{pmatrix} cos\theta & -sin\theta \\ sin\theta & cos\theta \end{pmatrix},$$
where σ_{xx}, σ_{yy} and σ_{xy} are the Cauchy stresses in each point $(x,\ y)$, which are evaluated by FE. We have computed the Cauchy stress field in polar coordinates by varying both the radial variable $\xi = r/\rho$ and θ. We have shown that the stress field seems to be heterogeneous for the two cases (sample with or without hole). Also, the stress field does not homogeneous near core region of the sample without hole. Far the hole, the Cauchy stress field tends asymptotically towards the one without hole. In the next step, we will attempt to approximate a stress field adapted to the sample geometry to be able use the experimental data arising from equi-bi-axial tensile test to identify or/and validate of hyperelastic models.

Keywords: Hyperelasticity, Equi-biaxial tensile, heterogeneous stress field, Finite element simulations.

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First-principles study on the origin of phase stability of long-period stacking ordered (LPSO) structure in Mg-M-Y (M = Ni, Cu, Co, and Zn) alloys

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Ever since a dilute magnesium alloy in which solute atoms (Zn, Y) are enriched in a periodic stacking fault to the (0001) plane of the hexagonal close-packed (hcp) structure shows high-strength and ductility [1-3], a much attention has been paid for the studies of materials that expected to be involved in strengthening mechanisms such as kink deformation. In a class of Mg alloys with transition-metal (M) and rare-earth (RE) metal, various crystal polymorphs such as 12R, 24R, 10H, 18R, and 14H with different numbers of Mg layers between the concentrated layers of solute atoms (M and RE) are present, and these are so-called long-period stacking ordered (LPSO) structure. Furthermore, recent structural analysis using transmission electron microscopy and first-principles calculations reveal that solute elements form M_6RE_8 ($L1_2$ type) clusters in the concentrated layer of LPSO phase. It is experimentally found that the degree of regularity of solute atoms depends on the choice of M and the difference in the amount (composition) of solute atoms, which is correlated to the observed structural polymorphs. However, the origin of the phase stabilities and formation mechanisms of LPSO structure has not been clarified yet.
In this study, to understand the microscopic origin of the phase stabilities of the structural polymorphs with different compositions of solute elements, we performed first-principle density-functional theory (DFT) calculations for Mg – M - Y alloy (M = Co, Ni, Cu, Zn) with 18R and 10H structures. We found that the structural distortion of the $L1_2$ cluster is uniquely determined by the choice of M atom, and explain how the geometries of $L1_2$ solute cluster affects the electronic state of near the Fermi level that crucially determines the stabilities of LPSO phases. The origin of the partial dislocation will also be discussed by focusing on the role of solute atoms and vacancy formations.
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Cosserat, micromorphic and gradient materials / 57

Fractional Strain-Gradient Plasticity

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Prompted by the mounting experimental evidence pointing to a discrepancy between the size-dependent yield strength of metals and predictions from conventional strain-gradient plasticity (SGP), e.g. [1,2,3], we have developed [4] a new *fractional strain-gradient theory of plasticity* (FSGP) that uses fractional derivatives of plastic strain as a means of quantifying the inhomogeneity of plastic deformation.

One natural way to express the size dependent yield stress can be written $\sigma_{\rm y} = \sigma_0 \left[1 + \left(\frac{\ell}{h}\right)^{\alpha}\right]$, where σ_0 is the yield stress in tension for a large scale and well annealed specimen, ℓ is a material length scale, h is an appropriate size measure of the plastically deforming region and α is a scaling exponent. Conventional SGP almost invariably predicts a size scaling exponent $\alpha = 1$ that, in many cases, grossly overestimates the experimentally-observed values.

We take this discrepancy to suggest that the differential structure of conventional strain-gradient plasticity is overly stiff and proceed to relax the excessive rigidity by recourse to fractional plastic-strain gradients. Specifically, by allowing the free energy to depend on a fractional derivative of strain, we show that the size-scaling discrepancy between conventional SGP and the experimental data in [1,2] is resolved. When applied in the shear layer configuration, the theory predicts a size scaling relation with exponent α equal to the fractional order of plastic strain-gradient differentiation. Through this identification, the observed experimental scaling can be exactly matched by an appropriate choice of fractional differential order.

The form of the non-local fractional plastic strain-gradient contribution to the free energy is explicitly given by a double-integral representation and its fractional differential character is set simply by an appropriate choice of exponents in the interaction kernel.

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Cosserat, micromorphic and gradient materials / 40

From simple to complex defects in Cosserat elasticity

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The simple line defects including dislocations (i.e. displacement discontinuity) and disclinations (i.e. rotational discontinuity) are studied and used to construct multiple arbitrary complex defects within an incompatible Cosserat elasticity under general loading conditions including stress and couple stress pertaining to in-plane analysis. The underlying types of line defects are governed automatically based on the corresponding deformation and rotation fields and the consistent boundary conditions without any ad hoc assumption. Moreover, the higher-order framework of Cosserat elasticity is extended towards nonlocal as well as higher-grade versions. Such extension is motivated to regularize and derive realistic fields in agreement with experimental observations as well as atomistic simulations. Finally, outline for anti-plane analysis and necessary library of line defects are discussed.

Acknowledgements
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Experimental identification and material characterization / 92

Fundamental study on deformation of paste around one aggregate in specimen under compressive stress by x ray CT and DVC

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In a concrete, aggregates are important for a strength, a volume change and a durability. In Japan, there are tried to apply many kinds of waste particles as the aggregate for the concrete because of reduce of natural resource. For the reason, it needs to reconsider behavior of particles in the concrete under various environment in detail. However, there were little methods for directly measuring behavior of the aggregate and the paste around it until now.
We have a special X ray CT apparatus with loads machine. This X ray CT apparatus can give the three-dimensional reconstructed images inside the concrete under below 300 kN of the load. It will be able to be cleared behavior inside the concrete by X ray CT images scanned under different loads and a digital volume correlation (DVC).
In this study, as the first step clearing behavior of the paste around an aggregate, it was the comparisons between strain distributions around an aggregate in the paste specimen with different one particle just before breaking.
Three paste specimens of 75 mm in diameter and 150 mm in height were used. One was made by only paste. Others paste specimen had a crushed stone of approximately 40 mm in diameter in the center for modeling the paste around one aggregate.
The first scan was done for the specimen under loading 1 kN. After that the load was increased at 0.5 mm / minutes until the vertical strain before breaking. And, the load was stopped and the specimen was scanned. At last, the specimen was scanned after destruction. the radiographic parameters were

set 210 kV and 100 micro A. An integral time of a detector was 0.5 seconds. One side of a voxel cube was 0.123 mm.
In case of the paste specimen without the particle, some topical places of a shrinkage strain are placed uniformly in this cross section but the shrinkage strains are not concentrated especially. For the reason, at the breaking time, many cracks were occurred intricately without clearly position.
However, Inside the paste specimen with the crashed stone, the large expansion strain was occurred around the immediate surface of the stone. At the breaking time, the large cracks were shown along the high share strain area.
As the result of this study, if the particle was inserted into the paste, the shrinkage strains will be blocked and the share strains will be occurred around the surface of particles. And these share strain will become some cracks at breaking.

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Gradient-enhanced model for simulation of transformation patterns in pseudoelastic shape memory alloys

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Shape memory alloys, such as the polycrystalline NiTi, often exhibit a softening pseudoelastic response, which is responsible for strain localization phenomena. Accordingly, the stress-induced martensitic transformation often proceeds through formation and propagation of Luders-like bands or more complex transformation patterns based on the applied loading conditions. In order to simulate the related phenomena, we have developed a gradient-enhanced finite-strain model of pseudoelasticity [1,2]. The model employs a micromorphic-type regularization, which facilitates its finite-element implementation. Specifically, the micromorphic counterpart of the volume fraction of martensite is introduced into the model, and the regularizing gradient term is expressed in terms of this additional global variable. The approach is similar to that employed by Maziere and Forest [3] in the context of Luders bands in metals exhibiting softening-hardening plasticity. The complete evolution problem is formulated within the incremental energy minimization framework, and the resulting non-smooth minimization problem is solved using the augmented Lagrangian technique.

Thermomechanical couplings have also been introduced into the model in order to describe the loading-rate effects in a physically sound manner. Specifically, the latent heat of transformation and the dissipated energy are introduced into the heat conduction equation as a source term. Secondly, the chemical energy is assumed to depend on the resulting local temperature and thus the local temperature influences the transformation criterion.

Finite-element simulations of representative 3D problems illustrate that the model correctly represents the loading-rate effects in a NiTi dog-bone specimen under tension and complex transformation patterns in a NiTi tube under tension.

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Gradient-extended crystal inelasticity with grain boundary interaction coupled to classical decohesion

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The macroscopic constitutive properties of a polycrystalline metal depend, among other things, on the size and shape of the individual grains and on the nature of interaction along the grain boundaries. A standard way of introducing a length scale in crystal inelasticity models is by incorporating gradient variables (slip gradients) in the free energy density, which typically results in an extra set of constitutive equations (commonly denoted microforce balance in the literature, refer, for instance, to [1]). These microforce balance equations require additional boundary conditions that are thermodynamically well motivated.

In addition, the corresponding interface conditions along grain boundaries must be able to account for the mismatch of crystal orientation of the neighboring grains as well as the more conventional mechanical interaction. Most importantly, it is desirable to incorporate the coupling between the gradient (microtraction) interaction and classical decohesion that is expected at sufficiently extensive macroscopic strain levels. In this presentation, we discuss the appropriate modeling framework and illustrate our approach by numerical results obtained utilizing the Finite Element Method. In the present contribution the crystallographic structure of additively manufactured Inconel 718 is represented [2].

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Linear elasticity and viscoelasticity / 124

Green's function molecular dynamics to calculate the effect of contact roughness on sub-surface stresses

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Contact between elastic bodies with self-affine rough surfaces can be studied through various modeling techniques. The most efficient are boundary element methods (BEM) that rely on fast fourier transforms (FFT), of the type of FFT-BEM or Green's function molecular dynamics. Attention in previous work has mostly focused on determining surface fields, despite body fields are of great importance to establish when and where elasticity breaks down.

In this work we focus on analyzing the effect of contact roughness on the body fields in elastic solids, modeled using Green's function molecular dynamics (GFMD). GFMD is a modeling technique that relies on damped dynamics to find the static elastic solution of contact problems. The analysis is

performed in reciprocal space, where the displacements of different modes decouple. To date, GFMD has been applied to three-dimensional incompressible bodies subject to normal loading. In this work, GFMD is extended such that it can be applied to a compressible body under generic loading. The body fields are then calculated analytically.

Simulations are then performed to relate the roughness of the contact to the body fields. Results show that despite area-load curves are insensitive to a change in Hurst exponent, as long as the load is normalized on the root mean square gradient, the subsurface fields depend on it. Including smaller wavelength in the description of the roughness affects the depth at which the maximum stress occurs up to a given threshold, below which subsurface stresses become insensitive to variations of the contact area.

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In-situ X-ray scattering experiments to measure deformation on multiple scales

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A well-founded understanding of the deformation on different material scales is key when formulating physically sound multi-scale constitutive models. In polymer structures, the macroscopic deformation is to a large extent dependent on the behaviour of the underlying molecular structure. The deformation induced evolution of the molecular structure in polymeric materials can be studied using non-destructive methods such as X-ray scattering. However, scattering experiments give indirect information about the microstrucure and in order to interpret the experimental data, appropriate modelling tools are required.

This work presents an experimental method combining *in-situ* mechanical loading and full-field deformation measurements using digital image correlation (DIC) with X-ray scattering that enables deformation to be measured simultaneously over a wide range of length-scales. Using this technique, it is possible to measure the deformation simultaneously at different length scales within the material. Moreover, the work presents modelling tools to extract information about the deformation from X-ray scattering data.

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Influence of randomness in topology and geometry on the stiffness of different networks generated from the same graph

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Provided, a random network is an appropriate idealization for the micro-structure of a material, effective material properties are controlled to a large extent by the network's characteristics.
We consider a regular square lattice graph, assigning exactly one diagonal with random direction (/ or \) to each square, Different realizations are distinguished by means of the ratio between the numbers of diagonals of different type $\bar{\rho}$ and a regularity measure μ. The Ising model with fixed

magnetization and parameters β and $\bar{\rho}$ is used for sampling according to these characteristics.
Different networks can be constructed from the same initial graph. Truss and beam networks are obtained by interpreting edges as linear elastic trusses or beams, respectively. Beam networks of type II rely on the corresponding dual graphs. Beam networks of type I are constructed by shorten the diagonals and connecting their endpoints with the center points of the edges which define the squares.
The networks are exposed to an overall strain $\mathbb{E}$. The overall response is discussed in terms of the strain energy density W, postulating $W = f_W(\bar{\rho}, \mu)$.
For all three types of networks, W correlates in a similar manner with $\bar{\rho}$ and μ. Effective media theory is used to link these results to characteristics of matrices representing graph properties, i.e., degree matrix, adjacency matrix and incidence matrix. Strategies for interpreting our results in the light of more general networks for which such an initial graph is either unknown or doesn't even exist are discussed.

