ICMM 9

9th International Conference on Material Modeling

BOOK OF ABSTRACTS

Prague, Czech Republic

1–3 September 2026

Faculty of Civil Engineering, CTU in Prague, 2026

icmm9.fsv.cvut.cz

Publication information

Publication title	9th International Conference on Material Modeling: Book of Abstracts
Editors	Martin Doškář, Marek Tyburec and Jan Zeman
Conference	9th International Conference on Material Modeling
Event details	1–3 September 2026; Prague, Czech Republic
Organizing institutions	Faculty of Civil Engineering, Czech Technical University in Prague
Official website	https://icmm9.fsv.cvut.cz
Last updated	2 September 2026

Recommended citation

Martin Doškář, Marek Tyburec and Jan Zeman, editors. *9th International Conference on Material Modeling: Book of Abstracts*. Prague, Czech Republic, 1–3 September 2026. Faculty of Civil Engineering, CTU in Prague, 2026.

Committees

Organizing Committee

Jan Zeman Czech Technical University in Prague
Martin Doškář Czech Technical University in Prague
Marek Tyburec Czech Technical University in Prague
Michael Somr Czech Technical University in Prague
Martin Horák Czech Technical University in Prague

Scientific Committee

Douglas J. Bammann Mississippi State University
Frédéric Barlat Pohang University of Science and Technology (POSTECH)
Stéphane Berbenni Université de Lorraine / CNRS, LEM3
Albrecht Bertram Technische Universität Berlin
Francesco Dell'Isola Sapienza University of Rome
Pawel Dłużewski Institute of Fundamental Technological Research, Polish Academy of Sciences (IPPT PAN)
Fionn Dunne Imperial College London
Yuri Estrin Monash University
Samuel Forest MINES Paris - PSL
Alexander Freidin Institute for Problems in Mechanical Engineering, Russian Academy of Sciences
Marc Geers Eindhoven University of Technology
Sanjay Govindjee University of California, Berkeley
István Groma Eötvös Loránd University
Mitsutoshi Kuroda Yamagata University
Dave McDowell Georgia Institute of Technology
Karol Miller University of Western Australia
Roberto Paroni University of Pisa
Matti Ristinmaa Lund University
Reuven Segev Ben-Gurion University of the Negev
Vadim V. Silberschmidt Loughborough University
Sivakumar M. Srinivasan Indian Institute of Technology Madras
Sebastian Skatulla University of Cape Town
Arun Srinivasa Texas A&M University
Bob Svendsen RWTH Aachen University
George Voyiadjis Louisiana State University
Quanshui Zheng Tsinghua University
Thomas Böhlke Karlsruhe Institute of Technology (KIT)

Contents

A Fast Fourier Transform-Based Method for Static Field Dislocation Mechanics Within a First Strain Gradient Elasticity Theory of Mindlin Type

Stéphane Berbenni[1]* , Thomas Böhlke[2]

[1] Université de Lorraine, CNRS, Arts et Métiers Institute of Technology, LEM3, Metz, F-57000, France

[2] Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Karlsruhe, 76131, Germany

* *Presenting author*

Here, a fast Fourier transform (FFT)-based micromechanical method for static Field Dislocation Mechanics (FDM) within a first Strain Gradient Elasticity (SGE) theory of Mindlin type is developed. The kinematic equations of dislocation defects are first presented in the framework of static FDM for periodic media. Using Stokes-Helmholtz decomposition, the incompatible elastic distortion is solved from a prescribed dislocation density field with a Poisson equation. The thermodynamic-based constitutive relationships are reported for stress and double stress tensors as functions of elastic strain and elastic strain gradient tensors, respectively. Homogeneous centrosymmetric materials are considered and are specified for cubic and isotropic materials. Then, the compatible elastic distortion field is obtained from solving equilibrium equations through a generalized Navier-type equation. The Fourier-based method is applied, which defines a generalized Green's function in Fourier space for first SGE of Mindlin type. Thus, the solutions for incompatible and compatible fields can be derived in Fourier space. The efficient Fast Fourier Transform (FFT) algorithm is used based on intrinsic Discrete Fourier Transforms (DFT). The numerical scheme is well adapted to the discrete grid to compute higher order partial derivatives with finite differences, which are transformed to the Fourier space. Therefore, using the inverse FFT, regularized dislocation density fields obtained from the present method are numerically computed for single straight dislocations like pure screw and edge dislocations. Stress and double stress fields are also calculated and compared with analytical results from the literature. Finally, some applications of the method focus on more complex dislocation configurations with distributions of dislocations, as dislocation dipoles and configurations with dislocation walls like low-angle grain boundaries (LAGBs).

Keywords. field dislocation mechanics, strain gradient elasticity, Mindlin, fast Fourier transform method

A Periodic, Non-Singular Dislocation Energy Kernel Based on Gradient Elasticity and Ewald Summation

Bernhard Heininger[1]*, Thomas Hochrainer[1]

[1] Graz University of Technology

* *Presenting author*

Plastic deformation of crystalline solids is primarily caused by the movement of line-like defects, the dislocations. In order to develop a coarse grained continuum description of dislocations (continuum dislocation dynamics, CDD) [1] we seek to derive a local density approximation as suggested in [3] directly from discrete dislocation data on periodic domains. This comprises obtaining the (average) energy from discrete dislocation configurations on periodic domains, while simultaneously avoiding the singularity at the dislocation core, as it results from classical linear elasticity. With regard to the latter, we employ a Helmholtz-type gradient elasticity theory which has been worked out for infinite domains in [2].

In the current work, we present the incorporation of periodicity into isotropic gradient elasticity of Helmholtz type to compute dislocation interaction energies and self-energies on periodic domains. Periodicity is introduced using the Ewald summation (or Ewald splitting) method, which is well known in numerical simulations of molecular dynamics and electrostatics. This approach combines the numerical advantages of periodic formulations with the physical consistency of non-singular elasticity, making it ideal for large-scale simulations of dislocation networks and other crystalline defects. We discuss the choice of the so-called splitting parameter in dependence of the domain discretization. Furthermore, we provide comparisons of energies obtained directly from DDD data with those obtained based on CDD density fields derived from the former.

Keywords. crystal plasticity, continuum dislocation dynamics, discrete dislocation dynamics, computational material modelling

References

[1] T. Hochrainer, S. Sandfeld, M. Zaiser, and P. Gumbsch, Continuum dislocation dynamics: towards a physical theory of crystal plasticity, *Journal of the Mechanics and Physics of Solids*, 63:167–178, 2014.

[2] M. Lazar, The fundamentals of non-singular dislocations in the theory of gradient elasticity: Dislocation loops and straight dislocations, *International Journal of Solids and Structures*, 50(2):352–362, 2013.

[3] M. Zaiser, Local density approximation for the energy functional of three-dimensional dislocation systems, *Physical Review B*, 92(17):174120, 2015.

Microcurl Modelling of Size Effects in Single Crystals

Samuel Forest[1]*, Anjan Mukherjee[2], Mohamed Jebahi[2], Mohamed Abatour[3]

[1] Mines Paris PSL CNRS, France
[2] Arts et Métiers Institute of Technology CNRS LEM3, France
[3] Transvalor, France

* *Presenting author*

The introduction of the dislocation density tensor into the constitutive modelling of single crystalline materials is a fundamental change in the modern approach to crystal plasticity, based on the pioneering works of Nye and Kröner. It makes it possible to address the effect of grain and particle size on the local and global material responses by means of appropriate characteristic lengths. The *Microcurl* model, a variant of Eringen's micromorphic medium, introduces the microdeformation as an ancillary variable to total plastic deformation. It is particularly well-suited for finite element simulations with a number of additional degrees of freedom per node that does not depend on the number of involved slip systems or slip system families [2]. The proposed constitutive framework contains both energetic and dissipative contributions of the dislocation density tensor [1]. Both components are required to identify the material parameters from several data: results of dislocation dynamics simulations of cyclic plasticity and experimental results from the literature including the bending torsion of a L-beam micro-specimen under various passivation conditions [4]. The model is finally used to distinguish geometric effects from actual size effects in the compression of thin metallic layers [3].

