CMM-SolMech 2022 conference

S05 Micromechanics of heterogeneous materials

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GRANULAR COMPUTING IN COMPUTATIONAL HOMOGENISATION PROBLEMS

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In the research on inhomogeneous materials, the necessity to take into account uncertainties is currently being under consideration. Sources of uncertainties occur in the micro scale as uncertain geometry parameters or constituent properties. Uncertainties propagate across scales. The uncertain microstructure parameters cause uncertainties in macro-scale material properties and in the response of structural systems made of inhomogeneous material, e.g. vibrations and instabilities. In the literature, in most cases, the probabilistic approach is applied to the uncertainty problems. However, such an approach requires the knowledge of statistical property distributions based on a number of experiments. An alternative is granular computing that can deal with incomplete data.

In the present paper, various linear and nonlinear inhomogeneous materials (composite, porous and auxetic ones) are analysed. It is assumed that the properties of constituents and parameters of the microscopic geometry are not deterministic and can be treated as granular ones. Assuming local or global periodicity of the structure, the representative volume element (RVE) approach is used to carry out computational homogenisation of materials with imprecise parameters. The RVEs are modelled by means of the finite element method (FEM). One can refer to the specified class of problems as granular computational homogenisation.

To deal with granular data, fuzzy sets and interval numbers are applied. The fuzzy sets are represented by alpha-cuts, allowing interval arithmetic instead of the fuzzy arithmetic. Response surfaces developed for deterministic effective elastic properties are applied to reduce the calculation effort while maintaining acceptable accuracy. Granular material properties of the components (Young's modulus, Poisson ratio and yield stress) and geometric parameters of the microstructure (pore or reinforcement diameter or its volume fraction) are the input parameters. The stiffness matrix coefficients for linear materials and stress/strain curves for non-linear materials are determined as output parameters. Homogenisation results are compared to the results obtained using analytical models available in the literature or direct FEM calculations. Numerical examples showing the efficiency of the proposed method are presented.

The scientific research was funded from the statutory subsidy of the Faculty of Mechanical Engineering, Silesian University of Technology, Poland.

SPACE-FRACTIONAL KIRCHHOFF-LOVE PLATE THEORY FOR BENDING ANALYSIS WITH SCALE EFFECT

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The study presents the recent research results related to the formulation of nonlocal structural elements developed by incorporating the assumptions of space-Fractional Continuum Mechanics. The considerations focus on the modelling of size-dependent thin plates. Through the application of fractional derivatives, this theory is able to capture the scale effect, which is determined by the order of fractional derivative and length scale. The presented space-fractional Kirchhoff-Love plate (s-FKLP) theory is applied to the static bending problem. The outcomes demonstrate how the non-locality parameters affect the static bending behaviour of the s-FKLP model. Moreover, a detailed parametric study on the influence of length scale and order of fractional continua will be included for plates with different boundary conditions.

ACKNOWLEDGEMENTS
This work is supported by the National Science Centre, Poland under Grant No. 2017/27/B/ST8/00351 and by Poznan University of Technology, Grant No. 0411/SBAD/0005.

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EXPERIMENTAL ANALYSIS AND NUMERICAL MODELLING IN THE FRAMEWORK OF FRACTIONAL CALCULUS OF SELF-HEALING PHENOMENA IN ROOFING FELTS

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Due to its low cost and relatively simple installation, roofing felt is a well-known material for decades and is still widely used as waterproof insulation incommercial and residential buildings. They are available in many types andvariants, differing in purpose, thickness, materials or finishing. In the presentation, we will focus on selected representatives of this group. Research methodology, results of determination of detailed mechanical behaviourand 'self-healing' capabilities of the material. Microscopic photos of the material structure and maps of the chemical composition of different types of roofingfelt will be presented. The presented results will show how heterogeneous and anisotropic the structure the roofing felt is. The presentation will demonstrate that exposition of damaged material to increased temperature may contribute to reuniting material. The results of the evaluation of the strength of the joint obtained in this way will be presented. Based on the obtained results computational modelling strategy utilizing hyperelastic fractional damage material model with memory presented by W.Sumelka and G.Z. Voyiadjis in [1, 2, 3] will be presented. Results of numerical analysis have been prepared with symbolic mathematical calculations software Wolfram Mathematica extended with AceGen/AceFem software in which implementation of the concept of hyperelastic fractional damage material model with memory has been prepared. The choice of AceFem software was dictated by its structure (the system combines symbolic and numeric approaches) and because its environment is designed to solve multi-physics and multi-field problems.

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MICROSTRUCTURE AND MODELING OF AUSTENITIC STAINLESS STEELS DURING FRACTURE AT CRYOGENIC TEMPERATURES

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The aim of the work is to analyse the evolution of the microstructure of the austenitic stainless steels, grades AISI 304 and 316L, in particular, to examine the phase transformation during the uniaxial tension and torsion tests. The fracture area is then studied using the scanning electron microscopy (SEM), the technique of backscattered electron diffraction (EBSD) and the X-ray diffraction by means of a synchrotron beam.
The experiment is carried out with the use of a non-standard test set-up. The examined specimen is mounted in the heat-insulated cryostat within the static tensile test machine. In order to ensure suitable temperature, the coolant (liquid helium, 4.2K) is conveyed from a dewar to the cryostat via special cryogenic transfer line.
The austenitic stainless steels are usually characterized by low stacking fault energy. Thus, they undergo such processes as the diffusionless phase transformation from gamma-austenite to alpha'-martensite, the discontinuous plastic flow (DPF), caused by the effect of accumulation of dislocations on the internal lattice barriers, and the process of formation and propagation of the microdamage fields.
The X-ray diffraction studies with the use of synchrotron beam revealed that the phase transformation is very dynamic, which leads to the propagation of the macrocrack in the continuum with 95% alpha'-martensite content. Moving away from the fracture surface, the volume fraction of the hard alpha' phase sharply decreases. At a distance of 2 mm, the martensite alpha' content is only 25%. The uniaxial tension generates coherent hetero-phase boundaries, favouring the Pitsch and the Kurdjumov-Sachs disorientations. Moreover, the resulting martensite alpha' intensively twins to achieve a good lattice fit to the austenitic matrix. The secondary phase nucleates at the intersections of the shear bands regardless of their nature, i.e. at the crossing of epsilon martensite plates or twin lamella.
Observation of the forming martensite provides information on its morphology. Martensite alpha' is characterized by a band structure, directionally correlated, which clearly indicates the need to take into account both volume and shear components in the micro-strain tensor caused by the phase transformation. These components correspond to the volume change during the phase transformation and to the local shearing effect. The micro-deformation tensor formulated in this way, subjected to integration and averaging over the volume, allows to derive the macroscopic strain tensor resulting from the fcc-bcc phase transformation. The resulting strain tensor will be included in the constitutive model of metastable materials operating at extremely low temperatures.