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Investigation of NiAl-9Mo fiber structures using FFT-based homogenization in a dual setting

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Computational homogenization schemes based on the fast Fourier transform [1] enable studying the micromechanical behavior of polycrystalline microstructures with complex morphology [2].
In the conventional strain-based setting, evaluating the single crystal elasto-viscoplastic constitutive law involves solving a non-linear system of equations which dominates the overall computation time. Owing to the stress-explicit formulation of the flow rule, the inverse material law is much cheaper to evaluate in the small-strain setting under certain constitutive assumptions, cf., e.g., Lebensohn et al. [2]. Based on a dual variational formulation of the cell problem, we investigate the anisotropic mechanical creep behavior of directionally solidified fibrous NiAl-Mo microstructures [4]. The performance of different advanced solution schemes is evaluated in the primal and dual setting.

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Irreversible thermal processes in a one-dimensional harmonic crystal.

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Due to the rapid development of nanotechnologies it became possible to investigate properties of materials at very small scales. In context with applications in microelectronic devices, crystalline structures are of high interest due to modern technological achievements, which make use of the unique properties of such materials as graphene, CNT's, BNNT's, etc. Their thermal properties were recently investigated and still give rise to many questions. This has led to development of wide variety of different heat conduction models. From a phenomenological point of view recent models lead to many controversies. In such models the formulation of the second law of thermodynamics should be revised. A most important issue is the selection of the independent variables for the constitutive law. This choice is dictated by the type of material and model one wants to deal with.

This work deals with the particular model of ballistic heat conduction developed on the basis of covariance analysis of lattice dynamics in 1D harmonic crystal. A thermodynamic analysis of the ballistic heat equation from two viewpoints: Classical Irreversible Thermodynamics (CIT) and Extended Irreversible Thermodynamics (EIT) is presented. The entropy is calculated for a sinusoidal initial temperature perturbation by using both approaches. A comparison between the entropy behaviors predicted for the ballistic, for the ordinary Fourier-based, and for the hyperbolic heat equation is made. A difference in irreversibility and asymptotic behavior of entropy for these three models is shown.

Using this approach, it becomes possible to bridge the gap between discreet and continuum systems and develop the continuum model which is based on the atomistic concept, consistent with modern phenomenological thermodynamics, and describe heat transport on nanoscale.

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Kinetics of dislocation induced phase ordering

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It is known that precipitation of new solid phases in a parent crystalline solid phase is assisted by the presences of defects. Typical nucleation sites for second-phase are grain boundaries, dislocations, impurities and crack tips. For example, during so-called delayed hydride cracking (DHC) in zirconium alloys, hydrogen migrates towards a crack tip to form zirconium hydrides. When the concentration of hydrogen in a Zr alloy exceeds the terminal solid solubility, at an applicable temperature, hydrides will form. However, temperature and hydrogen concentration are not the only parameters that dictate the nucleation and growth of hydrides. The evolution of hydride morphology and the type of hydride phases formed are strongly affected by the local microstructure and stress state. In DHC, hydrides are observed to nucleate in certain crystallographic directions and eventually form platelets oriented perpendicular to the applied load. Elastic stresses in solids may emanate from, e.g., crystallographic mismatch between phases, the presence of dislocations and applied loads. They affect the driving force for phase transformations. In addition, the precipitation path may be rather complex and can involve precursor, metastable as well as stable phases; all with their own crystal structure.

In the present study, we apply a phase field method to address some attributes of phase ordering near a dislocation in a generic elastic crystal undergoing phase transition. We use a three-component time dependent Ginzburg–Landau (TDGL) equation for describing the kinetics of precipitation of low-symmetry phases. The associated Landau potential comprises the elastic properties of the solid, the singularity that characterises the dislocation stress field, and the order parameter terms ensuring the stability of the phases with different symmetries. This allows us to study different scenarios where three low-symmetry phases may precipitate in the parent matrix phase. The line character of edge dislocations may justify that the study of the microstructural evolution is limited to a 2D-space. The system under consideration is quenched by introducing a single edge dislocation, with its Burgers' vector parallel to the modelled plane and the dislocation line perpendicular to it. Numerical calculations based on the finite volume method are undertaken to solve the TDGL equation. We then investigate the time evolution of the microstructure as oriented ordering takes place locally in the vicinity of the dislocation. We vary some of the coefficients of the Landau potential, thus changing the phase stability and the order of transition in the bulk material at equilibrium. For different sets of the coefficients, the influence of the interaction strength between the order parameter and displacement field is studied. The spatio-temporal evolution of the field variable is calculated until a near steady-state is reached. The results are compared with mean-field equilibrium solutions, and it is found that both stable and metastable phases evolve at the dislocation. This study is an extension of our previous work on stress-induced phase transition, in which we considered one- and two-component order parameter as field variables. The three-component order parameter is commonly used in phase field modelling of hydride precipitation in zirconium in the literature.

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Material Characterization and Viscoelastic Constitutive Modelling for Advanced Optoelectronics Sensor Packaging

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Material modelling and system simulation is an important and powerful tool for risk assessment and identification of design errors before production. Especially for optical sensor solutions for industry 4.0 or applications for the internet of things, this is critical, as they need to provide highly reliable performance at very small footprints. The packages need to withstand harsh temperature and humidity environments. Under these conditions, frequently observed failure modes include delamination, silicon die cracking, or gold wire bond breakage. In this study, we present the successful application of materials characterization and finite element (FE) modelling in package design.

Results on characterization and thermomechanical modelling of a laminate substrate based, transfer molded, microelectronic optical sensor package are presented. Material samples of a broad variety of customized materials were prepared by thermal cross-linking and characterized by dynamic mechanical analysis (DMA) and static thermo-mechanical analysis (TMA). Optical correlation methods were used to determine Poisson's ratios of polymeric thermosets with varying filler content and electrical conductivity. Engineering properties of glass fiber reinforced laminate substrates were characterized by nanoindentation and validated by DMA.
Using the obtained data, linear- and viscoelastic constitutive models were set up, which enable a finite element simulation of the stress fields caused by thermal strains. These results can be validated by means of single component testing, optical deformation measurements and direct stress measurement approaches.
Results on characterization and FE modelling of moisture uptake, swelling and diffusion into the polymeric compounds are presented. The determination of diffusion constants is described by a non-Fickian dual-step diffusion approach. For this purpose, spectrometric (FTIR-ATR) methods of monitoring the evolution of IR absorption modes were compared to gravimetric characterization

approaches. The applied methods can be used for full hygro-thermomechanical FE implementation and analysis.

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Material modelling and experimental investigation of semi-crystalline polymers at finite strains for varying degrees of crystallinity

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Thermoplastic polymers represent an important class of materials in many technically relevant applications and are well-suited for forming processes at elevated temperatures. Semi-crystalline polymers represent a subclass of these materials, which partly recrystallise, when being cooled from the melt. The mechanical properties of semi-crystalline polymers strongly depend on the degree of crystallinity, the temperature, and the moisture content. Due to these complex dependencies, a strong demand for the prediction and thus computational modelling of these materials arises.

Thus in this work, the tensile properties of semi-crystalline Polyamide 6 under large deformations are investigated for varying degrees of crystallinity, temperatures, and loading rates. To this end, digital image correlation (DIC) and thermography are employed. Based on the experimental results, a phenomenological constitutive framework at finite strains is derived in a thermodynamically consistent manner. In order to account for the biphasic nature, a rule of mixture of the energy contributions of amorphous and crystalline regions of the underlying microstructure is applied [1]. The degree of crystallinity serves as a constant input parameter. To capture the experimental findings, the crystalline phase is modelled by means of a hyperelastic-plastic material formulation based on the works [2, 3], where non-linear isotropic and kinematic hardening of Armstrong-Frederick type are incorporated. To account for the rate-depended material behaviour, the amorphous phase is represented by a hyperelastic-viscose material law in line with [4]. The model parameters are fitted in a staggered approach and the capabilities of the constitutive framework to accurately and efficiently predict the material response is demonstrated.

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Mechanics of Random Fibrous Networks: Modelling Deformation and Damage

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Fibrous networks are ubiquitous structures of many natural materials, such as cancellous bones and bacterial cellulose, and artificial ones (e.g. polymer-based nonwovens). Mechanical behaviour of these networks deviates significantly from that of traditional materials treated usually within the framework of continuum mechanics. The main reason for this difference is a discontinuous character of networks with randomly distributed fibres resulting in complex scenarios of fibre-to-fibre interactions in the process of their deformation. This affects patterns of load transfer, characterised by spatial non-uniformity and localisation.
Nonwovens are a typical example of artificial fibrous materials. Constituent fibres of their webs are distributed randomly. A discontinuous nature of random fibrous networks results in their non-trivial deformation behaviour and failure character. This study examines the effect of microstructure on macroscopic deformation and failure of random fibrous networks using a combination of experimental studies, microstructural analysis and advanced finite-element (FE) simulations. The network's microstructure was characterised in terms of its orientation distribution function obtained based on SEM and microCT images. The mechanical tests were performed at two levels – for single fibres and fabric samples. A parametric FE modelling approach – a tool to develop and characterise random fibrous networks – is also presented. It was used to incorporate microstructure of the network into the model by direct introduction of fibres (and their individual mechanical properties) according to their orientation distribution in the fabric together with a specific pattern of bond points. The model reproduced main deformation and damage mechanisms experimentally observed and provided the meso- and macro-level responses of the fabric. The suggested microstructure-based approach identified and quantified a spread of stresses and strains in fibres of the network for different levels of macroscopic stretching as well as its structural evolution during deformation and damage. The simulations also predicted changes in distributions of stresses and strains due to structural evolution and progressive failure of fibres.
In order to investigate damage and fracture mechanisms, various notches were introduced both into real-life specimens used in experimentation and discontinuous FE models specially developed [2-5] to mimic the microstructure of fibrous networks. The specimens were tested under tensile loading in one of the principal directions, with FE-based simulations emulating this regime. The developed discontinuous model with direct introduction of microstructural features of fibrous networks allowed assessment of strain distribution over selected paths in them in order to obtain strain profiles in the vicinity of notch tips. Evolution of calculated damage demonstrated a good agreement with images from experiments.

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Mechanisms of local structural transformations under uniaxial tension of iron nanocrystal

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The atomic mechanisms of nucleation and development of plasticity in an iron nanocrystal under uniaxial uniform tension along different crystallographic directions were studied. The calculations were carried out on the basis of the molecular dynamics method using many-body interatomic potentials. It was shown that dislocations and twins are the main carriers of plasticity in the nanocrystal under study. The nucleation of these defects is due to structural transformations that lead to a local change of the type of crystal lattice. Under uniaxial uniform tension along the $[1\,\overline{2}\,1]$ direction, a twin is formed in the nanocrystal. The bcc-fcc-bcc structural transformations of the crystal lattice occur at the front of their propagation. The growth of the single twin is accompanied by the nucleation of dislocations in its body. A significant number of twins are formed at the uniaxial stretching along the $[1\,\overline{1}\,0]$ direction of the nanocrystal. The bcc-fcc-bcc and bcc-hcp-bcc local structural transformations determine the propagation of twins in the nanocrystal body in this direction of tension. However, with further loading the contribution of twins to the development of plasticity decreases and a significant part of the twins are transformed into dislocations. The nucleation of plasticity has a pronounced dislocation nature at stretching of the nanocrystal along the $[1\,1\,1]$ direction. The first dislocations appear on free surfaces. The formation of subsequent new dislocations is associated with the arising of local regions with an fcc lattice in the vicinity of previously formed dislocations. The subsequent stretching of the nanocrystal leads to the escaping of a significant part of dislocations on free surfaces. In this case, a dislocation network is formed in the nanocrystal and the concentration of vacancies increases significantly.
It was found that the bcc-fcc-bcc type short-lived local structural transformations in regions with increased stresses arise at elastic stretching. Such transformations are associated with thermal fluctuations of the atomic system and their lifetime is comparable with the period of atomic oscillations. The lifetime of local regions with the fcc lattice on the front of twin propagation can be 5 or more times longer than the period of atomic oscillations and depends on the velocity of the twin propagation.
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Mesoscale modeling of grain growth in FCC metals with fully anisotropic grain boundary energy

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Local variations in grain boundary energy have a profound impact on the kinetics of grain boundary migration in polycrystals. The anisotropy of the grain boundary energy is mainly a consequence of the structure of the adjoining crystals and of the local grain boundary character. From these dependencies, a complete representation of the local grain boundary character requires five parameters: three parameters to describe the misorientation between the two adjacent crystals and two additional parameters to define the local orientation of the grain boundary plane with respect to some frame of reference. Accordingly, the grain boundary energy will tend to vary with the full set of five parameters. However, the full extent of this anisotropy is disregarded in the vast majority of numerical simulation models and properties such as the grain boundary energy are assumed isotropic and constant. If energy variations are indeed considered, it is almost exclusively done under severely limiting simplifications and assumptions. A range of different numerical methods, such as level sets, phase fields, vertex models and cellular automata, can be used for mesoscale modeling of the evolution of a grain boundary network [1]. Regardless of which approach is adopted, grain boundary energy is usually assumed either to be a constant parameter or it is taken as a quantity that varies according to a Read-Shockley type of energy model, based on a single misorientation parameter. Few numerical models consider the influence of a full five-parameter characterization of grain boundaries in evaluating anisotropic grain boundary energies.

The present work, recently published in [2], shows how numerical simulations of grain boundary migration can be performed at the mesoscale, in both 2D and 3D, based on a level set representation of the grain boundary network, while respecting the full extent of grain boundary energy anisotropy. Key components in the formulation are, for example, an efficient and simple scheme for unequivocal identification of crystal neighbors at junctions where an arbitrary number of crystals intersect. The implementation works without modifications in 2D as well as in 3D. The proposed level set formulation is also shown to provide grain boundary junction configurations that comply with classical equilibrium conditions. Full grain boundary energy anisotropy is considered by adopting a parametrization of the five-parameter grain boundary energy space, as previously proposed in [3].