Keywords. crystal plasticity, micromorphic, size effect

References

[1] Y. A. Amouzou-Adoun, M. Abatour, M. Jebahi, S. Forest, and M. Fivel, Enhanced plastic distortion based micromorphic model for flexible control of scaling effects, *International Journal of Solids and Structures*, 322: 113568, 2025, doi: 10.1016/j.ijsolstr.2025.113568.

[2] N. M. Cordero, A. Gaubert, S. Forest, E. Busso, F. Gallerneau, and S. Kruch, Size effects in generalised continuum crystal plasticity for two–phase laminates, *Journal of the Mechanics and Physics of Solids*, 58: 1963–1994, 2010.

[3] Y. Mu, X. Zhang, J. W. Hutchinson, and W. J. Meng, Dependence of confined plastic flow of polycrystalline Cu thin films on microstructure, *MRS Commun.*, 6(3):289–294, 2016.

[4] B. Zhang, K. L. Nielsen, J. W. Hutchinson, and W. J. Meng, Toward the development of plasticity theories for application to small-scale metal structures, *Proc. Natl. Acad. Sci.*, 120(44):e2312538120, 2023.

A CPFEM-Based Virtual Testing Approach for Characterizing Anisotropic Plastic Behavior of Additively Manufactured Low-Carbon Lath Martensitic Steel

Hoyoung Lee[1*], Jehyun You[2], Myoung-Gyu Lee[2]

[1] Hyundai Motors Group

[2] Department of Material Science & Engineering, Seoul National University

[*] *Presenting author*

Additively manufactured low-carbon lath martensitic steel can exhibit direction-dependent mechanical behavior due to process-induced microstructural heterogeneity. However, direct experimental characterization of the corresponding anisotropic constitutive response remains challenging. In this study, a microstructure-informed representative volume element (RVE) and crystal plasticity finite element modeling (CPFEM) are employed to perform virtual mechanical tests and to examine the macroscopic anisotropic plastic response. Based on the CPFEM results, a continuum-level constitutive description is constructed for use in engineering-scale simulations where experimental data are limited. The predicted constitutive response is then compared with experimental observations, showing reasonable agreement in the measured directional behavior. The results suggest that RVE-based CPFEM can provide a useful basis for identifying anisotropic constitutive behavior and for supporting continuum-scale modeling of additively manufactured steels.

Keywords. additive manufacturing, crystal plasticity, automotive applications

Characterizing and Modelling the Viscoplastic Anisotropy of Tin Single Crystals Using CPFEM

Alain Twisungemariya[1*], Veronique Doquet[1], Eric Charkaluk[1]

[1] Ecole Polytechnique, Laboratoire de Mécaniques du Solides, CNRS

[*] *Presenting author*

The reliability of electronic assemblies heavily depends on the durability of Sn-based solder joints grids. Due to their sub-millimeter scale, these joints solidify into nearly single-crystal dendritic β-Sn structures (over 90% in mass), with Cu and Ag-containing intermetallic particles. The low symmetry of the tetragonal (β) tin lattice induces a pronounced thermo-elastic and viscoplastic anisotropy, and since the solder joints undergo both cyclic and sustained stresses at high homologous temperatures ($T/T_m > 0.50$ at room-temperature), they exhibit highly orientation-dependent service lives, due to a combination of creep, ratchetting, and fatigue [1].

Characterizing the viscoplastic anisotropy of pure tin, through tests run on a sufficiently wide range of crystal orientations, and then capturing the observed behaviors through a Crystal Plasticity (CP) model, should be the first steps towards reliable modelling of the multiphase solder joints behavior. However, the corresponding literature is limited. Moreover, some authors tested directionally-grown tin single crystals in tension [3] or made nanoindentation tests on individual grains in tin polycrystals [2], these methods face some limitations: directional solidification mostly yields crystal orientations near [110] restricting the investigated range of orientations, while the complex stress field in nanoindentation often masks anisotropy.

In this study, a large set of single crystal dogbone-shaped tin specimens, with sufficiently varied orientations, ensuring the independent activation of most of the 10 potential slip families, were solidified, polished, and submitted to tensile cyclic or creep tests at room temperature. A combined analysis of the surface slip lines, and the strain fields measured by Digital Image Correlation or obtained by CPFEM simulations, the type of activated slip systems could be determined for most tests, and the hardening and viscous parameters of each one was identified. Such dialog between experimental data and CPFEM simulations showed that the hardening parameters are highly dependent on the type of active slip system which was not the case for the viscous parameters. Viscous stress exponents n are all between 3 and 5, which appears consistent with common underlying creep mechanisms: dislocation glide and climb plus cross-slip

Keywords. crystal plasticity, single crystal, digital image correlation, creep

References

[1] A. Bleuset and E. Charkaluk, Creep behavior of SAC305 quasi-single crystals at 185 °C, *EMMC19, Madrid, Spain*, 2024, May 29-31.

[2] B. Ernst, On the anisotropic indentation modulus and anisotropic creep behavior of β-Sn characterized by nanoindentation methods, *Mater. Sci. Eng. A*, 848, 2022.

[3] J. Weertman, Creep of tin single crystals, *J. Appl. Phys.*, 27, 1956.

Effects of Texture on Twin Propagation and Thickening in Magnesium Alloys

Filip Šiška[1*], Andrej Ostapovec[1], Daria Drozdenko[2], Patrik Dobron[2]

[1] Institute of Physics of Materials, Czech Academy of Sciences

[2] Department of Physics of Materials, Faculty of Mathematics and Physics, Charles University

[*] *Presenting author*

Twinning is the significant deformation mechanism in HCP metals and alloys. Due to its complex mechanisms, it is still not fully understood. Twinning spans several length scales within the microstructure, from the atomic level during initiation to the grain-scale during propagation and thickening. The twinning process significantly changes the stress and strain distribution within the microstructure by imposing lattice rotation and twin shear. Twinning analysis requires a multiscale modelling approach. The study presented here focuses on the grain-scale interaction of the propagating twin with the surrounding microstructure. The main focus is on the distribution of stresses and strains and their dependence on twins' geometrical characteristics and crystallographic orientations of surrounding grains. The numerical analysis is performed using the finite element method within the framework of the crystal plasticity model for HCP materials. The twin is treated as an inclusion inside the microstructure, which undergoes internal shear strain transformation. The microstructural effects are evaluated by the stress that has to be applied in order to keep the system in equilibrium.

Keywords. crystal plasticity, FEM, twinning, HCP alloys

Assessment of Numerical Schemes for Solving Higher-Order Gradient Crystal Plasticity Model

Yuichi Tadano[1*], Chikako Natsumeda[1]

[1] Saga University

[*] *Presenting author*

Mechanical behavior of metallic materials is strongly influenced by the size effect at the micrometer scale. The conventional crystal plasticity theories, which are widely used for the meso-scale modeling of polycrystalline metals, do not represent the size effect because these theories cannot consider the accumulation of dislocations. Therefore, a higher-order gradient crystal plasticity model has been proposed for taking the dislocation information into account to describe the size effect [2]. In this model, geometrically necessary dislocations (GND) are introduced into a hardening function of the slip system. In this model, the following governing equations for displacement and GND density fields should be simultaneously solved.

The high-order gradient crystal plasticity model, which couples the displacement and dislocation density fields, can be interpreted as a kind of mixed problem. In a mixed problem, the combination of analytical schemes for each field may strongly affect the analysis result. In fact, the finite element method (FEM) sometimes provides an improper solution in the higher-order gradient crystal plasticity analysis [1]. The reproducing kernel particle method (RKPM), which is a kind of meshfree method, is an alternative way to solve this model [3]. In this study, a quantitative investigation of effect of selection of element in the FEM and basis function in the RKPM on the high-order gradient crystalline plasticity analysis is demonstrated, and suitable numerical scheme to solve the higher-order gradient plasticity is discussed.