IMPACT OF FIBRE ORIENTATION DISTRIBUTION RECONSTRUCTION ACCURACY ON COMPOSITE'S BEHAVIOUR PREDICTION

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The composites reinforced with discontinuous fibres have found wide industrial applications due to their various advantages. The most popular method of processing such materials is injection or compression moulding, which typically leads to obtaining inhomogeneous fibre orientation distribution. Therefore, designing and predicting properties of composite structures made of discontinuous fibre reinforced composites may be challenging. In this case, measurement or numerical estimation of the fibre orientation state may be inaccurate which in turn can lead to errors in the computer models of the composite structures [1]. Since the orientation distribution is one of the key factors determining the overall material behaviour it is important to estimate how the accuracy of the orientation distribution reconstruction affects the predictions of computer models. Effective properties of short fibre composites can be determined by using various micromechanical models and numerical methods enabling to take into account arbitrary orientation distribution of fibres [2-4]. The present work is focused on Monte Carlo simulations involving the uncertain character of the orientation distribution of fibres. The results of the simulations are the distributions of the composite's stiffness characteristics in terms of the orientation distribution uncertainty level. The linear-elastic and elastic-plastic constitutive behaviours of composites have been analysed.

Acknowledgement: The research was financially supported by a subsidy from the Faculty of Mechanical Engineering and the Rector's Grant for Research and Development, Silesian University of Technology (Grant No. 10/040/RGJ21/0107).

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EFFECT OF TWINNING ON VOID GROWTH AND THE LATTICE ORIENTATION HETEROGENEITY IN HCP SINGLE CRYSTALS

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Void growth and coalescence in hexagonal close packed single crystals are studied using the crystal plasticity finite element method. A rate-dependent crystal plasticity constitutive theory has been implemented in the finite element model [1]. As potential plastic deformation modes for hcp crystals 3 basal, 3 prismatic and 6 pyramidal slip accompanied by 6 tensile twinning systems have been considered. A 2D plane strain model with one void has been employed. In Mg single crystals, the effects of lattice orientation, tensile twinning, and stress state on void growth are investigated. To better understand the influence of stress state on void growth, simulations based on imposing constant stress biaxiality through a specific truss element are performed for many specified values of the biaxiality ratio. Two loading conditions, prismatic and C axis loading are considered.
In the studies, it has been observed that under the prismatic loading, the major contribution of plastic deformation occurs by prismatic slip system. For the C axis loading, the easy deformation mechanisms of basal slip occur around the void along with tensile twinning in the transverse ligament during the initial deformation stage. For both orientations, void growth decreases as stress biaxiality decreases. However, the initial phase of void growth is significantly inhibited in the C axis loading due to texture hardening imparted by tensile twinning. In the case of prismatic loading, void coalescence is caused by necking of the internal ligament normal to the major principal stress direction, regardless of stress biaxiality, while for C axis loading, especially at lower biaxiality, failure occurs by shear localisation along an inclined band that links adjacent voided cells diagonally. This is because of the strong plastic anisotropy generated by tensile twinning. These observations are in good agreement with the results of [2].
Simulations have also shown that presence of void leads to the heterogeneity of accumulated plastic deformation in the surrounding crystal. This heterogeneity is affecting lattice rotation leading to the grain refinement by which single crystal may transform to polycrystalline medium. The effect of loading conditions and the initial crystal orientation on intensity of this phenomena will be also analyzed.

The research was partially supported by the project No. 2021/41/B/ST8/03345 of the National Science Centre, Poland.

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APPLICATION OF MECHANICAL EQUIVALENCE HYPOTHESIS TO COMPOSITE EFFECTIVE PROPERTIES ESTIMATION

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The main goal of this work is to propose a new mathematical model that would allow for correct and efficient estimation of the effective mechanical properties of a composite, based on the knowledge of properties and geometrical configuration of its constituents. This new method is based on the hypothesis of the total energy equivalence between a real non-homogeneous composite, and a fictitious pseudo-homogeneous material. The proposed approach uses the concept of even-rank effect tensors that map thermodynamic forces from the real multi-component to the fictitious configuration. In the present research, we consider an isotropic composite as a multi-phase material, where the matrix and inclusions behave in an elastic-plastic way. The influence of inclusions on the mechanical properties of a composite is described by a scalar parameter, which is a volume fraction of inclusions. This method relies on the existence of the Representative Volume Element (RVE). The true state of material within the RVE is mapped to a material point of the effective quasi-homogeneous continuum. In the case of an irregular particle-reinforced composite in which the distribution, shape and orientation of particles are fully disordered (chaotic), only the knowledge of the components' mechanical properties, and the inclusions volume fraction are needed to describe the elastic properties of a composite by analytical formulae. Moreover, the presented approach to composite effective properties prediction can be applied not only in the elastic range but also in the plastic and damage regions. The proposed model is verified through experimental testing, and compared to other homogenization methods. A good agreement between experiment and model results is obtained.