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Micromechanical modeling of Greenwood-Johnson mechanism of transformation plasticity

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We propose an innovative treatment of Greenwood-Johnson's [1] mechanism of transformation plasticity of metals and alloys, based on the neglect of elasticity and the powerful kinematic method of limit-analysis. This work allow to improve numerical simulations of thermomechanical processes, such as welding or quecning. In this purpose, Leblond et al. [2] had developed a model based on a simplified micromechanical approach, restricted to the application of low stress. In the new approach the representative unit cell considered in the homogenization process includes only the mother-phase surronding a growing nucleus of daughter-phase. Thus the new model consists of a hollow sphere under loading, the external loading arising from the macroscopic stress apllied and an internal one arising from the volumetric transformation strain of the enclosed nucleus. The treatment brings considerable improvement regarding classical one model of Leblond, not only by eliminating the need for ad-hoc hypotheses of limited validity, but more importantly by extending its results to more general situations involving large external stresses, comparable in magnitude to the yield stress of the weaker phase. Furthermore, this new formulation describes experimentally renowned effects that the old analysis could not show, such as the non-linear growth effect of the plasticity of transformation according to the applied stress. The theoretical results are compared to other theories, experiments, finite element micromechanical simulations. The first results of this work are regrouped in the article [3] and show the capacities of the model and its limits. To be able to envisage a more realistic situation, we carried out microstructure calculations for a distribution of the germs of the daughter phase. This allows to highlights the effects of interaction and spatial distribution of seeds. These calculations are performed using a numerical scheme by FFT [4,5], in order to evaluate the relevance of the new model. In addition, the methodology presented paves the way to incorporation, in a future work, of the effect of anisotropies of morphologic type upon transformation plasticity; this will be done through consideration of growing nuclei of daughter-phase of more general, spheroidal instead of spherical shape.

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Micromechanical modeling of micro-crack initiation due to dislocation pile-up in the ductile-brittle transition region of ferritic steels

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The transition behaviour of ferritic steels from ductile fracture at room temperature to brittle fracture at lower temperatures and/or increased rates of loading is a complicated mechanism depending additionally on microstructural parameters. The brittle fracture behavior is herein associated with the initiation and propagation of transgranular cleavage micro-cracks, which originate at broken grain-boundary carbides due to a dislocation pile-up at these sites by the so-called dislocation strengthening mechanism. Experimental observations show, that the shape, size, and position of the carbide particles as well as the dislocation pile-up influence the initiation and propagation of the micro-cracks significantly. Therefore, a discrete finite element model which takes into account all these microstructural features is necessarily needed.

In a former study [1] the influence of the size, volume fraction, strength and distribution of carbide particles on the crack initiation and propagation was investigated by a discrete micromechanical finite element model. Furthermore, in a recent cell model study [2] an effective strain gradient plasticity model by Peerlings [3] has been used to model the dislocation pile-up in the ferritic matrix under macroscopically uniform loading conditions and potential cleavage cracking was incorporated by a cohesive zone model.

In the present contribution, the complex interaction between dislocation-pile up at grain boundaries, cleavage initiation and ductile mechanism of failure is investigated under crack tip loading conditions incorporating highly inhomogeneous deformations in the fracture process zone. A parameter study exploits the sensitivity of the macroscopic fracture toughness on changes of microstructural parameters like the strength of the constituents and the grain size.

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Micromechanically motivated inter-granular cracking in polycrystalline aggregates

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This work studies the formulation of a micromechanically motivated incremental mixed-mode traction separation relations for cohesive zone modeling and employs it for the inter-granular crack initiation and propagation in micro-forming of metallic specimens. The mathematical formulation focusses on the growth of cylindrical pores which are basically the representative volume elements (see e.g. [1]). Incremental traction-separation relations are obtained through an upper bound solution, where micromechanical parameters such as size, shape and spacing of pores describe the level of damage and linkage of the pores characterizing the propagating cracks. The obtained relations are incorporated through UEL subroutines in Abaqus for the simulation of crack initiation and propagation in microstructures where the plastic deformation in grains are attained through strain gradient crystal plasticity framework (see e.g. [2], [3]). The coupled, nonlocal crystal plasticity model runs in the bulk park through Abaqus UEL routines as well. The numerical examples illustrate the size, grain boundary condition, and orientation distribution dependent cracking in three dimensional micron-sized polycrystalline examples. Moreover, the fracture behavior of the material through micromechanical parameters such as porosity are addressed as well.

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Micromorphic homogenization of mechanical metamaterials

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Mechanical metamaterials are generally multi-scale ‘designed’ materials, whereby the microstructure entails emergent unconventional effective engineering properties. Nowadays, remarkably complex mechanistic responses can be achieved, e.g. converting compression to twist, or converting progressive instabilities into motion. Mechanical metamaterials do not trivially satisfy the classical scale separation principle that underlies conventional homogenization strategies. Upon loading, these microstructures develop fine scale fluctuation patterns that directly influence the coarse scale

behaviour. These emerging patterns reveal long range order in the microstructure. This behaviour has a pronounced twofold influence on the macro-scale mechanical response: (i) the coarse scale behaviour no longer depends on the average deformation and stress state only; (ii) strong size effects emerge, since boundary conditions may significantly constrain the developing patterns.
This contribution presents a micromorphic homogenization framework for mechanical materials exhibiting such multiple geometric pattern transformations [1]. Cellular elastomeric materials typically reveal these mechanisms as the result of local microstructural instabilities. Multiple pattern transformations may emerge as the result of the applied load (e.g. compression in two orthogonal directions). A micromorphic computational homogenization framework [2] is here presented, which is extended in order to capture multiple pattern transformations, either in space or in time. The proposed solution ansatz consists of a smooth part, an uncorrelated micro-fluctuation field and multiple spatially correlated fluctuating fields. These correlated fields are determined from the computed bifurcation models, whereby their amplitudes constitute a (phase) field variable in the micromorphic continuum at the coarse scale. An example will be presented, revealing three distinct geometric patterns, including the experimentally observed flower-like pattern observed for these microstructures. It will be shown that the homogenization approach adequately captures the full-scale solution. Moreover, size effects due to constrained boundary layers and loading cases resulting in mixed modes in space and time are also studied, again compared with full-scale reference numerical simulations.

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Microstructure-based numerical analysis of deformation and fracture in metal matrix composites and coatings

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Plastic strain localization, fracture and residual stress formation in aluminum substrate with "aluminum matrix/substrate – carbide particles" composites and coatings subjected to thermomechanical loadings are investigated.
Plane strain material deformation across micro-, meso- and macroscales is simulated numerically by the finite-difference method. Constitutive models include elastic-brittle and isotropic elastic-plastic response of ceramic particles and metal matrices/substrates, respectively. Experimentally observed microstructure of the coated material is taken into account explicitly in calculations. Formation of local regions experiencing bulk tension under compression of the composite material is simulated to control crack initiation and growth in ceramic particles, with the irregular geometry of matrix-particle and coating-substrate interfaces being of a major factor of stress concentration. Effects of the coating thickness and distance between ceramic particles on the macroscopic strength of the composite and coated materials are studied.
Combined experimental-numerical technique is proposed to generate 3D microstructures of metal-matrix composite and coated materials. The procedure is based on the assumption for scale invari-

ance of rock grinding mechanisms and implies 3D camera shooting of macroscopic chip stone surfaces to simulate complex shape of ceramic particles. 3D microstructure models of materials with metal-matrix composite coatings were created. 3D thermomechanical problems were solved by the finite-element method, using ABAQUS Standard and Explicit. Formation of residual stresses and local tensile regions under cooling from the melt point to room temperature, compression and pure shear of aluminum microvolumes containing a carbide particle was studied.

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Microstructure-based simulations for mechanical behavior of additively manufactured aluminum alloys

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Additive manufacturing (AM) is an innovative technology which enables producing structural components of complex geometry. Although considerable progress in this field has been attained in the past few years, many problems remain to be unsolved yet. Particularly, there is still a great deal to learn about the deformation and fracture mechanisms developing in AM materials since their microstructure and mechanical properties are much different from those of as-received materials. The numerical analysis with explicit consideration of the material microstructure seems to be a reasonable tool for analyzing the AM material behavior which is difficult to be predicted within macroscopic models.
This paper presents a computational approach to investigate the deformation behavior of aluminum alloys produced by selective laser melting with an explicit account of the grain structure. In order to construct the microstructure models two approaches are used. First approach relies on the mathematical description of the microstructure evolution during AM, taking into account physical processes involved. The numerical solution is based on a combination of the finite difference method for modeling AM thermal processes and the cellular automata method for describing the grain growth. Another approach provides fast generation of synthetic 3D microstructures typical for AM aluminum alloys, using the method of step-by-step packing. The grains are associated with the crystal plasticity-based constitutive models taking into account the microstructure and texture effects. The microstructural constitutive models are then used as input data in the boundary-value problem. The combined effects of the grain structure, texture and loading conditions on the evolution of the microscale stress-strain fields in AM aluminum alloys are analysed.
This work is supported by the Deutsche Forschungsgemeinschaft (Grant No. PL 584/4-1) and the Russian Foundation for Basic Research (Grant No. 18-501-12020).

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Modeling coupled nonlinear response of smart viscoelastic materials and composites

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During the service life of smart viscoelastic materials and composites, the temperature rise caused by the self-heating under cyclic loading greatly affects their performance. It is imperative to investigate and understand the role of each influencing factors on the energy dissipation.
Passive viscoelastic materials such as polymer dissipate energy under cyclic mechanical loading and their temperature increases due to viscous behavior. Monolithic ferroelectric ceramics experience hysteretic polarization response under cyclic electric fields and dissipate energy. Recently, ferroelectric ceramics of fibrous and particle shapes are being embedded in polymer matrix to create flexible smart composites. In such multifunctional composites, both ferroelectric inclusions and viscoelastic matrix can dissipative energy when subjected external electrical and mechanical stimuli, which is converted into heat and thus increasing the temperature of the composites. The properties of materials generally depend on temperatures; thus, the dissipative effect leads to a fully coupled electro-thermo-mechanical response in smart composites.
This study presents a thermodynamically consistent constitutive modeling framework to predict the fully coupled time-dependent thermo-electro-mechanical behavior of monolithic materials. The proposed framework allows to analyze the evolution of time-dependent field variables due to fully coupled heat conduction and nonlinear electro- thermo-mechanical deformation of dissipative materials and structure. As an example, a viscoelastic polymeric beam under cyclic loading is considered and the temperature, stress and strain evolution is presented. The proposed constitutive structure can be easily incorporated into a micromechanical modeling framework to predict the effective electro-thermo-viscoelastic response of smart composites containing more than one dissipative constituent. A simplified micromechanical model is also proposed that takes into account the dissipation of energy from the viscoelastic constituents and hysteretic polarization response of ferroelectric ceramics. The studied active composite comprises of ferroelectric fibers dispersed in polymeric matrix. A nonlinear rate-dependent constitutive model for describing hysteric polarization and strain responses is used for the ferroelectric fibers, while the matrix is assumed to follow linear viscoelastic response. The constitutive model for the heat flux follows the classical Fourier law. The integrated micromechanical-FE framework is used to analyze coupled heat conduction and deformations of smart composite structures. The effect of frequency, amplitude of strain and strain on the energy dissipation is presented and the evolution of micro-macro field variables in the smart composite is analyzed. It was found that that polymers under mechanical loads and fibers under electric fields generates a lot of heat, and its energy dissipation density increases with the increase of loading amplitude and frequency. The surface temperature of the specimen due to energy dissipation increases nonlinearly at first cycles and then stabilizes. The hysteretic temperature rise of composite under different loading conditions can be predicted via FE simulations.

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Modeling evolving anisotropy using second order orientation tensors

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The Evolving Microstructure Model of Inelasticity (EMMI), a dislocation based finite deformation internal state variable model is extended to incorporate the effects of anisotropy. Following the approach of Prantil et al. an Orientation Distribution Function (ODF) based upon a texture vector is expanded into an infinite series of increasing tensorial order. The tensor is truncated to second order and the closure methods of Advani and Tucker results in a temporal evolution equation for the second order "structure" tensor. Choosing a specific form for the ODF to represent an extreme texture yields a power series that is well represented as the inner product of the structure tensor and the direction of current inelastic flow which is incorporated in the evolution equations of the hardening variables. The resulting model is compared with the anisotropic yield surfaces from the

experimental work of Brown, the evolving anisotropic hardening differences between compression and torsion for 304L SS, the large load path change experiments of Armstrong et al. and axial effects in large strain torsion experiments.

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Modeling of Hydrogen Absorption in a high pressure metal hydride storage tank via FEM simulation

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Hydrogen presents a viable option for long distance mobility and strategic energy storage with a huge potential over battery based e-mobility concepts. One of the biggest problems preventing the widespread application of hydrogen today is the storage of large quantities of hydrogen in a light, small and inexpensive container.
The storage of hydrogen by chemical absorption in a solid material, for example using transition metals forming metal hydrides, leads to higher volumetric densities compared to high pressure tanks. Combining high pressure and metal hydride storage increases the hydrogen capacity even further; therefore, such hybrid tanks present a very attractive storage solution. In such a tank, metal powder or pellets fill the tank, such that a sufficient void fraction is achieved to facilitate hydrogen flow and the expansion of the metal hydride bed during the absorption process. Absorption is an exothermic chemical reaction, and the reaction rate depends on temperature. In addition the metal hydride expands upon hydrogen uptake, thus the mechanical loading must be taken into account. One can see that the complex thermo-mechanical behavior during the chemical hydrogen absorption process under high-pressure needs to be thoroughly understood to design efficient and effective storage tanks.