Keywords. crystal plasticity, gradient plasticity, numerical method

References

[1] M. Kuroda, On large-strain finite element solutions of higher-order gradient crystal plasticity, *International Journal of Solids and Structures*, 48(24):3382–3394, 2011, ISSN 0020-7683, doi: 10.1016/j.ijsolstr.2011.08.008.

[2] M. Kuroda and V. Tvergaard, A finite deformation theory of higher-order gradient crystal plasticity, *Journal of the Mechanics and Physics of Solids*, 56(8):2573–2584, 2008, ISSN 0022-5096, doi: 10.1016/j.jmps.2008.03.010.

[3] Y. Tadano and N. Zenimoto, Kink strengthening mechanism due to multiple kink bands in long-period stacking ordered magnesium alloy, *Computational Materials Science*, 263:114428, 2026, ISSN 0927-0256, doi: 10.1016/j.commatsci.2025.114428.

Geometrical Interpretation of Commutative-Symmetrical Stretch Tensor Products and the Decoupling of Material (An)isotropy From Deformation-Induced Anisotropy

Klaus Heiduschke[1]*

[1] Alumnus of Institut für Mechanik, ETH Zurich

* *Presenting author*

Based on stretch tensor projections, the Lagrangean and Eulerian total, plastic/inelastic and elastic deformation ellipsoids, associated with Lagrangean or Eulerian commutative-symmetrical stretch tensor products [1, 2], can be interpreted geometrically as material deformations. The six internal degrees of freedom, reflected in three stretch eigenvalues and three principal directions of the symmetric stretch tensors, correspond to three semi-axes and three principal directions of the total, plastic/inelastic, elastic deformation ellipsoids. In the case of a plastic deformation ellipsoid, its six internal degrees of freedom can be controlled completely by a symmetric plastic-flow rule. And the Lagrangean and Eulerian total, plastic/inelastic, elastic deformation ellipsoids are related to each other by the Lagrangean and Eulerian commutative-symmetrical stretch tensor products, respectively. Since the multiplicative logarithmic strain space formulation [2] and the commutative-symmetrical stretch tensor products [1] represent both an Eulerian description and a Lagrangean description at the same time, their Eulerian characteristic may be employed to properly model the (overall) elastic isotropy and their Lagrangean characteristic may be utilized to decouple the material (an)isotropy from the deformation-induced anisotropy. This aspect is further discussed in particular with respect to material orthotropy. A new elasto-plastic/-inelastic interpretation of the continuum mechanics framework of the multiplicative logarithmic strain space formulation is presented in detail. This leads to new tensor definitions of the elastic and plastic/inelastic logarithmic Hoger stresses in addition to the well-known total logarithmic Hoger stress.

Keywords. anisotropic elasto-plasticity/-inelasticity, finite deformation-induced anisotropy, material (an)isotropy, multiplicative stretch tensor decomposition, multiplicative logarithmic strain space formulation

References

[1] K. Heiduschke, A commutative-symmetrical multiplicative decomposition of left and right stretch tensors, *International Journal of Solids and Structures*, 144–145:59–65, 2018, ISSN 0020-7683, doi: 10.1016/j.ijsolstr.2018.04.013.

[2] K. Heiduschke, On the multiplicative logarithmic strain space formulation, *Technische Mechanik* (*ICMM5 Edition*), 38:22–40, 2018, ISSN 0232-3869, doi: 10.24352/UB.OVGU-2018-004.

On Force Interactions for Electrodynamics-Like Theories

Reuven Segev[1*], Vladimir Gol'dshtein[2]

[1] Ben-Gurion University of the Negev, Department of Mechanical Engineering, Beer-Sheva, Israel
[2] Ben-Gurion University of the Negev, Department of Mathematics, Beer-Sheva, Israel

[*] *Presenting author*

In earlier works (see [2, 3, 4]), a framework for premetric p-form electrodynamics is proposed. Independently of particular constitutive relations, the generalized Maxwell equations are derived as a special case of stress theory in geometric continuum mechanics. In the proposed setting, generalized velocities are modeled mathematically as p-differential forms, interpreted physically as potential forms. In addition, for the expression of the mechanical power/potential energy, the stress field is assumed to have a particularly simple form.
In this work (see [1]), we extend the theory to propose expressions for the force and stress interactions acting on a charged/magnetized body due to external electromagnetic fields. The expression for the force distribution, viewed as a linear functional of virtual velocity fields, is obtained by computing the rate of change of the proposed potential energy under a virtual motion of the region. The expressions we obtain differ from those appearing in the standard references. For example, in the case of electrostatics in $\mathbb{R}^3$, letting F, w, D, and E, denote the force functional, virtual velocity of the material, electric displacement, and the electric field, respectively, the force functional is of the form

$$F(w) = \int_\Omega D_{j,j} E_i w_i \, dV + \int_\Omega D_j E_{i,j} w_i \, dV + \int_\Omega D_j E_i w_{i,j} \, dV.$$

It is noted that the last integral includes stress-like and torque-like interactions.
The cases of electrostatics and magnetostatics in $\mathbb{R}^3$ are presented as examples.

Keywords. electrodynamics, field theory, geometric continuum mechanics, stress, potential energy, forces

References

[1] V. Goldshtein and R. Segev, On force interaction for electrodynamics-like theories, 2026, arXiv:2601.10308v1 [math-ph].

[2] R. Segev, Continuum mechanics, stresses, currents and electrodynamics, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 374(2066):20150174, 2016, ISSN 1364-503X, doi: 10.1098/rsta.2015.0174.

[3] R. Segev, *Foundations of Geometric Continuum Mechanics*. Birkhauser, 2023, ISBN 978-3-031-35654-4.

[4] R. Segev, Electrodynamics and geometric continuum mechanics, *Continuum Mechanics and Thermodynamics*, 37:33, 2025, doi: 10.1007/s00161-025-01364-1.

Polyconvexity with Moments and Sums of Squares

Giovanni Fantuzzi[1], Didier Henrion[2], Martin Kružík[3], Ajay Murali[1], Stephan Weis[4*]

[1] University of Erlangen–Nuremberg, Department Mathematik, Erlangen, Germany
[2] University of Toulouse, LAAS-CNRS, Toulouse, France
[3] Czech Academy of Sciences, UTIA, Prague, Czechia
[4] Czech Technical University in Prague, Faculty of Electrical Engineering, Prague, Czechia

[*] *Presenting author*

Energy densities that are polyconvex are popular in material modeling and nonlinear elasticity. They can describe physically meaningful properties while guaranteeing mathematical well-posedness. High compression can be prevented by penalizing small determinants of the deformation gradient. Energy-minimizing deformations exists under growth conditions at infinity, given suitable boundary conditions. If the energy density is not polyconvex, then its polyconvex envelope is a relaxation that still respects physics.
Yet, computing the polyconvex envelope pointwise is generally difficult. Existing numerical approaches employ an infinite-dimensional moment problem and face significant challenges. We propose a numerical method to compute the polyconvex envelope of polynomial energy densities, based on the moment sum-of-squares hierarchy from polynomial optimization. Furthermore, we present a sufficient conditions to certify polyconvexity via sum-of-squares technology. A preprint [1] is available at https://arxiv.org/abs/2604.11124.

Keywords. elasticity, polyconvexity, sum of squares, polynomial optimization

References

[1] G. Fantuzzi, D. Henrion, M. Kružík, A. Murali, and S. Weis, Polyconvexity with moments and sums of squares, 2026, https://arxiv.org/abs/2604.11124.

Sweeping Process in Stress-Based Models of Elastoplasticity

Ivan Gudoshnikov[1*]

[1] Institute of Mathematics, Czech Academy of Sciences

[*] *Presenting author*

The connection between plasticity phenomenon in mechanics and the sweeping process was noticed since the very discovery of the sweeping process as a mathematical problem. Specifically, when the stress distribution is considered as a state variable, the "moving set" of a sweeping process reflects the interplay between the "elastic range" characteristic of an elastoplastic material, and the constraint of quasistatic equilibrium.
In the presentation we will discuss the implications of this idea for various types of plasticity (strain hardening, perfect plasticity [1], strain softening [2]), and pay attention to the accompanying challenges.