STRESS-STRAIN BEHAVIOUR OF METAL CELLULAR MATERIALS USING ARTIFICIAL NEURAL NETWORKS

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Cellular metallic materials are widely used in many application fields, like: automotive industry, structural engineering, filtering or battery industry. It is then crucial for engineers to be able to reliably assess certain cellular metals' properties or to have a material model for these materials. The aim of our research is a proposition of a model of stress-strain behaviour for cellular metallic materials under quasi-static compression. There are used experimental data from compression tests and artificial neural networks (ANNs) for this purpose. Data from the experiments constitute the data for training and testing of neural networks. We use an algorithm which builds, tests and evaluates different architectures of ANNs in order to find the network which most adequately models the stress-strain behaviour. Networks are the feedforward type with varying numbers of neurons in hidden layers. The following measures are used to evaluate the model's quality: mean square error (MSE), absolute relative error (MARE), and Pearson's coefficient for outputs and targets (R).

MODELLING OF PLASTIC DEFORMATION OF METAL CRYSTALS BY A QUASI-EXTREMAL ENERGY PRINCIPLE

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Solving of rate-independent polycrystal or single crystal plasticity problems is related to non-uniqueness of incremental solutions. The main difficulty in the crystal plasticity problems arises from indefinite and non-symmetric slip-system interaction matrix when a set of active slip-systems at a material point level has to be determined. The solution and the set of active slip-systems can be found using the computational approach based on the incremental energy minimization [1]. In order to find the solution using the incremental energy minimization, the selective symmetrization of the slip-system interaction matrix restricted to active systems has been proposed. However, a generic rate-problem in crystal plasticity is of non-potential type. The question arises how to select a physically meaningful solution among multiple possibilities when the known extremal principles do not apply.

The new concept to predicting the time-independent response of metal crystals is based on the recently proposed quasi-extremal energy principle (QEP) [2]. The quasi-extremal energy principle enables finding the solution to a generally non-potential problem. The main advantage with the respect to the previous computational approach to rate-independent crystal plasticity problems [1] is that the present approach does not require any symmetrization of the slip-system interaction matrix.

The computational algorithm originally developed for step-by-step minimization of the incremental energy supply, under the symmetry restriction imposed on the constitutive law, is now modified in order to solve the QEP problem. The minimization method applied to solve the QEP problem is based on the augmented Lagrangian method and is implemented within the Wolfram Mathematica environment.

The effectiveness of the modified algorithm is demonstrated by examples of the large deformation of a fcc single crystal under simple shear and uniaxial tension. The approach enables step-by-step selection of the current set of active slip-systems. It is shown that a numerically stable solution can be found for which the number of simultaneously active slip systems does not exceed five. The QEP results are compared to those obtained using approach based on the selective symmetrization and also those of conventional rate-dependent framework. Especially with the simulations in a high-symmetry initial orientation, where several equivalent solutions exist, significant differences are visible. Moreover, the numerical simulations have been compared to the available experimental results, showing the benefits of using the computational approach based on QEP.

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EXPERIMENTAL AND MULTISCALE CHARACTERIZATION OF ELASTIC VISCOPLASTIC COPPER UNDER CYCLIC LOADING

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The present research is driven by the needs of reliability of Printed Circuit Boards (PCB) requested especially for aeronautic, space or automotive applications. A PCB is a layered material containing mostly woven composites, copper but also active or passive components embedded in its core to achieve a higher interconnection density. As the electronic device must be reliable and since the copper trace is carrying the electrical signal, it is essential to ensure that copper will not present failure during its lifetime.

Copper trace thickness, thermal treatments or grain size, shape and orientations, manufacturing process are features which are strongly influencing the mechanical behavior. To account for microstructural features, we propose to adopt an elastic-viscoplastic self-consistent model for polycrystalline materials to link information at the grain level to the overall response.

In the present work, the copper response of thin film used in PCB is captured during cycling loading. For that purpose, a specific sample is developed with an elastic core, and two copper layers at the outer surface. At the same time, texture and grain sizes are measured. Next, an elastic-viscoplastic self-consistent scheme (EVPSC) is proposed for polycrystals. The approach relies on the tangent additive interaction law for elastic-viscoplastic materials. To model the cyclic response, kinematic hardening at the level of the slip system is introduced. Finally, a comparison between predictions of the EVPSC scheme and experiments is made. The model is able to reproduce the cyclic response of copper for various strain amplitudes. In addition, information at the level of the slip systems is provided, which is not the case for macroscopic models usually adopted in the literature for such applications.

Acknowledgment :
The financial support of EuroMétropole de Metz, of Département de la Moselle, of CIMULEC, of SYSTRONIC and of CSI SUD OUEST through the ID+ Lorraine foundation is acknowledged.

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THE EFFECT OF INCLUSION SPATIAL DISTRIBUTION: MODELLING AND EXPERIMENTAL VALIDATION

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The classical mean-field models are not sensitive to the space distribution of components within the representative volume element of heterogeneous material. Such effect can be accounted for by applying the extensions of the standard scale transition schemes by using either morphologically representative pattern (MRP) approach [1] or the interaction 'cluster' model [2]. According to the first model the inclusion packing effect is described by introducing a coating to the particle, equal to the half of mean minimum distance between inclusions in the representative volume. On the other hand the cluster model accounts for the interaction between each of two particles in the predefined cluster volume. For isotropic phases the MRP predictions are also isotropic, whereas for the cluster model the geometry of particle distribution is reflected in the anisotropic effective properties. The availability of such a modelling tool enables the selection of optimal microstructure in the material-by-design strategy.