A novel simulation model is developed, capable of simulating the hydrogen absorption process, including the heat flux of the reaction and the expansion of the solid material under high hydrogen pressures, accounting for real gas compressibility.
For this, the tank content (metal hydride and hydrogen) is modeled with finite elements as a homogenized two-phase material including a solid phase and a fluid phase, with the fluid pressure as an additional degree of freedom at the finite element nodes (besides temperature and displacement). In the model, the following effects are included:
- elastic deformation
- thermal expansion
- thermal conduction and convection
- hydrogen flow
- reaction heat as body head flux
- hydrogen absorption as seepage flow

After presentation of the model, a simplified tank with a steel outer hull and aluminum tubes containing the metal powder (so-called *tube in shell tank* design) is modeled via FEM simulation. A parameter variation on the tank design shows the absorption performance of such a system can be increased by optimizing the heat transfer from the internal tubes to the environment. Compared to the initial tank design for low pressure absorption an increase in the reacted fraction after 300 s of 400% is achieved by using high-pressure hydrogen and an optimized heat transfer system.

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Modeling of bainitic transformation by coupling phase-field, mechanical and diffusional contributions

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The bainitic transformation is one of the most complex transformations in steel. The transformation from austenite to bainitic ferrite is assumed to be displacive [1] in contrast to the pearlitic growth which is highly dependent on the carbon movement and therefore is ranked as a diffusive transformation. However, regarding the whole microstructure named bainite, consisting of bainitic ferrite, carbides and (residual) austenite, the movement of the carbon is of major importance. The displacive and directed growth of the bainitic ferrite leads to a supersaturated phase. In lower bainite the carbon within the ferrite separates [2] and precipitates as carbides. In upper bainite the carbon leaves the supersaturated bainitic ferrite and diffuses across the interface into the austenite. This may lead to carbides close to the interface between ferrite and austenite but may also stop the transformation from austenite to bainitic ferrite and produce residual austenite. In this work the phase field method is utilized to simulate the phase transformations of upper and lower bainite, including the phase transition from austenite to bainitic ferrite and the precipitation of carbides [3]. The directed growth of the bainitic ferrite is modeled by coupling the phase field equations to the mechanical equations and considering eigenstrains. Furthermore the phase field equations are coupled to a diffusion equation governing the carbon concentration. The underlying system of partial differential equations is based on a thermodynamic framework of generalized stresses for a two phase Ginzburg-Landau system and a Cahn-Hilliard equation [4]. We extend this framework for multiphase field models coupled to a viscous Cahn-Hilliard equation with diffusion across the interface and mechanical contributions [5]. The numerical examples show the qualitative mechanism of the upper and the lower bainitic transformation unified in a model as discussed above.

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Modeling of the cyclic deformation behavior of austenitic TRIP-steels

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The mechanical behavior of TRIP-steels (TRansformation Induced Plasticity) under monotonic loading conditions has been studied extensively both experimentally and by continuum mechanical modeling. The cyclic response received far less attention, although the mechanically induced martensitic phase transformation highly affects the cyclic deformation behavior [1,2]. A considerable cyclic hardening is observed in cyclic deformation curves, which evolves equivalently to the volume fraction of strain-induced martensite.

In the present contribution a phenomenological material model is proposed, which is able to capture these effects. The model is motivated by a rate independent two-surface plasticity approach proposed by Hallberg et al. [3] for monotonic loading. The first surface describes plastic yielding, whereas the second surface is of Drucker-Prager-type and represents the mechanically induced phase transformation. The formulation of the plastic behavior incorporates nonlinear kinematic hardening. The model is calibrated based on a consistent set of cyclic deformation experiments with constant strain amplitude. Results of the simulations, their qualitative and quantitative agreement with the experimental data as well as the capabilities and limitations of the model are discussed.

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Modeling of the oxidative aging of bitumen : a multi-scale and multi-physics problem

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Among other distress types that affect the service life of bitumen, especially in road applications, oxidation is considered one of the most complex phenomena. The complexity lies in its multi-scale and multi-physics nature.
For the oxidative aging process two reactions have been proposed. The first, fast-spurt reaction is related to the short-term aging during bitumen production, whereas the second, slow reaction path is responsible for the long-term aging during service life of road infrastructure.
Recently, a reaction-diffusion model has been derived in the framework of thermodynamics of irreversible processes (TIP). It manages to bridge between continuum theory and molecular scale. The model is able to account for oxidation mechanisms at molecular scale, with the assistance of activity models. In addition it can distinguish between different bitumen compositions.
An inspection of the potential of the existing model will be presented in short. More specifically, certain aspects and obstacles of modeling will be discussed using physically meaningful parameters such as molar fractions, molar volumes, solubilties etc. These fundamental information are obtained via corresponding chemical analysis, e.g., SARA fractionation. We discuss exemplary the influence of solubility on diffusivity, as well as the results of a sensitivity analysis with regards to the different parameters of the model.
The model so far accounts only for the spurt reaction. Herein, a first version of a model incorporating both reactions, is presented. The slow reaction-diffusion mechanism is rather complex due to its multipath chemical nature and its interdependence on the fast reaction.

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Modelling of cyclic plasticity and phase transformations during repeated local heating events in pearlitic steels

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Short term local friction heating in railway operation might occur when a railway vehicle's wheelset skids along the rail (for example in emergency braking). The consequent temperature elevation might be significant, up to 1000°C, and in the pearlitic rail and wheel steels this results in phase transformations. The temperature dependent differences in thermal expansion, density and mechanical properties between the phases result in residual stresses which can cause thermal damage in railway rail and wheel steels.

Previously, within our research group, Finite Element (FE) modelling incorporating phase transformation kinetics describing transformation and evolution of volume fraction of austenite, martensite, pearlite, ferrite, cementite and bainite has been developed. The mechanical behavior of these phases has been modelled using a plasticity model with isotropic hardening. The FE modelling has included the coupling between a thermal and mechanical analysis in order to compute residual stresses in the vicinity of the wheel-rail contact. The modelling of the kinetics and the mechanical behavior of the phases are improved in the current study, with the purpose to increase the accuracy of the predicted residual stresses in railway applications. The strains in each individual phase are calculated separately. To capture the dilatation effects on martensite tempering, two distinct un-tempered and tempered martensitic phases are introduced.

The experimental results for cyclic loading of pearlitic steels show that kinematic hardening is dominant. In this regard, the mechanical behavior of the phases is modelled by a plasticity model accounting for mixed nonlinear isotropic and kinematic hardening. In addition, identifications of the plasticity model parameters for ferrite, pearlite and martensite phases are conducted. The model is able to mimic test data from two heating cycles in a dilatometry experiment by accounting for phase transformations and phase dependent thermal expansion. The predicted residual stress fields generated due to heating events are reasonable and agree well with experimental observations.
Finally, the influence of rolling contact loading on the residual stresses, induced by friction heating, is investigated. The results show that over-rollings reduce the level of generated tensile residual stresses.

Nonlinear elasticity / 39

Modelling of hyperelastic material accounting for the Mullins effect

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Load bearing bonds become increasingly common in glass-façade structures. This is due to their beneficial characteristics, such as the more continuous load transfer between glass and the supporting elements compared to alternative connections, and the possibility to enable a more transparent design [1, 2]. Utilized adhesives show rubber-like, hyperelastic material response under large deformations. During experimental investigations stiffness reduction is observed referred to as Mullins effect.

Until now, German regulations for the dimensioning of load bearing bonds include very high safety factors [3] which could be reduced by using a more sophisticated prediction of the real material behaviour [4]. To provide better predictions, a material model representing the complex behaviour mentioned above is needed to enable a less time consuming and less cost intensive realistic calculation and design.

Many material models are available in literature; nevertheless, most of them are not able to simulate the described material behaviour, namely large deformations combined with stiffness reduction and multiaxial stress states. To overcome this issue, a new model is developed, which is based on the

Ogden formulation for hyperelastic materials. In the presented model, an internal variable is defined, which describes stiffness reduction during loading and unloading procedures. For the calibration of the corresponding material parameters different experiments such as simple tension, equibiaxial tension, and pure shear are considered during the fitting procedure. For validation, several examples, taking into account multiaxial stress states, are analysed and discussed.

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Keywords
Hyperelasticity; rubber-like material; stiffness reduction; Mullins effect; large deformations; material modelling

Heterogeneous materials / 134

Modelling the seismic velocities and anisotropy of polar ices exhibiting various microstructures: interplay between lattice preferred orientations, air pores, melt, and rock debris

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The interpretation of earthquakes produced by very large glaciers in Greenland and Antarctica (so-called icequakes), due to iceberg calving at the glacier terminus, crevasse opening, and/or sliding of the glacier over the bedrock, requires an accurate knowledge of the seismic response of polar ices. The effective elastic properties of polycrystalline ice, and associated seismic response, possibly anisotropic, strongly depends on the ice microstructure. For polar ices, important microstructural features include (i) the strongly pronounced crystallographic texture (LPO) with grains c-axes typically oriented towards the in-situ vertical direction or aligned with the vertical plane, (ii) the open porosity in the firn (down to ~100m depth), (iii) the air bubble (closed porosity) down to ~1000m depth, (iv) melt pockets in temperate ices, and (v) the inclusion of sand/rocks coming from the bedrock erosion in the ~100m bottom layer. All these microstructures are associated with a large mechanical contrast in the material.To estimate the seismic response of such ices, we make use of a mean-field homogenization model (elastic self-consistent model) that allows estimating the effective elastic properties of polar ices with respect to the microstructural parameters, and the interplay between these parameters. Associated anisotropic seismic response will be discussed and compared with observations.

Biomechanics and biomaterials / 91

Multiscale and multiphasic modeling of skin mechanics: Rationalizing experimental observations across length scales

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The mechanical properties of the human skin determine not only its essential protective function as the barrier to the outside world, but also the microenvironment of dermal cells. The macroscopic deformation behavior of skin tissue is characterized by the interaction between the collagen fiber network and the interstitial fluid, resulting in fiber alignment and large but reversible volume reduction upon tensile loading [1, 2]. Investigations on the local properties at the micrometer scale have shown that the extracellular matrix offers an extremely compliant cell environment, with apparent stiffness in the order of 1 kPa, measured by means of atomic force microscopy [3]. In *in vitro* cell cultures, this order of magnitude of the substrate stiffness was further shown to promote cell behavior similar to *in vivo* conditions [3]. In contrast, macroscopic tensile tests typically report skin stiffness in the order of MPa; such order-of-magnitude differences between microscopic and macroscopic measurements have been found for several soft biological tissues [4].

In this contribution, we investigate the observed scale dependence of soft biological tissue mechanical properties with focus on the human skin. Recent uniaxial characterization of skin at the macroscale [1] is combined with indentation tests at intermediate length scales to bridge the gap between macro- and microscale measurements in literature. The experimental results are rationalized using a mixed discrete-continuum model, containing a discrete representation of the collagen fiber network [2], parametrized using histological and macroscopic [1] data, and coupled with a continuum representation [5] of the embedding ground matrix.

Subjected to homogeneous displacement boundary conditions, the homogenized response of the mixed discrete-continuum model is shown to well-represent skin behavior under uniaxial tension. Simulations of indentation tests across length scales reveal the influence of the fiber characteristics on the scale-dependent stiffness, and model predictions are compared with experimental data. Furthermore, our analysis highlights important aspects of the experimental characterization and data analysis of soft tissues, shedding light on the differences in apparent stiffness reported by different investigators at both ends of the length-scale spectrum.

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Experimental identification and material characterization / 79

Normal traction-separation law and mixed mode loading

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A thermodynamically consistent interface model is generalized to predict arbitrary mixed mode loading histories. The model, only, makes use of a normal cohesive traction-separation law defined by the material's fracture energy, tensile strength and a dimensionless parameter. A master curve is established from these three quantities, with the shape of the law given by the dimensionless parameter. Calibrating the interface model for normal mode loading, it is demonstrated that the interface model predicts experimentally obtained cohesive traction-separation curves reported for a polyurea and two epoxy adhesives subjected to different temperatures and loading rates at shear mode loadings. The dimensionless parameter is found to determine the shape of the fracture curve and is invariant to mixed mode loading, temperatures and loading rates.

Cosserat, micromorphic and gradient materials / 29

Notes on high order continuum mechanics on manifolds

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For the general geometrical setting of differentiable manifold, stress theory for continuum mechanics of order k may be described as follows. One constructs the configuration space of all C^k embeddings of the body manifold into the space manifold as an infinite dimensional manifold, and defines forces as continuous linear functionals on the space of virtual velocity fields—elements of the cotangent bundle of the configuration space. Then, a mathematical representation theorem implies that forces are represented by vector-valued measures that generalize the hyper-stress object. The expression for the representation of a force by stresses is a generalization of the principle of virtual work in continuum mechanics. We recall that the jet of a vector field is the invariant mathematical object on manifolds that contains both the values of the vector field and their first k derivatives as one entity. It is emphasized that for the geometry of general manifolds, the higher derivatives cannot be separated invariantly from lower ones. Thus, the representation theorem states that the action of the force functional on a generalized velocity field is equal to the action of the hyper-stress on the k-jet of the velocity field. While a force on a body cannot be restricted to sub-bodies, just as in the standard formulation, a hyper-stress induces a unique force system on the collection of sub-bodies. It is noted that the collection of C^k-configurations (embeddings) is open in the infinite dimensional manifold of all C^k-mappings for all $k \geq 1$. Thus, force and stress theory emerge naturally from the kinematics.