Acknowledgements. This research is supported by the Czech Science Foundation project GA24-10586S and the Czech Academy of Sciences (RVO: 67985840).

Keywords. elastoplasticity, sweeping process, convex analysis, strain softening

References

[1] I. Gudoshnikov, Regularity lost: The fundamental limitations and constraint qualifications in the problems of elastoplasticity, *Discrete Contin. Dyn. Sys.*, 51(0):370–438, 2026, doi: 10.3934/dcds.2026034.

[2] I. Gudoshnikov, Elastoplasticity with softening as a state-dependent sweeping process: non-uniqueness of solutions and emergence of shear bands in lattices of springs, 2026, doi: 10.48550/arXiv.2508.16333, preprint, accepted to *Math. Eng.*

A Crystal-Plasticity Finite Element Framework to Assess the Fatigue Behavior of Turbine Blades Through Geometrically Necessary Dislocations Criteria and Conform Meshes

Sam Gadoin[1*], Aurélien Vattré[2], Christophe Bovet[2], Vincent Chiaruttini[3], Lucie Lanciaux[4]

[1] Safran Tech, ONERA
[2] ONERA
[3] Safran Tech
[4] Safran Aircraft Engines

[*] *Presenting author*

This current work is dedicated to the study of aircraft engine turbine's blades made in a directionally solidified nickel-based alloy. Due to its complex manufacturing process and to empirical conservative quality criteria of the manufacturer, numerous blades are scrapped. The versatility of the finite element method is used to model a whole aircraft engine turbine blade at the grain scale to quantify its fatigue behavior. This framework relies on a crystal plasticity large strain model, involving a multiplicative decomposition of the transformation. Plasticity is embodied by dislocation theory, in which both statistical dislocation and geometrically necessary dislocation (GND) densities are represented. A Kocks-Mecking law and the Orowan relation are used to quantify the plastic flow. The GNDs are computed through the curl of the plastic strain and projected on the sliding systems.
In previous works [2], a monotone behavior was defined to represent tensile stress tests on equiaxial REV. This work is dedicated to improve this law by adding a kinematic hardening [1] to explicit fatigue behavior of columnar REV. Fatigue Indicator Parameters are developed based on the dislocation densities to define lifespan criteria.

Keywords. crystal plasticity, fatigue indicator parameter, simulation, kinematic hardening, columnar grains, finite element, conform mesh, geometrically necessary dislocations

References

[1] C. Bayley, W. Brekelmans, and M. Geers, A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity, *International Journal of Solids and Structures*, 43(24):7268–7286, 2006, ISSN 0020-7683, doi: 10.1016/j.ijsolstr.2006.05.011, Size-dependent Mechanics of Materials.

[2] C. Bovet, V. Chiaruttini, and A. Vattré, Full-scale crystal plasticity modeling and data-driven learning of microstructure effects in polycrystalline turbine blades, 2025, doi: 10.2139/ssrn.5984981.

Atomistic Investigation of Anisotropic Radiation-Induced Embrittlement

Hojjat Mousavisogolitappeh[1*], Stanisław Stupkiewicz[1], Aneta Ustrzycka[1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences

[*] *Presenting author*

Radiation-induced degradation in structural alloys originates from defect formation and evolution at the atomic scale, which significantly alters mechanical behavior and fracture mechanisms. In this study, we present an atomistic investigation of anisotropic radiation-induced embrittlement in Fe–Ni–Cr alloys using molecular dynamics (MD) simulations [1, 2].

Neutron irradiation generates complex defect populations, including vacancy clusters, stacking fault tetrahedra (SFTs), and dislocation structures, which emerge from displacement cascades and govern subsequent microstructural evolution. To accurately represent the alloy system, simulations are performed using a validated Fe–Ni–Cr interatomic potential capable of capturing radiation-induced defect behavior. Radiation-induced defect structures are systematically created, and their influence on crack-tip behavior and fracture mechanisms is analyzed under controlled loading conditions.

Crack propagation is analyzed under Mode-I loading for different crystallographic orientations, namely (001), (011), and (111). The results reveal strong orientation-dependent fracture behavior governed by defect–dislocation interactions and slip system activity.

Furthermore, the results provide clear evidence of irradiation-assisted ductile-to-brittle transition (DBT), where increasing defect density suppresses plastic deformation and accelerates crack propagation. The transition is quantified using atomistic energy-based fracture metrics, in which the critical energy release rate is evaluated directly from MD simulations, thereby providing a consistent description of fracture energetics at the nanoscale.

This work provides a comprehensive atomistic framework for understanding the interplay between irradiation-induced defects, crystallographic anisotropy, and fracture behavior in Fe–Ni–Cr alloys, offering insights into the fundamental mechanisms governing embrittlement at the nanoscale.

Acknowledgements. The National Science Centre in Poland supports this work through Grant No UMO-2020/38/E/ST8/00453.

Keywords. crack propagation, radiation defects, MD simulations, Cr-rich alloy, T–S law, atomic-scale fracture energy, ductile-to-brittle transition

References

[1] H. Mousavi, S. Stupkiewicz, and A. Ustrzycka, Molecular dynamics study of the role of anisotropy in radiation-driven embrittlement, *International Journal of Plasticity*, 201:104686, 2026.

[2] A. Ustrzycka, H. Mousavi, F. Dominguez-Gutierrez, and S. Stupkiewicz, Atomistic study of radiation-induced ductile-to-brittle transition in austenitic steel, *International Journal of Mechanical Sciences*, 303: 110567, 2025.

Fatigue Life Prediction at the Microstructural Scale Considering Plastic Strain Localisation

Mathieu Musy-Haspel[1*], Aldo Marano[1], Samuel Forest[2], Lionel Gelebart[3]

[1] DMAS, ONERA, Université Paris-Saclay, F-92322, Châtillon, France

[2] Mines Paris PSL, Centre des matériaux, CNRS UMR 7633, Versailles, France

[3] Université Paris-Saclay, CEA, SRM, Gif-sur-Yvette, 91191, France

[*] *Presenting author*

During cyclic loading, particularly at low strain amplitudes, the time required for crack initiation can account for most of the fatigue life. Predicting the number of cycles to crack initiation is therefore a central issue in component design. In nickel-based superalloys such as Inconel 718, fatigue crack initiation is closely linked to the formation of Persistent Slip Bands (PSBs), within which plastic strain localizes. These bands result from the irreversible accumulation of dislocations, which gradually organize into structures leading to the formation of surface extrusions or intrusions, or stress concentrations at grain boundaries, along which cracks preferentially initiate.

The formation of these bands strongly depends on the local microstructure. It is therefore necessary to work at this scale in order to predict crack initiation life. The current state of the art generally relies on crystal plasticity simulations performed on numerical polycrystalline microstructures. The results are then used to construct Fatigue Indicator Parameters (FIPs), which are subsequently related to fatigue life through empirical laws identified from experimental data. However, the models and spatial resolution commonly used in these simulations remain poorly suited to representing strain localisation in the form of slip bands. In addition, the associated life criteria do not always directly account for the physical mechanisms governing crack initiation, particularly the irreversibility of plastic deformation.

This work aims to investigate the effect of plastic strain localisation on the prediction of fatigue life. A crystal plasticity model capable of capturing strain localisation in the form of persistent slip bands is employed. Numerical simulations are used to compute local ratcheting, which directly quantifies the irreversibility of plastic deformation along these bands. The locally accumulated irreversible energy, associated with dislocation accumulation in the PSBs, is evaluated as the dissipated energy weighted by the ratcheting quantity. This energy is then compared with the specific free surface energy, following the Tanaka–Mura–Wu formalism, to estimate fatigue crack nucleation life. This approach allows the consideration of plastic strain localisation, the accurate identification of likely crack initiation sites, and a direct link between the local microstructural mechanisms of localisation and fatigue life criteria. It is finally applied to numerical microstructures containing typical fatigue-sensitive features, such as carbides, coarse grains, and twin boundaries, to assess its ability to capture the criticality of these features and the competition between different crack initiation mechanisms.