To validate those proposals the numerical homogenization of representative cells is usually performed. Another possibility is to compare model predictions with the experimental data, although in such direct comparison we often cannot decouple the two effects: the proper recognition of the material model for a single phase and the scale transition rule. In our recent studies we performed tests on samples made of epoxy resin with a predefined distribution of spherical voids and varying volume fraction. The samples were prepared using a 3D printing technique [3]. The samples with regular cubic, body centre cubic and face centre cubic distributions of spherical voids were printed. They were tested in the regime of strain enabling to obtain elastic stiffness. DIC technique were used to measure material response under compression. As a reference the sample without voids was also printed and subject to testing. Anisotropy of the response related to both, printing direction and geometry of void placement was assessed. Acceptable accordance with mean-field models was found during testing.

The research was partially supported by the project No. 2016/23/B/ST8/03418 of the National Science Centre, Poland.

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MOVING LAYERS AND GRADED DAMAGE COUPLING WITH ELASTO-PLASTICITY

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The paper investigate the coupling between graded damage [1] and elasto-plasticity. The elastic properties of the material depends on a damage variable. The free energy depends on the strain, on internal variables and damage. Damage variable is positive and less then one and its gradient is bounded by a concave function of damage in order to limit its concentration [1].

The potential energy of the body, with prescribed boundary conditions, is introduced in order to define driving forces associated with the internal parameters. These forces are used to define the evolutions of internal parameters and damage by normality laws or equivalently with the help of convex potentials of dissipation.

Potential presence of discontinuities along the boundary between sound and damaged material are investigated. In particular, the free energy can be discontinuous along moving boundaries, where damage begin to growth. If such a discontinuity exists additional dissipation occurs, if not this imposes continuity conditions on the internal variable, and consequently plasticity and damage cannot evolve simultaneously in the damaged zone as shown previuosly in [2]. This fact is illustrated on analytical examples based on cylindrical or spherical geometries on elasto-plasticity.

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FRACTIONAL CALCULUS IN MATERIAL INSTABILITY FOR NON-LOCAL SOLIDS

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In material instability problems, especially when post-critical behavior is investigated in a non-linear case, the use of non-local constitutive equation is essential, in both time and space variables. Non-locality in space variables is classified as a weak and strong one. Conventionally, in studies of material instability, rate- and gradient-dependent terms are added to the constitutive equation referred as weak non-locality. Fractional calculus appears at the strong non-locality approach in form of Riemann-Liouville fractional integral, and then by Riemann-Liouville and Caputo fractional derivatives. The use of fractional calculus is naturally connected to hereditary (non-local time) constitutive modeling. When convolution type integral operators are used in the constitutive equations and creep and relaxations are considered as "inverted" phenomena, Rabotnov has introduced the so-called fractional exponential function as a kernel of the integral operator. His motivation was to meet experimental results and use an invertible operator. As an obvious analogy, fractional derivatives may also be introduced in spatial non-locality. Here convolution type operators could be used to encounter spatial non-local effects. Such approach leads to a strong non-local material model for space variables. The selection of the kernel is a key step. Altan and Aifantis have shown that a proper selection of it may result a weak non-local material. Of course it is a strange result. In classification instead of such formalities as the presence of derivatives or integrals, the focus should be on the physical background. The one should be of couple-stress effects in polar material bodies, the other of finite or long-range fading memory interaction. In stability analysis an eigenvalue problem should be solved and its regularity - separate static and dynamic bifurcations and a finite dimensional critical eigenspace - should be satisfied. When constitutive equations contain fractional derivatives, some requirements should be satisfied for them. In spatial non-locality Ortigueira's two-sided fractional derivative is a proper selection. For non-local time the derivative is a Riemann-Lioville type and the method of Radwan can easily be applied for stability investigation. In the paper various types of fractional derivatives are presented in solving material instability problems for non-local solids by using dynamical systems theory.

CONTACT ANALYSIS OF BRANCHED CRACK SURFACES BY THE BOUNDARY ELEMENT METHOD

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In the present work, materials with single and multiple branched cracks are modeled using the boundary element method (BEM). The method requires division of external material boundaries and crack boundaries into boundary elements. Variations of boundary coordinates, displacements and tractions are interpolated using shape functions and nodal values. The relations between boundary displacements and tractions are expressed by the displacement and traction boundary integral equations. Stress intensity factors (SIF) are computed using the path independent J-integral and the decomposition technique.
During loading of cracked materials, contact of crack surfaces can occur. Contact forces are determined using the iterative procedure. In each iteration, the relative displacements of pairs of nodes on opposite crack surfaces in the normal and tangential directions are computed. If the opening is negative then the edges of the crack overlap. In this case, the pair of nodes is subjected to small normal tractions, which reduce overlapping of crack edges. The iterative process is repeated until the crack opening for the whole crack is positive. The increase of the crack tractions is constant and it is assumed as a fraction of the applied external traction [1].
The aim of the work is analysis of contact forces on surfaces of branched cracks. An influence of crack geometry and direction of loading on SIF and contact forces is studied. Effective elastic properties of plates containing multiple branched cracks are determined. Materials with branched cracks randomly distributed and oriented are considered. A possible contact of crack surfaces is taken into account. The effective properties are calculated using representative volume elements (RVE) with a large number of cracks. The BEM allows simple generation of RVEs with cracks and gives very accurate results [2]. Average strains and stresses in the RVEs are computed using boundary displacements and tractions, which are directly obtained by the BEM. In order to compute effective properties different boundary conditions are imposed on the RVEs. The computed contact forces and overall properties are compared with theoretical predictions and available numerical results presented in the literature.