For the case where the hyper-stress measures are given in terms of differentiable fields and $k = 1$, one can extract from the stress object a tensor field that determines the traction on the boundaries of sub-bodies. Furthermore, one can perform an extension of "integration by parts" and obtain an analog to the classical differential equations of equilibrium. However, if $k > 1$, the extension of the process of "integration by parts" is no longer available. Thus, the traction and differential equations cannot be obtained.

As a partial remedy to this situation, we show that forces can be represented also by objects to which we refer as non-holonomic hyper-stresses. While hyper-stresses act on k-jets of velocity fields, non-holonomic stresses contain more information as they act on the k-times iterated jets of velocity fields. To illustrate the nature of iterated jets, we consider the 2-iterated jet. As the value of a 1-jet field at a point consists of a vector and a linear mapping, the value of a 2-jet field at a point consists of a vector, a linear mapping and a symmetric bi-linear mapping. On the other hand, the value of the second iterated jet at a point consists of the value of the first iterated jet at that point—a vector and a linear mapping—and the value of its derivative—another linear mapping and a bi-linear, not necessarily symmetric, mapping. Such a representation, allows in the smooth case, an integration by parts and computation of hyper-tractions.

Heterogeneous materials / 25

Numerical Modelling on Nanoscale Stiffness and Strength Behaviour of Supercrystalline Nanocomposite

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The main goal of this work is the implementation of a numerical model to investigate the mechanical properties of matrix-inclusion nanocomposites, particularly the stiffness behaviour and damage mechanisms. The supercrystalline nanocomposite investigated in this work consists of iron oxide nanoparticles and crosslinked oleic acid molecules, and it exhibits the highest stiffness and strength properties amount synthetic organic/inorganic nanocomposites to date [1]. Since experiments are expensive and time-consuming and some material parameters are difficult to determine, numerical modelling plays an important role in investigating nanomechanical properties of this material.

According to experimental observations, representative volume element (RVE) models are defined with a face-centered cubic (FCC) arrangement of the particles. While the stiffness of the particles can be assessed easily, the stiffness of the organic part is not measurable experimentally. Therefore a thorough study of various material properties and particle shapes has been conducted to meet the experimental results of composite micro-testing.

Furthermore, a sensitivity study shows that small changes on the RVE lattice do not significantly alter the overall stiffness behaviour, and, thus, suggests that such changes are not relevant to the experimental data scatter of this supercrystalline nanocomposite.

For the damage study, a cohesive zone model is applied along the nanoparticle-ligand interface, and a continuum damage model is applied for the organic matrix. The overall strength behaviours of RVE models, considering different particle geometries, are studied to gain more knowledge about the damage mechanisms of this nanocomposite, which cannot be identified experimentally. Additionally, defects, which are expected to explain the experimental data scatter, are introduced in RVE models to assess their influence on the overall strength behaviour.

Plasticity and viscoplasticity / 142

Numerical analysis of interactions between twins and precipitates in HCP alloys

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Magnesium alloys are gaining more attention in present days due to their appropriate combination of density and stiffness which makes these materials suitable for lightweight applications. However, formability of magnesium alloys is affected by the presence of twinning deformation that is induced by the lack of slip systems. Initiation and evolution of twinning can be influenced by the presence of precipitates in the microstructure. The interactions between twins and precipitates are not yet fully

understood. The present study is focused on a numerical analysis of twin-precipitate interaction. The evolution of stress and strain fields in the twined region are studied with respect to twin and precipitate geometry.

Numerical aspects of material modelling / 9

Numerical aspects of micromechanical fatigue simulations of FRP - Limits of degradation and adaptive cycle jump approach

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Finite element based micromechanical fatigue damage models are a promising approach for getting a deeper insight into the underlying physical principles of fatigue damage in fibre reinforced plastics (FRP). The fatigue damage behaviour of FRP is very progressive and accompanied by load redistributions. Capturing these effects requires a transient analysis in conjunction with the usage of progressive damage models. In addition to this, for economic needs, the FE simulation should be computationally efficient. To meet the different and partly contrasting demands on fatigue damage analyses, the most models make use of numerical tweaks. For example, considering the fully damaged state of a material point, the material parameters are tried to be reduced to zero, but – for numerical convergence and stability reasons – they are degraded to a small fraction of the initial properties, only. Additionally, besides the gradual material degradation depending on the number of applied load cycles, also sudden failure within a load cycle due to exceeding the strength limit of the material may takes place which, nevertheless, is not considered in each micromechanical fatigue damage model. Although a transient analysis tracking the cycles of the fatigue load is necessary, passing through every single cycle is computationally extremely expensive. A solution to this challenge is the cycle jump approach introducing another numerical parameter: The cycle jump determines the number of cycles over which the damage state is extrapolated.
Regardless of the underlying damage model quality, the aforementioned parameters might have such a high influence that they might spoil the overall model quality and predictability. Thus the influence of the following numerical parameters on the obtained progressive damage behaviour of FRP is investigated for transverse tensile fatigue loads: 1) whether or not the model considers static failure within a simulated load cycle, 2) the degree of material property degradation after sudden failure and 3) the size of the cycle jump. The simulated damage behaviour is evaluated using experimentally observed crack patterns published in the literature. The results reveal a significant influence of the degree of material degradation and of the cycle jump on the simulated matrix crack formation at both, higher and lower fatigue loads. Static failure within a simulated load cycle primarily affects the damage behaviour at higher fatigue loads. The presentation gives recommendations of the parameter choice for plausible progressive fatigue damage simulation results. Regarding the cycle jump, an adaptive algorithm is proposed and implemented. This approach leads to plausible fatigue damage results paired with a significant reduction of computation time comparing to a cycle-by-cycle analysis.

Creep, damage and fatigue / 74

Numerical implementation of an anisotropic continuum damage model

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In this talk, a thermodynamic formulation for modelling anisotropic damage of elastic-brittle materials based on Ottosen's 4-parameter failure surface is proposed. The model is developed by using proper expressions for the Gibbs free energy depending of two second order symmetric tensors - the stress tensor and the damage tensor - and the complementary form of the dissipation potential. The theory of invariants is utilized in constructing the potential functions. The formulation predicts the basic characteristic behaviour of concrete well and results in a realistic shape for the damage surface. Implementation of the model to the finite element program ELMER as a material model subroutine has been carried out. Simulation results for some well known test-cases will be shown.

Plasticity and viscoplasticity / 14

On material-convective elasto-plasticity

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The modelling of finite elasto-plasticity must be based on proper strain tensor definitions—for the total strain e contributions as well as for the partial (elastic ${}^{e}\mathsf{e}$, plastic ${}^{p}\mathsf{e}$, ...) ones. The six internal degrees of freedom of a properly defined symmetric (total or partial) strain tensor may be interpreted as three principal values (eigenvalues) and three orthogonal principal axes (eigendirections), whose eigenvalues are functions of the present and reference edge lengths of the corresponding present $d\hat{v}$ and reference $d\hat{V}$ principal infinitesimal volume elements. For rate-type theories of plasticity, the plastic strain tensor ${}^{p}\mathsf{e}$ must be integrated from the plastic flow rule ${}^{p}\dot{\mathsf{e}}^{GN}$ translational- and rotational-convective with the material. The material-convective translation speed of a material point $\mathbf{x}$ (particle) is given by the material velocity $\mathbf{v}=\dot{\mathbf{x}}$ and the material-convective rotation speed by the antisymmetric material spin tensor $\Omega=-\Omega^{T}=\dot{\mathsf{R}}.\mathsf{R}^{T}$, which is the Eulerian time derivative of the material rotation tensor R. The material rotation tensor follows from the polar decomposition of the deformation gradient $\mathsf{F}=\mathsf{v}.\mathsf{R}=\mathsf{R}.\mathsf{U}=\hat{U}_k\hat{\mathbf{e}}_k\otimes\hat{\mathbf{E}}_k$ into the proper orthogonal (orthonormal $\mathsf{R}^{-1}=\mathsf{R}^{T}$ and right-handed $|\mathsf{R}|=1$) rotation tensor $\mathsf{R}=\mathsf{R}^{-T}=\hat{\mathbf{e}}_k\otimes\hat{\mathbf{E}}_k=\sqrt{\mathsf{F}^{-T}.\mathsf{F}^{-1}}.\mathsf{F}=\sqrt{\mathsf{F}.\mathsf{F}^{T}}.\mathsf{F}^{-T}=\mathsf{F}.\sqrt{\mathsf{F}^{-1}.\mathsf{F}^{-T}}=\mathsf{F}^{-T}.\sqrt{\mathsf{F}^{T}.\mathsf{F}}$ and the Eulerian left $\mathsf{v}=\mathsf{v}^{T}=\sqrt{\mathsf{F}.\mathsf{F}^{T}}=\mathsf{R}.\mathsf{U}.\mathsf{R}^{T}$ or Lagrangean right $\mathsf{U}=\mathsf{U}^{T}=\sqrt{\mathsf{F}^{T}.\mathsf{F}}=\mathsf{R}^{T}.\mathsf{v}.\mathsf{R}$ symmetric stretch tensors. The spectral representation of the deformation gradient $\mathsf{F}=\hat{U}_k\hat{\mathbf{e}}_k\otimes\hat{\mathbf{E}}_k=\hat{U}_k\hat{\mathbf{e}}_k\otimes\hat{\mathbf{e}}_k.\mathsf{R}=\hat{U}_k\mathsf{R}.\hat{\mathbf{E}}_k\otimes\hat{\mathbf{E}}_k=\dfrac{d\hat{\mathbf{x}}_k\otimes d\hat{\mathbf{X}}_k}{\|d\hat{\mathbf{X}}_k\|^2}$ unveils the polar decomposition as well as the definition of the principal quantities (marked with a *hat*): the stretch eigenvalues $\hat{U}_k=\|d\hat{\mathbf{x}}_{(k)}\|/\|d\hat{\mathbf{X}}_{(k)}\|$, the Eulerian unit eigenvectors $\hat{\mathbf{e}}_k=d\hat{\mathbf{x}}_{(k)}/\|d\hat{\mathbf{x}}_{(k)}\|$ with respect to the present configuration κ and the Lagrangean unit eigenvectors $\hat{\mathbf{E}}_k=d\hat{\mathbf{X}}_{(k)}/\|d\hat{\mathbf{X}}_{(k)}\|$ with respect to the reference configuration κ_0. Exclusively the Eulerian $d\hat{\mathbf{x}}_k=\|d\hat{\mathbf{x}}_{(k)}\|\,\hat{\mathbf{e}}_{(k)}$ or Lagrangean $d\hat{\mathbf{X}}_k=\|d\hat{\mathbf{X}}_{(k)}\|\,\hat{\mathbf{E}}_{(k)}$ principal edge vectors, the Eulerian $d\hat{\mathbf{s}}_k=\|d\hat{\mathbf{s}}_{(k)}\|\,\hat{\mathbf{e}}_{(k)}$ or Lagrangean $d\hat{\mathbf{S}}_k=\|d\hat{\mathbf{S}}_{(k)}\|\,\hat{\mathbf{E}}_{(k)}$ principal surface area vectors and the Eulerian $\hat{\mathbf{e}}_k$ or Lagrangean $\hat{\mathbf{E}}_k$ unit eigenvectors of the corresponding Eulerian $d\hat{v}$ or Lagrangean $d\hat{V}$ principal infinitesimal volume elements are collinear: $d\hat{\mathbf{x}}_k\sim d\hat{\mathbf{s}}_k\sim\hat{\mathbf{e}}_k$ or $d\hat{\mathbf{X}}_k\sim d\hat{\mathbf{S}}_k\sim\hat{\mathbf{E}}_k$ and related by $d\hat{\mathbf{x}}_k=\hat{U}_{(k)}\mathsf{R}.d\hat{\mathbf{X}}_{(k)}$, $d\hat{\mathbf{s}}_k=\dfrac{\hat{U}_1\hat{U}_2\hat{U}_3}{\hat{U}_{(k)}}\mathsf{R}.d\hat{\mathbf{S}}_{(k)}$ and $\hat{\mathbf{e}}_k=\mathsf{R}.\hat{\mathbf{E}}_k$. Hence, the Lagrangean principal infinitesimal volume element $d\hat{V}$ is rotated to the Eulerian $d\hat{v}$ by the material rotation tensor R. The relation $\Omega=\mathsf{w}-\frac{1}{2}\mathsf{R}.\big(\dot{\mathsf{U}}.\mathsf{U}^{-1}-\mathsf{U}^{-1}.\dot{\mathsf{U}}\big).\mathsf{R}^{T}$ between the antisymmetric Eulerian tensors of material spin Ω and vorticity $\mathsf{w}=-\mathsf{w}^{T}=\frac{1}{2}\big(\dot{\mathsf{F}}.\mathsf{F}^{-1}-\mathsf{F}^{-T}\dot{\mathsf{F}}^{T}\big)$ unveils the difference between the Green-Naghdi rate $\dot{\mathsf{s}}^{GN}=\dot{\mathsf{s}}-\Omega.\mathsf{s}+\mathsf{s}.\Omega$ (defined with the material spin Ω) and the Zaremba-Jaumann rate $\dot{\mathsf{s}}^{ZJ}=\dot{\mathsf{s}}-\mathsf{w}.\mathsf{s}+\mathsf{s}.\mathsf{w}$ (defined with the vorticity w) for Eulerian symmetric second-order tensors s. Therefore, the time integral $\mathsf{s}=\int_{material-convective}\dot{\mathsf{s}}^{GN}\,dt+\mathsf{s}_0$, translational and rotational convectively integrated with the material, is associated with the Green-Naghdi rate $\dot{\mathsf{s}}^{GN}$ and not with the (non-material) Zaremba-Jaumann rate $\dot{\mathsf{s}}^{ZJ}$. In particular, the Lagrangean ${}^{p}\mathsf{E}$ and Eulerian

${}^p\mathsf{e} = \mathsf{R}.{}^p\mathsf{E}.\mathsf{R}^T$ symmetric plastic strain tensors must be time integrated material-convective from the corresponding Lagrangean ${}^p\dot{\mathsf{E}}$ and Eulerian ${}^p\dot{\mathsf{e}}^{GN} = \mathsf{R}.{}^p\dot{\mathsf{E}}.\mathsf{R}^T$ plastic flow rules in order to result in the proper tensors ${}^p\mathsf{E} = \int {}^p\dot{\mathsf{E}}\, dt + {}^p\mathsf{E}_0$ and ${}^p\mathsf{e} = \int_{material-convective} {}^p\dot{\mathsf{e}}^{GN}\, dt + {}^p\mathsf{e}_0 = \mathsf{R}.{}^p\mathsf{E}.\mathsf{R}^T$, respectively. Only if these integrals are defined translational- and rotational-convective with the material, then the resulting plastic strains ${}^p\mathsf{E}$ and ${}^p\mathsf{e}$ fulfil the geometrical interpretability of proper (plastic) strain tensors. Otherwise, if the plastic rate integrals are not convected with the material (e.g. by using Zaremba-Jaumann rates or the like), the components of the resulting plastic strains just become house numbers without any physical meaning.