Keywords. fatigue life prediction, crystal plasticity, plastic strain localisation, slip bands

Revealing Fracture-Resistant Design Principles in Harmonic-Structured High-Entropy Alloys Using Quasi In-Situ Experiments and Integrated Modeling

Tang Gu[1]*  , Ruo-Fei Yuan[2], Yun-Fei Jia[2]

[1] Institute of Polytechnic Science and Aeronautics (IPSA), Ivry-sur-Seine, France
[2] East China University of Science and Technology (ECUST), Shanghai, China

* *Presenting author*

Harmonic-structured (HS) metallic materials have attracted increasing attention due to their outstanding strength–ductility synergy. However, the grain-scale fracture mechanisms governing damage initiation and propagation in HS microstructures remain insufficiently understood, limiting the establishment of predictive design strategies for strength–toughness optimization. In this work, HS CoCrFeMnNi high-entropy alloys with systematically tailored fine-grain (FG) shell fractions were fabricated to elucidate intrinsic fracture-resistant mechanisms. Quasi in-situ tensile experiments combined with electron backscatter diffraction (EBSD) and crystal plasticity finite element–cohesive zone modeling (CPFEM–CZM) reveal that FG regions exhibit higher crack susceptibility due to pronounced strain gradients, particularly at coarse-grain (CG)/FG interfaces and within FG zones. These strain gradients evolve with increasing deformation and intensify local stress concentrations through deformation incompatibility, promoting preferential crack nucleation and early crack propagation. In contrast, CG regions display superior intrinsic deformability and enable sustained plastic energy dissipation. As cracks propagate into CG domains, the activation of multiple slip systems generates elevated geometrically necessary dislocation densities near crack tips, leading to enhanced back stress, crack blunting, and increased fracture tolerance. A critical FG fraction of 31.4% is identified, which effectively suppresses premature crack nucleation in FG regions while preserving high strength unattainable in low-FG HS counterparts. This optimized dual-phase synergy ensures an enhanced balance between strength and fracture resistance. The present study quantitatively elucidates the role of FG fraction in damage tolerance and establishes microstructural design principles for fracture-resistant architectured and high-entropy alloys.

Keywords. harmonic structure, high entropy alloy, crystal plasticity, cohesive zone model, fracture mechanisms, back stress, energy dissipation

References

[1] T. Gu, J.-R. Medy, V. Klosek, O. Castelnau, S. Forest, E. Hervé-Luanco, F. Lecouturier-Dupouy, H. Proudhon, P.-O. Renault, L. Thilly, *et al.*, Multiscale modeling of the elasto-plastic behavior of architectured and nanostructured Cu-Nb composite wires and comparison with neutron diffraction experiments, *International Journal of Plasticity*, 122:1–30, 2019.

[2] R.-F. Yuan, Y. Zhang, Y. Zhang, B. Dong, Y.-J. Wang, Z. Zhang, T. Gu, Y.-F. Jia, and F.-Z. Xuan, Revealing fracture-resistant design principles in harmonic-structured high-entropy alloys using quasi in situ experiments and integrated modeling, *International Journal of Plasticity*, page 104600, 2025.

Modeling Metamaterials by Second-Order Rate-Type Constitutive Relations Between Only the Macroscopic Stress and Strain

Vít Průša[1]*

[1] Faculty of Mathematics and Physics, Charles University

* *Presenting author*

Following [2], we discuss a novel thermodynamically based approach for constructing effective rate-type constitutive relations describing finite deformations of *metamaterials*. The effective constitutive relations are formulated as *second-order* in time rate-type Eulerian constitutive relations between only the Cauchy stress tensor, the Hencky strain tensor, and objective time derivatives thereof. In particular, there is no need to introduce additional quantities or concepts such as "micro-level deformation", "micromorphic continua", "enriched continua", or elastic solids with frequency dependent material properties.
The linearisation of the proposed fully nonlinear (finite deformations) constitutive relations leads, in Fourier space, to the same dispersion relations as those commonly used in metamaterial theories based on the concepts of frequency dependent density and/or stiffness. From this perspective the proposed constitutive relations reproduce the behaviour predicted by the frequency dependent density and/or stiffness models, but yet they work with constant — that is motion independent — material properties. The behaviour predicted by the linearised models is documented through numerical experiments exploiting the dispersion-relation preserving discretisation proposed in [1].
Finally, we argue that the proposed fully nonlinear (finite deformations) second-order in time rate-type constitutive relations do not fall into the traditional classes of models for elastic solids (hyperelastic solids/Green elastic solids, first-order in time hypoelastic solids), and that the proposed constitutive relations embody a new class of constitutive relations characterising elastic solids.

Acknowledgements. The author thanks the Czech Science Foundation, grants no. 20-11027X and no. 25-16592S, for its support.

Keywords. elasticity, metamaterials, rate-type equations

References

[1] L. Fusi, O. Křenek, V. Průša, C. Rodriguez, R. Tozzi, and M. Vejvoda, Discrete versus continuous—linear lattice models and their exact continuous counterparts, *International Journal of Engineering Science*, 224: 104530, 2026, ISSN 0020-7225, doi: 10.1016/j.ijengsci.2026.104530.

[2] V. Průša, C. Rodriguez, L. Trnka, and M. Vejvoda, Modeling metamaterials by second-order rate-type constitutive relations between only the macroscopic stress and strain, *European Journal of Mechanics - A/Solids*, 116:105879, 2026, ISSN 0997-7538, doi: 10.1016/j.euromechsol.2025.105879.

On the Size Effect in Cellular Foam Materials: A Combined Numerical and Experimental Investigation

Fenil Maganbhai Lathiya[1*], Geralf Hütter[1], Stephan Kirchhof[2], Björn Kiefer[1]

[1] TU Bergakademie Freiberg, Institute of Mechanics and Fluid Dynamics, Germany
[2] Faculty of Mechanical Engineering, Hochschule für Technik und Wirtschaft Dresden – University of Applied Sciences, Dresden, Germany

[*] *Presenting author*

The mechanical behavior of foam materials is of great interest in lightweight engineering due to their excellent stiffness-to-weight ratio. However, the presence of a microstructure with a characteristic length comparable to component dimensions leads to size effects that are not yet fully understood. The literature reports conflicting observations; for instance, experimental studies have shown that smaller specimens can appear stiffer (a positive size effect) [1], while other investigations have reported the opposite trend where smaller specimens appear more compliant (a negative size effect) [3]. This ambiguity motivates a deeper investigation into the underlying mechanisms. This contribution aims to shed light on the sign and magnitude of size effects in foams by combining insights from recent numerical and experimental work. Virtual testing on ceramic foams, which avoids experimental artifacts, has indicated a clear negative size effect across different loading modes [2]. In parallel, direct numerical simulations of foam-like structures have revealed that both positive and negative size effects can emerge depending on the specific loading conditions applied [4]. Our ongoing research extends these investigations to polymeric foams with the goal of creating a profound experimental database as a basis to the development of generalized continuum theories to describe these size effects.

Acknowledgements. Funding by the Deutsche Forschungsgemeinschaft (DFG) under the grant number HU 2279/7-1 is gratefully acknowledged.

Keywords. foam, cellular materials, size effect, virtual testing

References

[1] W. B. Anderson and R. S. Lakes, Size effects due to cosserat elasticity and surface damage in closed-cell polymethacrylimide foam, *J. Mater. Sci.*, 29(23):6413–6419, 1994.

[2] S. Kirchhof, A. Ams, and G. Hütter, On the question of the sign of size effects in the elastic behavior of foams, *J. Elast.*, 153:1–24, 2023.

[3] C. Liebold and W. H. Müller, Applications of higher-order continua to size effects in bending: Theory and recent experimental results, In *Proc. 7th Int. Conf. Coupled Probl. Sci. Eng.*, 2016.