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Acknowledgement: The scientific research was financed from the statutory subsidy of the Faculty of Mechanical Engineering, Silesian University of Technology, Poland

TOWARDS OPTIMAL SPACE-FRACTIONAL EULER-BERNOULLI BEAM DESIGN

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The strong trend of miniaturizing caused that nano- micro-structures has gained much attention in recent years, which raises the need to propose reliable design procedures. There are two problems that required special consideration, the model and the design procedure itself. The paper presents a nano-beam structure design by optimizing its shape.

Due to the size of beam components which become comparable to characteristic dimensions of underlying microstructure, the local effects frequently are necessary to be considered. It raises the problem of reliable mathematical modelling. There is a variety of approaches proposed to capture the scale effect using phenomenological non-local models: micropolar theories, material surfaces/surface elasticity theories, integral-type theories, general non-local theories, strain-gradient theories. However, in the present study, we follow the space-fractional non-local formulation (sFCM) proposed by Sumelka [2014] where, the local behaviour of the material, thus microstructure, is described by two parameters, namely, length scale and order of continua. In the study, the space-fractional Euler-Bernoulli beam model proposed by Stempin [2020] is used.

The goal of the presented design procedure is to find a structure shape to fulfil stress/displacements/mass requirements. The structure modification is done by changing its height (moment of inertia) along the beam axis within a given range. The optimization is carried out for various configurations of the sFCM property to compare the microstructure effect on the final design. As an optimizer Limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm implemented in the SciPy package was chosen. The statics was solved using a dedicated procedure developed in Python. Due to the varied model properties, the governing equations for the particular points were built dynamically.

SHEAR BAND FORMATION IN POROUS THIN-WALLED TUBES SUBJECTED TO DYNAMIC TORSION

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We have performed 3D finite element analysis of the dynamic torsion of thin-walled tubes in order to investigate the effect of porous microstructure on the formation of adiabatic shear bands. For that purpose, we have incorporated into the finite element models the representative porous microstructure of four different additively manufactured metals -aluminium alloy AlSi10Mg, stainless steel 316L, titanium alloy Ti6Al4V and Inconel 718- obtained using the X-ray tomography technique following the methodology developed by Marvi-Mashhadi et al. (2021). The calculations were performed at strain rates ranging from 100 s-1 to 10000 s-1, for void volume fractions varying from 0.001% to 2%, and void sizes varying between 6 micrometers to 100 micrometers. The matrix material is linearly elastic and obeys von-Mises plasticity with the hardening/softening described as a function of strain, strain rate and temperature. Moreover, we assumed the deformation process to be adiabatic. Two matrix materials namely Titanium and HY-100 steel were considered. The finite element model is primarily based on the experimental configuration of the dynamic torsion experiments of Marchand and Duffy (1988). To the authors' knowledge, this is the first study ever that simulates the torsion test in porous materials with the actual representation of voids. Systematic analysis of up to 10 realizations of each of the four microstructures considered shows the effect of the stochastic location of the voids on the shear band formation. In addition, a detailed parametric analysis varying the void volume fraction for a given porosity distribution, voids number and size for a given void volume fraction, thermal softening, strain rate sensitivity and loading rate has been carried out. This provides quantitative analysis on the effect of local void volume fraction and voids size distribution on the critical nominal strain leading to shear band inception. It is observed that the critical nominal strain at which the shear band forms strongly depends on the maximum diameter of the voids present than the initial void volume fraction.

Acknowledgements
The research leading to these results has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme. Project PURPOSE, grant agreement 758056.

MESOSCOPIC SIMULATIONS OF FRACTURE IN RC BEAMS USING DEM

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Concrete is generally referred to as a strongly heterogeneous and discontinuous material. It may be considered at the meso-scale as a composite material wherein four key constituents (phases) may be isolated: aggregate, cement matrix, interfacial transition zones (ITZs) between aggregates and cement matrix and macro-pores. ITZ, which are adjacent to aggregates, reveal pronounced compositional differences as compared to the cement matrix. Recently, great efforts were made to accurately and efficiently capture the failure behaviour of concrete structures at the aggregate level by meso-scale models for a deeper understanding of the mechanisms of damage initiation and fracture evolution. The simulations of fracture in reinforced concrete (RC) were carried out with a mesoscopic model, based on the discrete element method (DEM) [1,2].
First, quasi-static 3-point bending experiments were performed on RC beams 80x40x40 mm3 (length, height and depth). The reinforcement ratio was high (rho=1.8%). Three-dimensional (3D) evolution analyses of the size and distribution of pores and cracks were carried out with an X-ray micro-computed tomography system SkyScan 1173 of high resolution that is a very valuable non-destructive tool for studying a 3D material interior. The tomography system was coupled with a quasi-static loading machine to continuously follow fracture changes without loading breaks [3]. The reinforced beam failed in shear due to a diagonal shear crack. Next, the experiments were simulated with the four-phase DEM model, assuming the real full meso-structure of the beam [1,2]. The steel reinforcement was also faithfully reproduced (i.e. ribs were reproduced in DEM geometry), thus the proper interface behavior between concrete and steel was taken into account. In DEM calculations, the focus was both on a macroscopic (load-displacement curve, macro-cracking) and mesoscopic beam response (micro-cracking). Special attention was laid on the formation and propagation of the main macro-crack and secondary cracks. A satisfactory agreement was archived between experimental and numerical results. In addition, the evolution of the contact force network was comprehensively studied. The findings offer a new perspective as to the understanding of macro- and micro-cracking formation in RC under loading.

Key Words: DEM, reinforced concrete, bending, micro-CT, aggregate level.