Numerical aspects of material modelling / 155

On numerical modelling of chemical reaction fronts in solids

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Our study is based on the concept of the chemical affinity tensor. It quantifies how stresses and strains influence the chemical reaction rate and the reaction front velocity [1]. The stresses affect the front velocity through the normal component of the chemical affinity tensor acting as a driving force and can accelerate, retard, or even stop the transformation front. In the last case reaction blocking occurs. For this case a stability analysis of the reaction front interface is made. Analytical examinations of the stability are complicate even for simple geometries and linear elastic material models. For materials with complex rheology at finite strains the stability analysis must be performed numerically.

One of the FEM approaches to simulate moving interfaces is based on regenerating the mesh on each time the interface moves. Apart from creating an extremely fine mesh for sufficient accuracy, this technique requires us writing non-trivial algorithms for automation and additional computational resources for the remeshing process. An alternative way is based on a method that allows the interface to pass through the elements and to move independently of the mesh, the so-called CutFEM approach [2,3]. The procedure is used to simulate the propagation of chemical reaction fronts and special attention is paid to the behavior of the interfaces and to stability in the vicinity of the reaction blocking state. Finally we compare CutFEM approach with a more standard remeshing technique.

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Plasticity and viscoplasticity / 140

On the evolution of Hooke's law during plastic deformations of fiber reinforced materials

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In anisotropic finite elastoplasticity an internal variable is needed to describe the evolution of the elastic law during yielding. One choice is to assume elastic isomorphy, i.e., identical elastic behavior before and after the deformation. This assumption applies almost perfectly within crystal plasticity, it still applies to polycrystals as long as the evolution of the crystallografic texture is reasonable small, but it does not apply to materials where the elastic anisotropy is linked to the material deformation. This effect is called material plasticity. Such phenomenon occurs in fiber reinforced materials where the fibers and the matrix material deform together plastically. This leads to a change of the material symmetry class of the elastic law. Considering the case of two or three orthogonal fiber directions, the material would initially show an orthotropic elastic behavior. After a large shear deformation this is no longer the case. The symmetry class would become smaller.
For the investigations, a representative volume element (RVE) in a finite element setup has been used as a numerical lab to determine the elastic stiffnesses before and after finite deformations. Matrix and fiber are considered in the RVE. By a method due to Weber, Glüge, Bertram (2019) one can determine the distance of any stiffness tensor to some particular symmetry class like orthotropy, hexagonality, etc. This algorithm has been modified to monitor the evolution of the elastic anisotropy related to material plasticity.

Optimization and inverse problems in multiscale modelling / 139

Optimal q-states values for monte carlo potts model simulation of grain growth

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Abstract: Monte Carlo Potts model simulation, based on Potts model and Metropolis algorithm, was carried out on a 2D square lattice on a matrix of size 1000 x 1000 for a wide range of Q-states, which represent grain orientations in simulated microstructures, for over 50,000 million iterations. The simulations have shown good agreement with theory with respect to grain growth kinetics and grain size distribution. Further, the largest grain size and the average grain size were computed, at the end of 50,000 Monte Carlo Steps, for various Q-states, which have indicated normal grain growth and microstructure homogeneity. The simulations have also shown that the best value of grain growth exponent is obtained when Q-states is either 32 or 64. Excellent visual microstructure representations have been achieved which clearly shows grain structures with different orientations and grain boundaries while displaying close similarity with real microstructures.
Keywords: Monte-Carlo simulation; Potts Q-States; Metropolis Algorithm; Grain Growth Exponent; Grain Size Distribution.

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Parameter identification of DP800 based on a gradient-enhanced ductile damage model at finite strains

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A gradient-enhanced and finite deformation ductile damage model is proposed. Following a multi-surface approach, von Mises plasticity with nonlinear isotropic hardening is coupled to exponential Lemaitre-type damage. Evolution of plasticity and damage is each governed by effective driving forces. The concept of effective stresses, following from the postulate of strain equivalence, is analogously extended to an effective damage driving force, i.e. the effective damage driving force increases as plasticity evolves. For the gradient-enhancement of the model in the context of finite element simulations an additional field variable denoted as non-local damage is introduced and linked to the local damage variable by a penalty term. By introducing different damage influences, or rather different damage functions weighting the volumetric and isochoric contributions in the free energy, the model can be adapted to capture the ductile damage response of various materials.
A parameter identification using both, the experimentally measured forces and the displacement field obtained through digital image correlation (DIC) is performed. The particular material studied is DP800 steel and the investigations show that the model established is capable of reproducing the material behaviour. The calibrated material model is validated using different experiments and inhomogenous boundary value problems.

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Phase field theory of dislocation patter formation

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There is a long-standing discussion regarding the physical origin of dislocation patterning. During the past 50 years an amazing variety of different approaches proposed, many of which are based on analogies with pattern formation in other physical systems. It has been argued that dislocation patterns form because the dislocations try to minimize the elastic energy. This approach may be contrasted with the idea that dislocations in a deforming crystal represent a driven system far from equilibrium where patterns may form as dissipative structures. One can state that none of the models mentioned are really proved by experimental evidences and they are not linked to the theory of individual dislocations.

In the talk a 2D phase field continuum approach of the collective evolution of dislocation is proposed that is directly derived from the properties of individual dislocations. It is shown that the phase field theory has an unusual feature because due to the nontrivial mobility function that has to be introduced the steady state solution of the evolution equations does not correspond to the minimum of the phase field functional.

Linear stability analysis and numerical solution of the equations predict dislocation patterning under rather general conditions. The structure of the equations indicates that the pattering is neither “energetic” nor “dynamics” assumed in models proposed earlier.

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Physically based material model applied on additive manufactured superalloy 718

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The thermo-mechanical response in metallic materials depends not only on the current temperature and strain rate but also on the microstructure such as the grain size and precipitation of secondary phases. In the precipitate hardening family of superalloys, such as alloy 718, the precipitation of secondary phases has a significant impact on the stress-strain behavior of the alloy. The volume fraction and size of the nucleated particles need, therefore, to be taken into account when describing the stress-strain behavior in thermo-mechanically loaded samples. In the novel manufacturing technique additive manufacturing (AM), where components are built by adding layer by layer of material, either from a powder or a solid wire, which are fused together usually using a laser or electron beam, this is of typically interest. With this technique, the material experiences different temperature histories in different regions of the sample and the phase composition will vary across the final component. The technique is under development and has a great industrial interest, especially for the aerospace industry where small batches of components with complex geometries are produced. However, several questions need still to be answered to fulfill today's demands, particularly for thermo-mechanically loaded structures such as turbine blades or rocket nozzles. In these cases, modeling is a very important tool for further success. Using the finite element method, the thermo-mechanical-metallurgical response to the heating cycles of AM production can be computed. The final residual strain state and the phases in the component are of typically interest when predicting the final geometry, the maximum load capacity, and the fatigue properties, as well as to anticipate crack initiation during manufacturing or post heat treatments.

In this work, a physically based material model that takes the microstructure into account is applied in a finite element model simulating the process of AM. The model predicts the precipitation of secondary particles in superalloy 718, which is coupled with the flow stress behavior of the alloy. It is believed that the final residual stress state and the geometry of the component can be predicted better by using a model that takes the variation of hardened precipitates into account.

Nonlinear elasticity / 33

Physically based modeling of strain induced crystallization in natural rubbers

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Strain induced crystallization is a phenomenon observed in natural rubbers subject to high stretches where polymer molecules strongly align in the loading direction and form crystallites. Strain-induced crystallites are supposed to play an important role in the elastomer reinforcement and enhance the resistance to crack growth in natural rubbers. In this contribution, the analytical network averaging concept [1] is applied to model the phase transition during strain induced crystallization. To this end, a physically-based constitutive model describing the non-isothermal strain induced crystallization is proposed. Accordingly, the spatial arrangement of polymer subnetworks is driven by the crystallization nucleation and consequently alters the mesoscopic deformation. The crystallization growth is elucidated by diffusion of chain segments into crystal nuclei. The crystallization results in a change of temperature and an evolution of the heat source. The proposed model demonstrates good agreement with experimental data with respect to all measurable values such as stress, crystallinity or heat source.

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Plasticity and viscoplasticity / 68

Plastic flow and dislocation strengthening in a dislocation density based formulation of plasticity

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Formation and evolution of dislocation microstructures including dislocation multiplication is well known to be the essential work hardening mechanism in the stage II regime in face-centered cubic crystalline materials. The complexity of dislocation interaction mechanisms have only recently been revealed by DDD simulations [1], which demonstrate the relevance of an interplay of dislocations between slip systems for dislocation multiplication mechanisms and dislocation reactions leading to work hardening. In contrast, most dislocation based continuum models relate dislocation multiplication to plastic slip on the same slip system. However, this yields self-replication of dislocation density, which contradicts the observations in the DDD simulations.

Regarding the kinematic evolution of curved dislocation lines, recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [2]. These evolution equations provide a physically based approach in describing the motion of curved dislocations in three-dimensional systems. However, an open task is still the physically meaningful modeling of dislocation multiplication mechanisms and the incorporation of formulations, which reproduce the stability of the dislocation network originating from dislocation reactions.

In this contribution, we introduce a dislocation based continuum theory incorporating dislocation reaction mechanism, i.e. glissile, lomer and collinear reactions as well as cross-slip. We account for an interplay of the two competing mechanisms: (I) dislocation multiplication and (II) limitation of the dislocation mobility by the network. The results are evaluated by discrete dislocation dynamics data and discussed in the context of different existing continuum approaches.

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Coupled field problems / 146

Predicting buckling initiation in layered hydrogels using transient swelling models

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The phenomenon of swelling induced buckling in hydrogels is an intriguing scientific problem that has generated considerable attention over the last decades. However, most of the analytical and numerical studies in the literature investigate buckling during equilibrium swelling. In this work,

we aim at quantifying the effect that the transient nature of swelling has on the point of onset of buckling for confined hydrogel plates with stiffness gradients.

A material modelling procedure accounting for the transient nature of gel swelling is outlined in the context of a finite element framework. The model is implemented as a user material for the finite element software Abaqus, where the analogy between heat transfer and gel diffusion is utilized. The implemented model is benchmarked against analytical results for transient swelling of a homogeneous gel with excellent results.

Using the obtained model, the onset of buckling in layered hydrogel plates is studied for plates with various initial thickness and stiffness values. The obtained swelling ratio at onset of buckling and the initial wavelength of the resulting buckling pattern was compared with results obtained using analytical equilibrium swelling models. The initial thickness of the hydrogel plate was seen to change the effective swelling ratio at the onset of buckling, with lower swelling ratios for thicker plates. In addition, for gels with a low stiffness, the wavelength of the resulting buckling pattern was found to be reduced as the initial plate thickness was increased. Comparing with models assuming equilibrium swelling, the importance of transient effects increase significantly as the initial plate thickness is increased.

This work highlights the importance of accurate material models accounting for transient effects when aiming for finite element modeling procedures that can predict the behavior of buckling hydrogels in a quantitative manner.