[4] A. Malik, G. Hütter, M. Abendroth, and B. Kiefer, Micromorphic FE² simulation of plastic deformations of foam structures, *Int. J. Mech. Sci.*, 265:108877, 2024.

Numerical Modeling of the Mechanical Behavior of New Architectured Materials Based on Bi-Crystallographic Analogies

Nicolas Lallemand[1*], Thiebaud Richeton[1], Justin Dirrenberger[2], Stéphane Berbenni[1]

[1] Université de Lorraine, CNRS, Arts et Métiers Paris Tech, LEM3, F-57000 Metz, France
[2] PIMM, Arts et Métiers, Cnam, CNRS UMR 8006, 151 bd de l'Hôpital, 75013 Paris, France, Institut universitaire de France (IUF), France

* *Presenting author*

Additive manufacturing has allowed the development of architectured materials in the industry. However, despite their advantages, such as their low density and good energy absorption, the use of cellular materials as structural components is still hindered by concerns toward their mechanical stability and resistance [1]. In particular, highly periodic stretch-dominated lattice structures are subjected to the emergence of localization bands, which causes mechanical instabilities and early structural failure. A framework for improving the mechanical resistance of those lattice metamaterials consists in basing the design guidelines on an analogy between the macroscopic lattice structures and the crystalline microstructures [2]. For example, the introduction of defects like interfaces between different lattice orientations has been shown to hinder localization band propagation in an analogous manner to the interaction between grain boundaries and slip bands in polycrystals [2]. The objective of this study is to expand this framework by further exploring the analogy between both materials. The novelty of this approach stems from the implementation of the bi-crystallographic Coincidence Site Lattice (CSL) theory, commonly used in grain boundary engineering, to the design of bi-crystal inspired truss. Here, the CSL based bi-crystal parameters give access to bi-crystal inspired truss with a strong diversity of interface connectivity, through the nodes shared by the two lattice orientations. This allows to evaluate the influence of specific interfacial connectivity on both local and global mechanical behaviors. The reliability of this design methodology is assessed through finite element calculations. In fact, these simulations enable to assess the interface's influence on strain localization and on the lattice-based architectured material's stretch or bending-dominated deformation mode.

Acknowledgements. The authors thank the French National Research Agency (ANR) for their financial support, under grant number ANR-23-CE08-0032 (MIRACLES project).

Keywords. architectured materials, bi-crystal inspired, interface, coincidence site lattice

References

[1] M. Benedetti, A. du Plessis, R. O. Ritchie, M. Dallago, N. Razavi, and F. Berto, Architected cellular materials: A review on their mechanical properties towards fatigue-tolerant design and fabrication, *Materials Science and Engineering: R: Reports*, 144:100606, 2021, doi: 10.1016/j.mser.2021.100606.

[2] M.-S. Pham, C. Liu, I. Todd, and J. Lertthanasarn, Damage-tolerant architected materials inspired by crystal microstructure, *Nature*, 565(7739):305–311, 2019, doi: 10.1038/s41586-018-0850-3.

Well-Posed Continuum Damage Models Without the Agonizing Gradient

Celine Lauff[1], Matti Schneider[2*], André Schlichting[3], Thomas Böhlke[1]

[1] Karlsruhe Institute of Technology (KIT)
[2] University of Duisburg-Essen
[3] Ulm University

* *Presenting author*

Classical local damage models which represent softening behavior come with a serious bottleneck: Their computational response at component level depends on the used mesh, a result of the underlying mathematical ill-posedness of the localization phenomenon implied by softening.
Traditional remedies include non-local or gradient-enhanced formulations which effectively preclude localization by introducing a suitable length scale. However, these formulations come with a few downsides: Integrating them into finite element (FE) codes is rather intrusive, they are not necessarily well-posed in terms of uniqueness and they cannot be up-scaled, i.e., homogenized. The alternative route via adding a viscous term nullifies the elastic region of the model.
We discuss a damage-modeling approach based on measure theory, i.e., describing the distribution of "damaged mass". Based on the established framework of continuum thermodynamics, the model is formulated by specifying both the free energy and the dissipation in a direct way. The involved potentials are, by definition, convex, and lead to a well-posed mechanical problem. Put differently, the model leads to a mesh-independent response which may be computed in a numerically robust way. Moreover, due to their local nature, these models may be readily integrated into conventional user subroutines of industrial FE codes.

Acknowledgements. Matti Schneider acknowledges the support from the European Research Council within the Horizon Europe program - project 101040238. Celine Lauff and Thomas Böhlke acknowledge the partial support by the German Research Foundation (DFG) within the International Research Training Group "Integrated engineering of continuous-discontinuous long fiber reinforced polymer structures" (GRK 2078) – project 255730231.

Keywords. damage mechanics, local damage model, softening, well-posed, generalized standard material

Constitutive Modeling of Coupled Dissipation Processes in the Mechanics of Shape Memory Alloys

Miroslav Frost[1*], Alexej Moskovka[1], Petr Sedlák[1], Hanuš Seiner[1], Petr Pelech[2], Barbora Benešová[2]

[1] Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czechia
[2] Charles University, Faculty of Mathematics and Physics, Department of Mathematical Analysis, Prague, Czechia

[*] *Presenting author*

Shape memory alloys provide an example of materials whose mechanical response combines several deformation contributions. In addition to elasticity, dissipative processes associated with martensitic phase transformation and microstructural reconfigurations can be activated during loading. This leads to a rich mechanical response that is also temperature-dependent and gives rise to the so-called shape memory phenomena. At the same time, such a combination of several interdependent deformation processes poses a significant challenge for formulating a plausible constitutive model [1].
Based on thorough experimental characterization, we propose a novel constitutive model that captures the main, rate-independent features of the (thermo)mechanical behavior of NiTi shape memory alloys, including non-conventional plasticity in martensite. By employing the formalism of the Generalized Standard Materials framework, we can treat dissipative deformation processes in a unified manner, avoiding the explicit formulation of force-flux relations for each and any combination of activated processes. On the other hand, the fact that some specific transformation processes can occur only in a particular sequence requires (also due to the non-smooth character of the dissipation function) a refinement of the constitutive relations (evolutionary inclusions), which is then also reflected in the numerical treatment of the constitutive update algorithm.
In the talk, we will briefly summarize the (thermo)mechanical response of NiTi shape memory alloys, identify and characterize the main dissipative deformation processes, and introduce the formulation of the constitutive model within the Generalized Standard Materials framework. A numerical implementation of the model to the finite element method will be proposed and validated. The mathematical aspects on the model formulation will be presented in a subsequent contribution by P. Pelech.

Acknowledgements. This work has been financially supported by the Czech Science Foundation [Project No. 24-10366S] and by the Operational Programme Johannes Amos Comenius of the Ministry of Education, Youth and Sport of the Czech Republic, within the frame of the project Ferroic Multifunctionalities (FerrMion) [Project No. CZ.02.01.01/00/22_008/0004591] co-funded by the European Union.

Keywords. generalized standard material, dissipation function, strongly coupled processes, shape memory alloys

References

[1] M. Frost, B. Benešová, and P. Sedlák, A microscopically motivated constitutive model for shape memory alloys: formulation, analysis and computations, *Math. Mech. Solids*, 21(3):358–382, 2016, doi: 10.1177/1081286514522474.