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MICROSTRUCTURAL MODELING OF ANISOTROPIC AND TENSION-COMPRESSION ASYMMETRIC DUCTILE METALS

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HCP materials (i.e. magnesium, zirconium, titanium and beryllium alloys) have unique mechanical behavior in comparison to conventional cubic metals such as steels and aluminum alloys and exhibit remarkable tension-compression asymmetry. In this work in order to analyze the combined effect of anisotropy and tension-compression asymmetry in HCP ductile materials, finite element simulations of a cubic 3D cell with a void inside were developed. The whole geometry of the numerical cell is subjected to periodic boundary conditions and nonlinear kinematical constraints are imposed as boundary conditions in order to maintain macroscopic stress ratios as constant values during the whole loading history of the cell. The behavior of the matrix material is described by the CPB06 anisotropic criterion developed by [1]. The numerical results are compared to those considering 3D homogeneous cell (without void) with the same initial void volume fraction as the voided one and governed by the anisotropic porous yield criterion developed by [2]. The influence of prescribed hydrostatic stress, strength differential parameter and strain hardening exponent on void volume fraction and macroscopic stress evolution is discussed and compared in both homogeneous (without void) and non-homogeneous cells.

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ANALYSIS OF COMPOSITES WITH INTERPHASES

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The objective of this presentation is the inclusion of the interface to investigate the influence of surface effects on the effective properties of random particulate composites. For the interface the Gurtin-Murdoch approach is applied. The focus is on accounting for the surface bending stiffness. The main aspect is the identification of the formula defining energy associated with the surface bending. The real nano-particle and its surface are replaced by equivalent inhomogeneity with properties incorporating the surface effects. Closed-form expressions for the effective moduli of a composite with a matrix and randomly distributed spherical inhomogeneities are presented. The shear moduli of nanoporous materials as a function of void volume fraction is analyzed and evaluated in the context of other theoretical predictions.

ON THE REPRESENTATIVENESS OF THE STATISTICAL VOLUME ELEMENTS IN COMPUTATIONAL HOMOGENIZATION

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Most homogenization theories rely on the concept of the representative volume elements (RVEs), which are the sub-volumes of the macroscopic body large enough to represent the properties of the whole. In the case of periodic media, such an element is simply identified as a repeatable unit cell. If its size is smaller by orders of magnitude than the macroscopic body size, then the well-known asymptotic approach can be used to compute macroscopic material properties. However, in the case of random composites such repeatable cell does not exist. Moreover, the RVE should be of the macroscopic size, otherwise, the homogenization results are statistically scattered, i.e. they depend on the specific sub-volume size, shape and the boundary conditions used. Nevertheless, for the sake of computational feasibility, in the case of random composites, the statistical volume elements (SVEs) are analyzed rather, with the size smaller than RVE. Many realizations of the SVEs must be analyzed then and the homogenization results must be averaged. The natural question arises: what is the relation between the size and number of SVEs which must be analyzed in order to obtain a meaningful averaged macroscopic response? In the current work, we discuss some concepts in this area available in the literature (e.g. [1]-[3]) and we propose some new criteria based on energetic considerations and related to the boundary conditions applied to the SVEs [4].

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MECHANISMS OF STRENGTHENING BIOGENIC STRUCTURES UNCOVERED IN SHELLS OF MOLLUSKS

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Biogenic materials reveal a number of engineering strategies aimed at building a structure with balanced functional and mechanical properties. The shells of mollusks are a representative example. They are made of a light, but relatively weak material, which is calcium carbonate. The ability to self-organize the crystalline varieties of CaCO3, calcite and aragonite, allow to form a hierarchically complex microstructure specialized in anisotropic mechanical response. The electron backscatter diffraction (EBSD) studies revealed a deliberate modification of the microstructure of ribs in the bivalve shells of Pinna nobilis species. Calcite prisms obliquely oriented to the direction of the predicted load improve hardness, and the compressive strength which reaches an outstanding value of 700 MPa [1]. The formation of ribs with modified microstructure relative to adjacent areas locally strengthens the shell and, on the other hand, allow to maintain the flexibility needed to tight sealing against predator. Gastropod shells have a different, much more complicated structure. The cross-lamellar structure is dominant. It is built of plates, units of the first order, that are further subdivided into second-order lamellas. These, in turn, are made up of third-order bars. When studying shells of the Sinustrombus sinatus species, the smallest, basic, structural units were carefully analyzed. The high-resolution electron microscopy (HRTEM) images reveal that the examined lamellas are not single aragonite grains, but are divided by densely spaced twin plates. The energetically favorable twin disorientation is formed with an accuracy of 1°. The obtained HRTEM images were analyzed by the geometric phase method (GPA). The original implementation of the GPA made it possible to relate the registered crystalline lattice to a reference one containing an ideal twin boundary. In this way, deformation fields within the third-order structural units were identified. The embedded twin plates have been found to undergo strong compression in a direction perpendicular to the longest dimension. It leads to strain at the level of -0.1%. The high frequency with which twins are placed induces prestressing of the basic structural units. The uncovered mechanism significantly improves both the fracture toughness and the strength of the protective armor.

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FFT SIMULATION OF VOID GROWTH AND COALESCENSE

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Introduction and motivation:
Void nucleation, growth and coalescence are the phenomena responsible for ductile fracture observed in metal alloys.
There is a vast number of parameters whose influence on ductile fracture should be taken into account, such as stress triaxiality, plastic anisotropy or strain hardening. In particular, when voids much smaller than grain size are considered, the interaction of crystal orientation and void shape should be taken into account.

Methodology:
The material models were generated using the MFRONT software and the simulations of a microstructure under mechanical loading were conducted using the AMITEX_FFTP Fast Fourier Transform based solver. The most important advantage of FFT solvers as compared to commonly used finite element method (FEM) is their computational efficiency.

Results:
The numerical simulations of a volume element with voids were carried out. Considering void nucleation was outside the scope of the present work. The voids were introduced explicitly. The mechanical loading was applied in order to observe their growth and coalescense. The influence of various parameters mentioned in the introduction was studied. The results were compared against available experimental and numerical data (FFT, FEM).