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Principle of cluster minimum complementary energy of FEM-cluster-based reduced order method: fast updating the interaction matrix and predicting effective nonlinear properties of heterogeneous material

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Based on the FCA (FEM-Cluster based reduced order model Analysis) method proposed in [1], the principle of minimum complementary energy and its cluster form of the reduced order model for the efficient prediction of effective mechanical properties of heterogeneous material are developed. The proposed reduced order model is a RUC (Representative Unit Cell) of the microstructure which subjected to applied uniform eigenstrains and the PHBCs (Periodic Homogeneous Boundary Conditions). By using the known interaction matrix, an alternative form of the principle of cluster minimum complementary energy is constructed and proved very efficient for updating the interaction matrix and the effective elastic modulus when the material properties of clusters change. Moreover, the proposed principle of cluster minimum complementary energy is applied for the incremental nonlinear analysis of the cluster reduced order model, and thus greatly improves the prediction of nonlinear effective properties of the RUC in online stage computed in [1]. Several numerical examples illustrate the effectiveness and efficiency of the FCA approach with the proposed principle of cluster minimum complementary energy.

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Plasticity and viscoplasticity / 102

Quantitative evaluation of subsequent yield behavior in hexagonal metal

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A quantitative evaluation of the subsequent yield behavior of a polycrystalline hexagonal metal based on the crystal plasticity model is presented. The non-normality effect, that is, the difference between the normal to the yield surface and the plastic flow direction under a non-proportional loading condition, is numerically investigated, and it is shown that the non-normality effect of hexagonal metals is stronger than that of cubic metals. Additionally, the intensity of the non-normality of hexagonal metals depends on the amplitude of the offset strain, which is the pre-strain before non-proportional loading, while that of cubic metals is almost constant with respect to the offset strain. The contribution of each slip system to the non-normality effect is investigated. It is clarified that the difficulty of switching the dominant slip system when the strain path changes plays an important role and is the principal mechanism behind the strong non-normality effect of a hexagonal metal. The effect of the initial texture on the non-normality effect is also discussed.

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Second gradient material model for the bubble dynamics

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In this work, Mindlin's second strain gradient continuum theory for linear isotropic elastic materials is extended using principle of virtual power to incorporate the effect of geometric and material nonlinearities. Additional terms in the Cauchy stress and hyper-stresses due to geometric nonlinearity are obtained, which are not present in the linear second gradient theory. We have used certain length scale parameters to introduce the gradient effects. Further, the extended model is applied to study the radial dynamics of a gas filled phospholipid encapsulated thin microbubble submerged in fluid. The material is assumed to be homogeneous, isotropic and incompressible. Using the incompressibility condition, the nonlinear governing equation (in terms of outer radius of the bubble) for the radial dynamics of bubble is obtained as an extension to the conventional Rayleigh-Plesset equation to accommodate the gradient and second gradient effects. As the bubble is of micron size order, the surface effects including the interface curvature is expected to play crucial role in the behavior of microbubbles excited by ultrasound. Using the governing equation, nonlinear frequency response curves are obtained for different excitation pressures and a detailed parametric study has been carried out in terms of length scale parameters. The Poincare sections are also obtained from the time series data to identify the aperiodic behavior of the bubble in certain frequency regimes.

Creep, damage and fatigue / 147

Simulation of crack propagation in porous rocks with a phase-field fracture model

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In this work, we suggest a modified phase-field model for simulating the evolution of mixed mode fractures and compaction bands in porous rocks. For the purpose of validation, the behaviour of samples of artificial rock, with either a single or double saw cuts, under compression has been studied. The simulated results are compared to experimental data, both qualitatively and quantitatively. It is shown that the proposed model is able to capture the commonly observed propagation pattern of wing cracks emergence followed by secondary cracks and compaction bands. Additionally, the typical types of complex crack patterns observed in experimental tests are successfully reproduced, as well as the critical loads.

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Simulation of intragranular slip localization with softening crystal plasticity: from the local formulation to strain gradient plasticity

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The validity of constitutive mechanical models for crystalline solids must be assessed in regard of their ability to describe their heterogeneous deformation mechanisms. Hence, in the case of plastic slip, they need to satisfactorily predict the formation of various slip localization modes observed in crystalline materials. Locally softening mechanisms triggered by dislocation glide can promote enhanced slip on already active slip planes, leading to the formation of slip localization bands. Materials such as hyperquenched or irradiated metals provide a compelling example, as they exhibit dislocation channeling, a strongly softening mechanism, and subsequent intense slip localization.

Our work investigates the ability of local continuum crystal plasticity theory to simulate such intense slip localization within polycrystals. A generic strain softening model is implemented within a massively parallel FFT solver framework to study intragranular strain localization throughout high resolution polycrystalline simulations. Asaro and Rice bifurcation analysis has shown that softening crystal plasticity theory allows for two slip localization modes: slip and kink bands. In order to study their formation in our simulations, a systematic analysis of strain localization modes has been carried out: equivalent plastic strain and lattice rotation fields are processed to create binary maps of slip and kink bands populations, estimate their volume fraction and mean strain level.

Simulation results show the formation of intragranular localization band networks and associated localization maps are used to identify accurately slip and kink bands populations. The distinct evolution of kink bands influenced by lattice rotation is highlighted. It is evidenced that selection between slip or kink localization modes is only due to grain to grain incompatibilities with classical crystal plasticity models, as they do not account for their actual physical differences. As a result they predict the formation of a large amount of kink bands, in contradiction with experimental observations.

In addition to strong lattice rotation, kink bands are also associated with lattice curvature which has been linearly related to the curl of plastic deformation by Nye. A specific class of strain gradient plasticity models proposed by Gurtin including the full curl of plastic deformation in constitutive equations is used among the same FFT polycrystalline simulations. It is evidenced that these

models change qualitatively the nature of simulated slip localization. They significantly reduce the amount of simulated kink bands. Besides they prevent the formation of well-defined continuous kink bands, which are replaced by a dense succession of thin slip bands. Associated localization maps confirm that these "curl(Hp)" models reproduce more accurately the formation of slip lines in polycrystals.

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Simulation of pore shrinkage with crystal plasticity and dislocation transport

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Single crystal superalloys usually contain pores of sizes 5-10 μ-m after casting and heat treatment. These pores can be reduced under compression by combined creep and diffusion in a subsequent treatment called Hot Isostatic Pressing (HIP). The paper presents a methodology to simulate pore shrinkage under HIP conditions in two dimensions (2D).
At the scale of the pores, which is also the scale of the sub-grains (<50 μ-m) the dislocation sources cannot be assumed to be homogeneously distributed. Thus, the applicability of classical crystal plasticity is questionable. In this case, the transport of dislocations under an applied stress from the location where they are nucleated must be explicitly modelled. This is done by solving the transport equations for the dislocation densities and the elasticity equations in 2D. The dislocations are assumed to be nucleated at Low Angle Boundaries. They glide or climb through the sub-grains with a stress dependent velocity.
The transport equations are solved by the Flux-Corrected Transport method [1], which belongs to the predictor-corrector class of algorithms. In the first step, an artificial diffusion is introduced, which suppresses spurious oscillations of the solution. In a second step, the solution is corrected in such a way that no additional extremes appear and that the extremes do not grow. The algorithm is validated by simulating the transport of simple distributions with a constant velocity field.
With the dislocation velocities and the computed dislocation densities, the inelastic shear rate at the slip system level is computed by integrating the Orowan equation. In the 2D-setting, three slip systems are considered. The contributions of these slip systems are summed up to obtain the total inelastic strain rate. Dislocation glide and climb and the coupling of climb with vacancies diffusion are considered.
The resolution of the equilibrium equations from the inelastic strains turned out to be prone to numerical instabilities. As an alternative, the stresses are directly computed from the distribution of geometrically necessary dislocations following the method presented in [2]. The resulting boundary value problem is solved by the Least-Square Finite Element method [3].
Examples of simulations are presented for a representative region under creep tension and for a pore shrinking under external pressure.

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Simulation of ratcheting and mean stress relaxation in polycrystal aggregates using crystal plasticity

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When a sample is cyclically loaded with an asymmetric stress or strain boundary condition, ratcheting as well as mean stress relaxation are observed. Classical macroscopic models produce both quantities in excess as opposed to experimental findings [1]. Purely phenomenological solutions have been proposed in the framework of macroscopic plasticity models, and studies have been devoted to the intragranular behavior, but little attention has been paid to model such phenomena using polycrystal aggregates especially going up to the regime of stabilized stress-strain loops at the grain level. It will be shown that the interaction between different grains is enough to account for such complex phenomena using crystal plasticity for FCC crystals. Light will be shed on how different grains accommodate each other and how the classical definition of constant ratcheting rate cannot be reached in a polycrystal. More importantly, a detailed study will allow us to show that, for a prescribed stress loading, the absence of ratcheting on a macroscopic level does not mean that local steady state is achieved [2]. Diagrams will also be built to give an insight on how to stay in the ratcheting regime or to switch to elastic-plastic accommodation. With regards to mean stress relaxation, a start will be taken from a single crystal model depicting different relaxed stable regimes. Then a transition from a single to a representative polycrystal will be presented focusing on the capacity of the polycrystal model to reproduce experimental behavior. Different mean stress relaxed hysteresis regimes will be depicted and attention will be paid to the local evolution of plasticity.

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Creep, damage and fatigue / 21

Simulation of the failure of quasi-brittle specimen with defects using the TLS damage model : Scale effect analysis

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Predicting the maximum load that a (quasi-)brittle specimen can sustain is an important scientific and practical issue. A natural approach is to search for a criterion. Strength and toughness criteria are well suited for simple specimen having either no defect or an existing crack. When defects (notches, or cavities, ...) are present, the criterion is more complex to set up.
Two approaches are considered in this work: the first is the coupled criterion which is introduced by [1]. It could be qualified as semi-analytical since it starts from analytical consideration finalized by (simple) numerical treatment.

The second one is pure numerical approach which allow us to perform a full numerical quasi-static analysis of the specimen with an increasing loading. The failure load is defined as the maximum load above which no quasi-static solution may be found (and the specimen goes into dynamics). Since we are discussing quasi-brittle failure, we use a damage model. It is well known that regularization is needed when addressing failure with such a model, otherwise failure may be reached for infinitely small loading. Here we consider the TLS (Thick Level Set) approach of graded damage modeling. A material length scale is introduced explicitly, and the model is closely connected to the cohesive zone model (CZM) [2]. Note that the coupled criterion contains a length scale since it is written in terms of toughness, strength and Young modulus from which a characteristic length may be extracted.
In this work, failure load is determined using the two approaches which is then compared to ones obtained experimentally. Then the influence of scale effect is investigated. More precisely, we analyze the role played by length ratio (notch or cavity size over characteristic length) on the predicted failure load.

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Cosserat, micromorphic and gradient materials / 36

Stress vs strain gradient continuum theories

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Germain's general micromorphic theory of order n is extended to fully non-symmetric higher-order tensor degrees of freedom. An interpretation of the microdeformation kinematic variables as relaxed higher-order gradients of the displacement field is proposed. Dynamical balance laws and hyperelastic constitutive equations are derived within the finite deformation framework. Internal constraints are enforced to recover strain gradient theories of grade n. An extension to finite deformations of a recently developed stress gradient continuum theory is then presented, together with its relation to the second-order micromorphic model. The linearization of the combination of stress and strain gradient models is then shown to deliver formulations related to Eringen's and Aifantis's well-known gradient models involving the Laplacians of stress and strain tensors. Finally, the structures of the dynamical equations are given for strain and stress gradient media, showing fundamental differences in the dynamical behaviour of these two classes of generalized continua. Special attention will be paid to the suitable boundary conditions for stress gradient media.

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Stress, strain and fabric evolution in granular mechanics experiments

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The combination of grain-resolved 3D x-ray diffraction (3DXRD) and x-ray tomography enables detailed studies of granular mechanics across three scales; sample, individual grains and an intermediate, “continuum” scale. Grains stresses, and thus force transfer, can be studied in bulk granular systems using 3DXRD that, along with the granular kinematics and contact structure from tomography, allowing local comparisons of stress and strain and investigation of local evolution of elasto-plastic properties linked to the underlying granular fabric. Results from experiments involving confined uniaxial compression and triaxial compression of granular systems will be presented to illustrate the method and the new information that can be gained towards better understanding of granular mechanics.

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The roles of adhesion strength, internal heat generation and elevated temperatures in normally loaded, sliding rough surfaces

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Galling is a severe plastic deformation process, occurring between highly loaded, sliding surfaces. The galling mechanism is associated with macroscopic plastic flow, surface roughening and the formation of protrusions. Due to the elevated operating temperature and strict controls placed on coolant chemistry preventing the use of lubrication, valves within the primary coolant loop of pressurised water reactors (PWRs) are particularly susceptible to galling. Cobalt-based StelliteTM hard-facings provide excellent galling resistance but present a radiological issue through the activation of cobalt containing wear products. Cobalt-free replacement alloys are therefore sought. Iron-based hard-facings have been found to not be equivalent to StelliteTM 6, with a significant reduction in galling resistance at temperatures above 150 - 200℃ (well below the 300℃ operating point of a typical PWR) [1,2], the mechanistic explanation of which remains elusive.

Barzdajn et al. [3] developed a crystal plasticity framework for assessing the deformation of 316L stainless steel under normally contacting loading, and translating this into macroscopic galling frequency measurements compatible with ASTM G-196 [4]. The work presented here develops this further, incorporating adhesion strength, plastic and frictional heat generation, and elevated temperature, again in the context of single phase, 316L stainless steel.

Deformation of the surfaces was found to be dominated by the surface geometry, with no significant effect due to variations in adhesion strength. Plastic and frictional heating were found to have minimal effect on plastic deformation, owing to the rapid conduction of heat away from the deforming areas preventing any localised softening. Corresponding galling frequency results were calculated and shown to be insensitive to both adhesion strength and heat generation. The role of elevated temperature was then examined and compared with experimental results available in the literature [5], accounting for the contribution of surface roughness and wavelength. Qualitative agreement with literature was found, demonstrating a reduction in galling resistance at elevated temperature. However, the reduction was not as severe as that found experimentally, suggesting other mechanisms are responsible for the reported collapse in galling resistance.