Numerical Solution of Coupled Dissipation Processes in the Mechanics of Shape Memory Alloys

Miroslav Frost[1], Alexej Moskovka[1], Petr Sedlák[1], Hanuš Seiner[1], Petr Pelech[2*], Barbora Benešová[2]

[1] Czech Academy of Sciences, Institute of Thermomechanics, Prague, Czechia
[2] Charles University, Faculty of Mathematics and Physics, Department of Mathematical Analysis, Prague, Czechia

[*] *Presenting author*

Shape memory alloys are often modeled via non-smooth potentials in the Generalized Standard Materials framework [2]. The non-differentiability of the minimized functional then makes the numerical analysis challenging. Alternate minimization scheme (AMS) is widely used as it reduces dimension of the problem and has been studied thoroughly when the split variables are not coupled by a non-smooth term, see e.g. [1]. Recent paper [3] extends the analysis to variables coupled by a non-smooth dissipation potential, which is a typical case for SMAs; the AMS converges to a limit which depends on the splitting and the solution differs from the one given by the full minimization scheme (FMS). As explained by M. Frost in the preceding contribution, the specific choice of splitting is dictated by physics and therefore the AMS (unlike FMS) reproduces the correct material response. While non-smooth dissipation potentials are iconic for SMAs, the free energy is usually considered to be continuously differentiable. Yet, a simple constraint on the state variables makes the indicator function appear in the energy function, and the resulting problem is then non-smooth in both rates and states. The limiting behavior of the AMS is then no longer covered by the results obtained in [3] and the strategy for describing the effective problem for AMS has to be modified.
In the talk, we will reduce the constitutive model of SMAs given in the preceding contribution by M. Frost in order to make it mathematically feasible and highlight its important properties. We illustrate on simple examples why the FMS and AMS yield different solutions and describe the effective problem for AMS.

Acknowledgements. This work has been financially supported Operational Program Johannes Amos Comenius of the Ministry of Education, Youth and Sport of the Czech Republic, within the frame of the project Ferroic Multifunctionalities (FerrMion) [Project No. CZ.02.01.01/00/22_008/0004591] co-funded by the European Union.

Keywords. shape memory alloys, non-smooth potentials, alternate minimization

References

[1] J. Bolte, S. Sabach, and M. Teboulle, Proximal alternating linearized minimization for nonconvex and nonsmooth problems, *Math. Program.*, 146:459—494, 2014, doi: 10.1007/s10107-013-0701-9.

[2] B. Halphen and Q. S. Nguyen, Sur les matériaux standard généralisés, *J. Mecanique*, 14:39—63, 1975.

[3] A. Mielke, R. Rossi, and A. Stephan, On time-splitting methods for gradient flows with two dissipation mechanisms, *Calc. Var.*, 64(63), 2025, doi: 10.1007/s00526-024-02849-8.

Effects of Nanocrystalline Grain Size and Hydrogen on Stress-Induced Martensitic Transformation in NiTi Shape Memory Alloys: A Phase-Field Study

Kehinde Ajayi[1]*, Adil Benaarbia[1], Charlotte S. Becquart[1], Ludovic Thuinet[1]

[1] Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207—UMET—Unité Matériaux et Transformations, Lille, France

* *Presenting author*

Despite advances in modelling NiTi shape memory alloys, it is still not trivial to model and understand the convoluted impact of variants, grain size, hydrogen amount and thermomechanical coupling in hydrogen-containing systems. This work introduces a thermodynamically consistent phase-field framework integrating Calphad-assessed Ni–Ti thermodynamics with DFT-derived NiTi–H energetics from Tang [3] and Holec *et al.* [2], respectively, to compute phase-specific Gibbs free energies and driving forces for B2 $\rightarrow$ B19′ transformation under dilute hydrogen conditions. Our simulations show stabilisation of austenite by nanocrystalline grain size and hydrogen during stress-induced martensitic transformation. In hydrogen-free NiTi, increasing the grain size lowers the critical applied stress for martensite nucleation, sharpens the transformation plateau, and raises maximum global martensite volume fraction. Hydrogen consistently increases nucleation stress and slope, delays the onset of the forward plateau, and reduces the martensite volume fraction, effects which are amplified at smaller grains. These predictions demonstrate that nanocrystalline grains enhance hydrogen-induced hindrance to martensite nucleation and propagation, leading to incomplete superelastic recovery. They align with experimental results [1], offering mechanistic insights for hydrogen-resistant nanostructured shape memory devices. Finally, we will present the effect of heterogeneous hydrogen distributions, which are encountered for instance during hydrogen loading of the samples, on the onset of the transformation.

Keywords. NiTi shape memory alloy, hydrogen effects, nanocrystalline grains, stress-induced martensitic transformation, phase-field modelling, superelasticity, austenite stabilisation

References

[1] A. Baturin, A. Lotkov, V. Grishkov, I. Rodionov, and V. Kudiiarov, The effect of hydrogen on martensite transformations and the state of hydrogen atoms in binary TiNi-based alloy with different grain sizes, *Materials*, 12(23):3956, 2019, doi: 10.3390/ma12233956, Open access.

[2] D. Holec, M. Friák, A. Dlouhý, and J. Neugebauer, Ab initio study of point defects in NiTi-based alloys, *Physical Review B*, 89(1), 2014, ISSN 1550-235X, doi: 10.1103/physrevb.89.014110.

[3] W. Tang, Thermodynamic study of the low-temperature phase B19′ and the martensitic transformation in near-equiatomic Ti-Ni shape memory alloys, *Metallurgical and Materials Transactions A*, 28(3):537–544, 1997, doi: 10.1007/s11661-997-0041-6.

Modeling the Interaction Between Localized Transformation and Functional Fatigue in Shape Memory Alloys

Mahdi Neghabi[1*], Jędrzej Dobrzański[1], Mohsen Rezaee-Hajidehi[1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland

[*] *Presenting author*

NiTi shape memory alloys (SMAs) are widely utilized in various engineering applications due to their unique properties, such as superelasticity and shape memory effect. The operational lifespan of SMAs in most of the applications involves enduring cyclic mechanical/thermal loadings, which highlights the great importance of identifying their fatigue behavior. Due to the martensitic transformation, fatigue in SMAs is mainly classified into two aspects. The first aspect is known as functional fatigue, which involves the degradation of functional properties such as recoverable strain, transformation stress, and the area of the hysteresis loop. The second aspect is referred to as structural fatigue, which pertains to the evolution of damage within the material.

In superelastic NiTi, stress-induced martensitic transformation typically proceeds in a localized manner through propagation of diffuse interfaces (macroscopic transformation front) that separate low-strain austenite from high-strain martensite. In view of the high strain incompatibilities that exist within the transformation front, and thus large local stresses, it can be inferred that transformation localization plays a key role in the fatigue behavior of the material. Experimental studies have shown that repeated nucleation and propagation of localized bands accelerate superelastic degradation and promote earlier fatigue crack initiation and failure, highlighting a direct link between localization and fatigue performance. While existing constitutive models capture general degradation trends, they fail to distinguish the fatigue evolution in homogeneous versus non-homogeneous (localized) transformations. To address this limitation, this study presents a novel functional fatigue model that integrates the effect of localized transformation into the fatigue constitutive description. The model adopts a gradient-enhanced formulation, in which the gradient of the martensite volume fraction is included to represent the interfacial energy associated with the transformation front. The evolution of fatigue-related variables, namely the irreversible volume fraction of martensite and plastic strain, is explicitly coupled to transformation localization. This coupling is introduced by enriching their evolution laws with the gradient of the martensite volume fraction, so that localized transformation fronts accelerate their accumulation and thereby intensify functional degradation.

A representative numerical study investigates the influence of specimen geometry on fatigue behavior, specifically comparing thin and thick NiTi strips. Experimental observations indicate that, as specimen thickness increases, the transformation front becomes more diffuse, whereas thinner specimens tend to exhibit a sharper transformation front with more branching. It has been revealed that the thicker specimen maintains a higher fatigue life. The developed model is capable of capturing these important morphology-dependent localization effects and their implications for functional degradation effects.

Keywords. shape memory alloys, superelasticity, instabilities, functional fatigue

A Unified Formulation of Gibbs Free Energy for Solids and Fluids

Thomas Böhlke[1]*  , Frank Duderstadt[2]

[1] Karlsruhe Institute of Technology (KIT)

[2] TKMS, Kiel

* *Presenting author*

The Gibbs free energy plays a central role in the modeling of materials within both solid and fluid mechanics, dating back to the seminal work of Gibbs (1873). While its formulation in fluid mechanics is well established and largely undisputed, the situation in solid mechanics is considerably less uniform. Over the past decades, a variety of formulations have been proposed, see, e.g., Truesdell and Toupin (1969), Landau and Lifschitz (1975), Lurie (2005), often based on different choices of kinematic variables, stress measures, and thermodynamic potentials. These approaches are frequently incompatible and may lead to conceptual inconsistencies and therefore have been criticized, see, e.g., Silhavy (1997), Dreyer and Duderstadt (2008), particularly when attempting to establish a unified description that consistently encompasses both solids and fluids.