SPURIOUS SOFTENING PREDICTED BY THE MORI-TANAKA SCHEME FOR ELASTIC-VISCOPLASTIC COMPOSITES

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The Mori-Tanaka (MT) scheme is a well-established mean-field model suitable for modelling deformation of heterogeneous materials. Despite being one of the simplest mean-field models, it is characterized by fairly good predictive capabilities under low computational cost. That is why it may successfully compete with other, more elaborate multiscale approaches. The so-called incremental MT model is obtained after proper linearization of the constitutive equations of the phases and may serve for description of the behaviour of inelastic composites. Consequently, it can be applied to modelling, e.g., composite materials within the finite-element framework.

The paper is restricted to elastic-viscoplastic composites under the small-strain assumption. An intrinsic feature of the additive tangent MT scheme, proposed by Molinari for such materials, has been found, namely spurious softening in the macroscopic response [1]. The resulting non-monotonic macroscopic stress-strain response is non-physical and also has a negative impact on the overall efficiency and robustness of the computational scheme used in multiscale finite-element computations. Existence and magnitude of the identified spurious effects depend on material and loading parameters and on different isotropization strategies. For instance, the so-called soft isotropization employed to compute the viscoplastic Hill tensor promotes spurious softening effects. The softening is also observed in the case of the hard isotropization and in anisotropic case but for a much narrower range of material parameters. The predicted overall response is prone to softening for low strain rates, high elastic contrast and for high volume fractions of inclusions. Nevertheless, careful design of the additive tangent MT scheme leads to computationally robust mean-field model which enables efficient finite-element computations.

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INVESTIGATING THE EFFECT OF GRAIN ORIENTATIONS ON THE DEVELOPMENT OF NEAR BOUNDARY GRADIENT ZONE

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Electron Back Scattered Diffraction (EBSD) is used to study the microstructure evolution during progressive tensile deformation of an aluminium magnesium alloy. Localized plastic deformation is observed in the vicinity of prior-deformation grain boundaries, which are referred to as Near Boundary Gradient Zones (NBGZs). Several grain pairs, comprising of orientations from different regions of the standard stereographic triangle and with different Schmid factors are utilized to quantify the development of orientation and misorientation gradients within the NBGZs. A dislocation density based Strain Gradient Crystal Plasticity (SGCP) framework is used to predict the evolution of microstructure and local mechanical properties, with realistic virtual microstructures as input. The simulated contours show a direct correlation between the Geometrically Necessary Dislocation (GND) density and local misorientation, as well as between the Statistically Stored Dislocation (SSD) density and effective plastic strain, within the NBGZ. Both experiments and simulations reveal that length of the NBGZ scales directly with the Schmid factor; higher NBGZs develop in softer grains with higher Schmid factor and vice-versa. Additionally, our analysis shows that grain size acts as a dominant length scale governing the NBGZ development; a phenomenon showing pronounced effect in the softer grains.

TWINNING AS A DISPLACIVE TRANSFORMATION: A COUPLED PHASE-FIELD AND CRYSTAL PLASTICITY MODEL

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Deformation twinning is a prevalent inelastic deformation mechanism in some specific metals and alloys. Due to the critical differences in the underlying mechanism and the characteristics of deformation twinning with respect to plastic slip, modeling the phenomena of deformation twinning poses additional challenges to be dealt with in comparison with plastic slip. In this study, a finite-element-based model of coupled deformation twinning and plastic slip is developed by combining the phase-field method and crystal plasticity [1]. A distinctive feature of the proposed model is that twinning is treated as a displacive transformation, resembling a phase transformation, and thus the corresponding kinematics is characterized by a volume preserving stretch followed by a rigid-body rotation, which is in contrast to the conventional approach based on a simple shear. This treatment is relevant especially when the conjugate twinning systems are crystallographically equivalent.
A two-dimensional computational model is developed for magnesium with an HCP crystal structure. The model includes one twin deformation variant, i.e., two conjugate twinning systems, and three effective slip systems, i.e., one basal and two pyramidal slip systems. The features of the model are illustrated by studying various problems, including twin evolution, twin transmission across grain boundaries, and the overall response of a unit-cell containing several grains.

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ON MICROSTRUCTURAL LENGTH SCALES IN METALLIC MATERIALS

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In multiscale modelling of metallic materials, the micro-macro transition is frequently used sequentially and need not be related to a specific dimension range. However, the mechanical properties transferred from the micro to macro level may depend on microstructural length scales. The main challenge is to introduce into the material model such intrinsic length scales that possess a physical meaning and are suitable for predictive modelling of size effects. This lecture concerns the inelastic behaviour of metallic materials at the micron or sub-micron scale, with a focus on the modelling of microstructure formation and evolution during the deformation process. Three different approaches are presented along with the examples of size-dependent microstructures. In the first approach, illustrated by martensitic microstructures in shape memory alloys undergoing phase transformation, microstructural length scales are determined by the incremental energy minimization that includes the interfacial energy investigated at different levels of multiscale modelling. In the second approach, in phenomenological modelling of the microstructure evolution and strain hardening of metals during severe plastic deformation, dimensions of ordinary dislocation cells and cell blocks have a significant influence on the flow stress. In the third approach, illustrated by the characteristic wavelength of dislocation patterns in plastically deforming metal crystals, the intrinsic length scale in gradient plasticity is derived from phenomenological laws of plasticity of metals. The quantitative agreement between the predicted and observed indentation size effect has been found satisfactory.