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Thermo-Viscoplastic Material Modelling for Self-heating Loads and its Experimental Verification

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Classification

A material classification scheme based on experimental observations connects rate-dependency with an equilibrium hysteresis. When a specimen is subjected to a stepwise relaxation process on the load path and the states of equilibrium form a hysteresis, a general viscoplastic material model is to be applied [Haupt, Continuum Mechanics and Theory of Materials, Springer, 2002].
Micromechanically deduced material models for metals covering viscoplastic deformation with hardening effects were introduced for instance by Bodner/Partom (J. Appl. Mech., 1975) and Chaboche (Int. J. Plast., 1989). Investigations of such material models are typically restricted to isothermal loading regimes or for a mechanical load path with a superimposed temperature cycle validating the temperature dependency of the mechanical material parameters.
These approaches simplify the full thermomechanical problem to an uncoupled problem for the independent field variables displacement and temperature and therefore neglect the quantitative contribution of the deformation process to the temperature evolution. The solution of the coupled thermomechanical problem is recently becoming more present in the literature not least because of the accurate experimental accessibility of the temperature field due to contact-free thermography [Chrysochoos, Quant. Infrared Thermography J., 2012]. The influence of a hardening model variation on the temperature characteristic was discussed in [Broecker et al., Cont.Mech. and Thermodynamics, 2013] and the reasoning by comparing the energy storage ratio to experimental data extended.
In a setting of small deformation gradients and a presumed constant ambient temperature the expected change of temperature in a specimen varies in a range of $n \cdot \left[10^{-2} \dots 10^{0}\right]$ K, which is related to the actual specimen shape and load regimes. In terms of a chaloric evaluation, pure thermoelastic tension leads to small negative values for n, while in deformation processes dominated by dissipative phenomena n becomes in general positive.

Principles

The dissipative nature of viscoplastic deformation is visualizable by friction and damping elements of similar rheological networks [Johnsen et al., J. Mech. Phys. Solids, 2019]. To account for an evolving temperature in this sense, the second funda mental law of thermodynamics together with the energy and entropy balance leads to the inequality for the internal dissipation.
The concept of inner variables results into individual evolutionary equations for each variable and is used to relate self-heating quantities to deformation mechanisms. Due to the association of internal

variables to certain deformation processes the material related internal dissipation can be additively decomposed.
The set of rate-type equations incorporate Fourier's law for the heat conduction and the corresponding thermal boundary conditions and is solved by a predictor-corrector procedure.

Conclusion
This contribution addresses the possibility of material model validation by an emerging temperature field. Therefore different material modelling approaches are thermomechanically considered. The definition of accompanying experiments are discussed and the temperature characteristics of copper specimens are assessed by the analytic approach. Connections to other scalar valued indicators on the validity of the applied model are drawn.

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Thermomechanical behaviour of compacted graphite iron: microstructure-based modelling

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According to recent estimates, around 25% of the worldwide casting production is ductile iron. Compacted graphite Iron (CGI) is an important engineering material, used extensively in the automotive industry thanks to its good thermal and mechanical properties. Despite being first studied in 1948, its performance under long-term or high temperature conditions is not yet fully understood. This is partially attributed to its complex microstructure including short, stubby graphite particles embedded in the iron matrix (termed as *vermicular graphite*) as well as circular ones known as *nodular graphite*. Therefore, significant efforts have been recently made to characterise these microstructures and their role in the overall mechanical behaviour of CGI.
In this work the effect of microstructural morphology on thermomechanical behaviour of compacted graphite iron is investigated. To this aim, CGI specimens produced with different solidification rates are studied. The microstructural differences between these samples are characterised with scanning electron microscopy and further quantified employing post-processing of obtained scans. Also, their response to mechanical loading at room and high temperatures is investigated. Accordingly, the thermal and mechanical behaviour of this material is modelled employing a micromechanical approach. Representative volume elements comprising a ferritic matrix and various graphite particles represented as ellipsoids are studied using a finite-element approach. The developed numerical strategy allows for a parametric analysis of the effect of microstructural features such as the shape, size, location and orientation of graphite particles. Further, the interaction between graphite particles is analysed with an emphasis on the onset of local damage and fracture at microscale. Overall, the obtained results are expected to be useful in the future design of this engineering alloy.

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Topology optimization based on finite strain viscoplasticity

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In this talk, we present a framework that incorporate viscoplastic material response and large deformation theory into topology optimization. The objective of the optimization is to maximize the viscoplastic energy absorption of structures subjected to impact loads. And because energy absorption generally is affected by load magnitude and load rate, dynamic, finite strain and rate effects are accounted for in the design process.

The motion equation is formulated and solved in a total Lagrangian finite element setting in which the implicit Newmark scheme is used for the temporal discretization. The kinematic and constitutive models are based on finite strain isotropic hardening viscoplasticity. To solve the resulting coupled nonlinear residual equations, a nested Newton method is used together with an adaptive time-stepping procedure. The design is updated by the method of moving asymptotes (MMA), which requires sensitivities of the objective and constraint functions. For transient and path-dependent problems, these sensitivities are path-dependent.

The optimization algorithm is also extended to inverse homogenization material design, i.e. we present an optimization procedure for designing architected periodic viscoplastic microstructures. Instead of a formal homogenization approach, we perform numerical tests on a single unit cell subjected to periodic boundary conditions to evaluate its macroscopic mechanical properties. The microstructures are designed so as to maximize their macroscopic viscoplastic energy absorption, and exhibit near zero transverse contraction when subjected to large uniaxial tensile loads.

We formulate well-posed topology optimization problems by restriction via the Helmholtz partial differential equation filter, a periodic version is used for the inverse homogenization studies. Sharp boundaries between solid and void regions are obtained through RAMP penalization and Heaviside thresholding. The design domain is discretized with 8-node linear brick elements, which enables three-dimensional optimization problems to be solved but for simplicity, we use plane conditions to solve two-dimensional problems. The examples of optimized macroscopic structures and optimized periodic microstructures clearly demonstrate the importance of the load magnitude and the loading rate.

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Towards void coalescence criteria for porous single crystals

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Ductile fracture through void growth to coalescence is a common failure mode of metal alloys. Void growth regime corresponds to diffuse plastic flow, relevant for low porosity, and numerous homogenized models have been developed to describe the effect of porosity on the macroscopic behavior of porous materials, including the effect of the anisotropy of the matrix material around voids. Void coalescence corresponds to localized plastic flow between adjacent void, thus relevant for high local porosity, and has been far less described in the literature. Void coalescence criteria can be used to provide lower-bound estimates of fracture strains, but are only available for isotropic and Hill-type anisotropic matrix materials, for simplified void distributions, which may be too crude for realistic situations often involving random arrangement of voids at the single crystal scale.

Therefore, the effects of single crystal anisotropy and random distributions of voids are assessed in this study regarding void coalescence criteria. First, a simple semi-analytical coalescence criterion for porous single crystals with periodic arrangement of voids is proposed using effective isotropic yield stresses associated with a criterion derived for isotropic materials. Effective yield stresses are

defined using Taylor theory of single crystal deformation, and rely ultimately on the computation of average Taylor factors. Arbitrary sets of slip systems can be considered. The coalescence criterion is shown to be in good agreement with numerical limit-analysis results performed using a Fast-Fourier-Transform based solver. Secondly, the influence of void distribution on coalescence criteria is investigated numerically, for an isotropic matrix material and single crystals, regarding the definition of a representative volume element, and an extension of available void coalescence criteria derived assuming periodic arrangement of voids is proposed and validated against these numerical results.

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Underlying deformation mechanism for high energy absorption capability in porous magnesium with oriented pores: A crystal plasticity finite element study

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Porous metals with parallel cylindrical pores exhibit significantly superior mechanical properties compared with porous metals with isotropic pores depending on the loading direction [1]. Especially, recently developed porous magnesium with oriented pores shows remarkably high energy absorption capability during compression parallel to elongated direction of pores [2]. Distinctive features of microstructure in this porous magnesium are (i) elongated pores in the solidification direction, (ii) elongated coarse grains in the solidification direction, and (iii) peculiar crystallographic texture where one of the normal directions of {10-13} planes is closely oriented to the solidification direction. Crystal plasticity analysis in the previous research [2] indicated that the different deformation modes were activated depending on loading direction, which leads to strong anisotropy in the deformation behavior. Furthermore, detailed numerical investigation indicated the contribution of texture development by intra-granular misorientations to high energy absorption capability [3]. Based on these understandings of deformation mechanism from the viewpoint of crystal plasticity, a possible strategy for further improvement of energy absorption properties by pre-loading was proposed [3]. That is, detailed understandings of underlying deformation mechanism could provide guidelines for the further development of porous metals with improved properties.
In this study, the underlying deformation mechanism for high energy absorption capability in porous magnesium with oriented pores is summarized based on a series of crystal plasticity finite element simulations. The present numerical method considers the deformation modes in magnesium which includes basal slip, prismatic slip, first order pyramidal <**a**> slip, second order pyramidal <**c**+**a**> slip and {10-12} tensile twinning systems. The analysis model, which reproduces elongated pore structure, grain morphology, and initial texture, was constructed based on microstructural observations [2]. Material parameters in a crystal plasticity constitutive model, which were identified by fitting to experimental stress-strain curves of the porous magnesium in four different loading directions, are reasonable agreement with the parameters in past crystal plasticity studies on pure magnesium. By using the analysis method for the porous magnesium, influences of loading direction, oriented pore, grain morphology, and initial texture on deformation behavior were studied.

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Unified constitutive models for high pressure die casting aluminium alloy from cooling during casting to thermomechanical loads in service

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Optimizing the design of automotive parts to meet emission requirements, reduce consumption and stay competitive requires both the control of the manufacturing processes and the in-service design. The cylinder block is a central component of the powertrain, integrating many functions that result in geometric complexity requiring the use of a high-pressure die casting manufacturing process with a prior insertion of liners into the mould. The resulting structure is therefore subjected to a severe cooling phase generating residual stresses and strains that can significantly modify the mechanical balance of the structure and have an impact on its in-service fatigue resistance. In order to make the design stage more reliable and to optimise the cylinder block geometry, it is of primary importance to be able to determine the mechanical evolution of these components made out aluminium alloys from the cooling during casting to thermal-mechanical loads in service.

The aim of the study is to provide a reliable and continuous modelling of the mechanical behaviour of an aluminium alloy (AlSi9Cu3Mg) from the foundry process and then under operating conditions. The required modelling will have to consider plasticity and viscosity over a wide range of temperature and strain rate to provide a good representation of the deformations and residual stresses resulting from the process and their evolution in-service on the structure. The main objective of this paper, as a first step towards this objective, is then to focus on constitutive models' formalisms allowing to reproduce accurately uniaxial tests (tension, cyclic tension-relaxation, cyclic tension-compression and creep at different strain rates) carried out at temperatures close to the solidus (560℃) but also at lower ones close to the real use in service (around 200℃).

The aluminium alloy considered in this study presents a static recovery that is integrated into an elasto-viscoplastic model with appropriate hardening components [1]. The transition from the liquid phase at the beginning of the cooling process to the solid metal once below the solidus temperature must also be carefully introduced using this model in the case of an industrial structure design [2]. We have therefore introduced a simple self-consistent scheme [3] integrating the coexistence of a liquid and a solid phase. For the former, a simple constitutive model from the literature was used. Finally, a global methodology of identification of the model parameters has been investigated based on sensitivity analysis. This leads to the discussion of the optimal experimental database needed to obtain a relevant set of parameters.

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Validation of Local Crystal Plasticity Models in Micro-Scale Deformation of Aluminum

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The forming of polycrystalline metallic alloys induces highly heterogeneous plasticity evolution at the microstructure scale. Significant localization is observed especially at the grain boundaries, which might create complications in the surface quality, formability, and fracture behavior of the formed products. In principle, a quantitative and reliable prediction of the localizations by micromechanical models, e.g. crystal plasticity finite element models (CPFEM), can eliminate the need for tedious experiments and offer a better control of the final quality of the products. However, in reality various difficulties might occur for such a realistic prediction. In this work, we test the performance of classical crystal plasticity modelling approach in addressing the localizations over large areas (100+ grains) under large strains (> 0.1). The model is compared with uniaxial tension experiments producing micro-scale strain maps. While the method can simulate successfully the local deformation of few grains, the capability decreases at larger scales. Substantial mismatch between the model and the experiments are evident especially for grain boundary localizations. Possible sources of the mismatch and the remedies in modelling are discussed in detail.

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Variational material modeling of the transformation induced plasticity in polycrystalline steel

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The effect of transformation induced plasticity (TRIP) describes the coupling of plastic deformations and solid/solid phase transformations in steel. A result of this complex microstructural evolution is an improved elongation and strength of the so-called TRIP steels, which is the reason for their attractiveness for industrial applications, e.g., in the automobile industry.

The presented material model is based on the principle of the minimum of the dissipation potential. Considering kinematic hardening, the model describes the simultaneous evolution of plastic strains and of the volume fractions of an austenite and of several martensitic variants. Based on [Junker 2014], the polycrystalline structure is considered by an evolving orientation distribution function, which results in a much faster computation compared to our former investigations; see [Waimann 2015]. Our talk ends with the presentation of numerical results, which proof the model's ability to display the complex material behavior.

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