LAMINATION-BASED EFFICIENT TREATMENT OF WEAK DISCONTINUITIES FOR NON-CONFORMING FINITE-ELEMENT MESHES

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When modelling discontinuities (interfaces) using the Finite Element Method, the standard approach uses a conforming finite element mesh in which the nodes lie directly on that interface. However, this approach can prove cumbersome if the geometry is complex, in particular in 3D. Some methods use a finite element mesh that is independent of the geometry (a non-conforming mesh), but they are challenging to implement and may require user intervention in the finite-element code, for instance, adding extra global degrees of freedom. In this work, we propose a new, efficient method for non-conforming finite-element treatment of weak discontinuities by using laminated microstructures. The method is inspired by the composite voxel technique [1] that has been developed for FFT-based spectral solvers in computational homogenization. The idea behind our method is simple - each finite element that is cut by an interface is treated as a simple laminate. The volume fraction of the phases and the lamination direction are determined by considering the actual geometrical arrangement of the interface within the element. The approach is illustrated by several computational examples relevant to the micromechanics of heterogeneous materials. Elastic and elastic-plastic materials at small and finite strain are considered in the examples. The performance of the proposed method is compared to two alternative, simple methods showing that the new method is in most cases superior to them while maintaining the simplicity. The finite-element implementation and computations have been carried out in the AceGen-AceFEM environment.

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MODELLING OF PLASTIC STRAIN-INDUCED MARTENSITIC TRANSFORMATION IN AUSTENITIC STAINLESS STEELS USING INCREMENTAL MEAN-FIELD HOMOGENIZATION SCHEMES

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Austenitic stainless steels are commonly used as structural materials in high-field superconducting magnet systems because they retain high strength, ductility and toughness at very low temperatures and are paramagnetic or antiferromagnetic under the Néel temperature in their fully austenitic state. Nevertheless, especially at cryogenic temperatures, they are susceptible to strain-induced martensitic transformation which modifies the material properties, induces change of volume and additional strain hardening, and leads to a ferromagnetic behaviour. Thus, the correct prediction of the performance of these materials at very low temperatures is of great interest for the conception and design of high-field superconducting magnet systems. Here we propose adequate constitutive models for the evolving biphase material based on a Hill-type incremental formulation. Two different mean-field homogenization schemes have been implemented: Mori-Tanaka and self-consistent approaches. For each individual phase a mixed kinematic-isotropic nonlinear hardening model is used. The kinematic contribution is implemented using Chaboche's model, and the isotropic hardening is modelled by the superposition of equivalent exponential hardening laws. Moreover, the phase transformation is modelled by two different kinetic laws: the nonlinear model proposed by Olson and Cohen (1975) and a linear model proposed by Garion and Skoczen (2002). Furthermore, material parameters have been identified by using experimental data from tensile tests for AISI 304L and AISI 316LN at cryogenic temperatures (the kinetic laws being coupled with the homogenization approach). The models are implemented in ABAQUS/Implicit and simulations of fracture toughness tests are being performed. This work aims at demonstrating the capability of combining incremental mean-field homogenization schemes with phase transformation to simulate austenitic stainless steels submitted to severe mechanical solicitations.

FFT BASED NUMERICAL STUDY OF ELASTIC WAVE PROPAGATION IN HETEROGENEOUS MEDIA: APPLICATION TO POLYCRYSTALS

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Two Fast Fourier Transform (FFT) based numerical approaches are developed to study acoustic wave propagation in heterogeneous solids. First, a method is proposed to obtain the dispersion relation of acoustic waves in heterogeneous periodic media in which the microstructure is explicitly considered using a voxelized Representative Volume Element (RVE). The dispersion diagram is obtained solving an eigenvalue problem for Bloch waves in Fourier space. The second method is an implicit FFT based algorithm for solving elasto-dynamic problems in which an incident perturbation can be imposed using Green's functions.

Both methods are used then to analyze the propagation of acoustic waves in elastic polycrystals, showing the strong effect of crystal anisotropy and polycrystalline texture on the propagation. The Bloch wave approach aims at obtaining the dispersion diagrams and group wave velocities of the polycrystal and is well suited for wave lengths greater than grain size. The elasto-dynamic algorithm allows to obtain the propagation of a wave through the RVE in the time domain, and study wave attenuation as a function of the incident wave length.

ELASTIC DISK WITH ISOPERIMETRIC COSSERAT COATING

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Nowadays several technologies involve coating of a bulk materials with a thin layer made up of another material so that the physical properties of the system can be properly designed and enhanced. Their use is so widely spread around many fields, ranging from daily objects design to industrial manufacturing processes and to surgery application, that a strong effort has been devoted to the analysis of associated problems. From a mechanical point of view a coating layer diffuses the load on an attached solid in a non-local way, introduces a characteristic length, and deeply affects the mechanics response and failure mechanisms of the coated object so that the development of general mathematical model for the behavior of this systems plays an important role in the understanding and design of coated systems. In the framework of linear elasticity, the case of an elastic thin layer perfectly bonded to an elastic disk is analyzed in the present work providing a general mathematical tool to study the effect of the coating on the mechanical response of the coat/bulk material system which may find application in micro and nano technologies, for instance in the characterization of nanowires via nanoindentation. More specifically, an Euler-Bernoulli beam is perfectly attached on the boundary of a circular elastic disk. The beam is then acting as a coating for the disk where the axial inextensibility of the beam enforces an isoperimetric constraint for the inside disk which is constraint to maintain its perimeter during the deformation process. The mechanical model for the coat/disk system is formulated for general loading scenario relaying on the complex potential formalism where the beam is modeled as a Benveniste-Miloh interface equipped with the same bending stiffness of the beam and surrounding the inside bulk material; in this fashion the problem can be solved entirely on the disk relaying on complex potential formalism and Kolosov-Muskhelishvili potentials. The particular case of two equal and opposite traction distributions, each applied on a small boundary segment (thus modeling indentation of a coated fiber) has been studied and analytical solutions have been also compared to photoelastic experiments performed on polymethyl methacrylate samples ad-hoc designed and manufactured at the Instability Lab at the University of Trento.

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