In this work, existing formulations of the Gibbs free energy for solids are critically analyzed and compared with their counterparts in fluid mechanics. Building on these considerations, a geometrically nonlinear formulation of the Gibbs free energy is proposed. The proposed formulation provides a unified thermodynamic structure that avoids the inconsistencies of earlier approaches and offers a transparent transition between solid-like and fluid-like behavior. Several applications are discussed to illustrate the versatility of the framework and its implications for constitutive modeling in nonlinear continuum mechanics.

Keywords. Gibbs free energy, non-linear continuum mechanics

References

[1] W. Dreyer and F. Duderstadt, On the modelling of semi-insulating GaAs including surface tension and bulk stresses, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 464:2693–2720, 2008, see EMS http://rspa.royalsocietypublishing.org/content/suppl/2009/02/17/464.2098.2693.DC1.html.

[2] J. W. Gibbs, A method of geometrical representation of the thermodynamic properties of substances by means of surfaces, *Transactions of the Connecticut Academy of Arts and Sciences*, 2:382–404, 1873.

[3] L. D. Landau and E. M. Lifschitz, *Elastizitätstheorie*. Walter de Gruyter, 1975.

[4] A. I. Lurie, *Theory of Elasticity*. Springer, 2005 (Original 1970, Nauka, Moscow).

[5] M. Silhavy, *The Mechanics and Thermodynamics of Continuous Media*. Springer, 1997, ISBN 978-3-642-08204-7.

[6] C. Truesdell and R. A. Toupin, The classical field theories, In *Principles of Classical Mechanics and Field Theory / Prinzipien der Klassischen Mechanik und Feldtheorie*, volume III/1 of *Encyclopedia of Physics / Handbuch der Physik*, pages 226–793. Springer, 1960.

A Monolithic Mixed Finite Element Formulation for Thermomechanical Small-Strain Elastoplasticity with Temperature-Dependent Properties

Ahsan Kaleem[1*], Ignacio Romero[1]

[1] 1. IMDEA Materials Institute, Getafe, Spain; 2. Department of Mechanical Engineering, Universidad Politécnica de Madrid, Madrid, Spain

[*] *Presenting author*

Thermomechanical elastoplasticity has been extensively studied; however, many formulations are developed within weakly coupled frameworks and often assume temperature independent material behavior. Fully coupled thermomechanical approaches have also been investigated, but most are formulated in the finite-strain setting and are frequently solved using staggered solution strategies [2]. While temperature-dependent constitutive models have been proposed, they typically are restricted to elastic analyses or consider only a subset of material parameters for inelastic cases. Moreover, existing fully coupled formulations with temperature-dependent properties are commonly developed for specific engineering applications rather than as reproducible benchmark frameworks [1].
Despite these advances, their combined treatment in small-strain thermomechanics remains unexplored, particularly with reproducible benchmark problems. This work presents a fully coupled small-strain thermomechanical formulation for rate-independent elastoplastic materials with combined isotropic and kinematic hardening, in which all constitutive and thermal material properties are explicitly temperature dependent. The governing balance equations and constitutive relations are derived and discretized within a monolithic finite element framework. To avoid volumetric locking associated with nearly incompressible plastic deformation, a mixed displacement–pressure formulation with a stabilization term is employed. The implementation is verified against two benchmark problems with available analytical and semi-analytical solutions, demonstrating excellent agreement. Building on this verification, a suite of benchmark problems is introduced to systematically examine the influence of temperature-dependent material properties on the predicted thermomechanical response. The proposed framework is intended to provide a comprehensive and openly documented benchmark reference for the development, verification, and assessment of numerical methods for coupled thermomechanical problems in small-strain elastoplasticity.

Acknowledgements. This study is part of project PLEC2023-010190, funded by the Spanish Ministry of Science and Innovation, MCIN/AEI/10.13039/501100011033.

Keywords. small-strain thermomechancis, elastoplasticity, benchmarks

References

[1] B. Ali, Y. Heider, and B. Markert, Predicting residual stresses in slm additive manufacturing using a phase-field thermomechanical modeling framework, *Computational Materials Science*, 231:112576, 2024, doi: 10.1016/j.commatsci.2023.112576.

[2] J. Simo and C. Miehe, Associative coupled thermoplasticity at finite strains: Formulation, numerical analysis and implementation, *Computer Methods in Applied Mechanics and Engineering*, 98(1):41–104, 1992, doi: 10.1016/0045-7825(92)90170-o.

Experimental and Numerical Characterization of Johnson–Cook Model for Dog-Bone S355 Structural Steel at High Strain Rates and Elevated Temperatures

Hamed Hampaiyan Miandoab[1*], Tomasz Jankowiak[1], Wojciech Szymkuć[1], Michał Malendowski[1]

[1] Poznan University of Technology, Institute of Structural Analysis, ul. Piotrowo 5, Poznań, 60-965, Poland

[*] *Presenting author*

The use of finite element software is essential for analyzing engineering materials, as the precision of the results generated depends on how effectively the material models simulate real-world behavior. In this research, the mechanical properties of industrial S355 steel were evaluated across a range of strain rates, and the Johnson–Cook (JC) plasticity model parameters were established through both experimental and numerical methods. The investigation covered a temperature range of $20\,^{\circ}\mathrm{C}$ to $700\,^{\circ}\mathrm{C}$. The JC plasticity model constants were identified through a variety of experiments and evaluations, including compression, Split Hopkinson Pressure Bar (SHPB) testing, and thermal analysis. These established constants were incorporated into finite element analysis (FEA) software to simulate both the plastic deformation of the material and the initiation of damage during virtual experiments. Furthermore, a descriptive model for the dynamic strain aging (DSA) was proposed to characterize the plastic flow behaviors of S355 steel based on various ranges of temperatures and strain rates. Subsequently, the model predictions were compared with the results obtained from experimental test sets, which showed good agreement.

Acknowledgements. Funded by the National Science Centre, Poland under the OPUS call in the Weave programme under the grant 2022/47/I/ST8/02394 (marked as LA project 24-14577L, Material and structural response to dynamic actions in fire in the Czech Republic).

Keywords. SHPB, Johnson-Cook model, elevated temperature, high strain rates, dynamic strain ageing

Hard-Magnetic Soft Materials: Theory and Implementation

Marco Amato[1]* , Martin Horák[1] , Ondřej Faltus[1] , Milan Jirásek[1]

[1] Czech Technical University in Prague

* *Presenting author*

Magnetorheological elastomers (MREs) are active soft materials that respond to external magnetic fields, enabling applications in soft robotics, flexible electronics, and biomedical devices. Their behavior is governed by coupled magnetoelastic interactions, requiring complex computational models. Zhao et al. [2] proposed a simplified approach by treating the magnetic response as a material parameter, effectively decoupling the magnetoelastic problem into a purely elastic one.
However, Dorfmann and Ogden [1] pointed out inconsistencies in this formulation, particularly regarding the constitutive relations, stress symmetry, and frame indifference. In this work, we refine Zhao's model by integrating Dorfmann's critiques to achieve a fully consistent decoupling. We identify force-like boundary conditions necessary to maintain physical accuracy and develop a finite element framework to solve the problem in both multiphysics and purely static scenarios. This approach enhances computational efficiency while ensuring a rigorous representation of MRE behavior. Our findings provide a more robust theoretical foundation for MRE modeling, with implications for the design of adaptive structures, biomedical actuators, and next-generation soft robotic systems. By addressing key theoretical and numerical challenges, this work advances the applicability of MREs in engineering and applied sciences.

Keywords. magnetorheological elastomers, magnetoelasticity, Finite element method, constitutive modelling

References

[1] L. Dorfmann and R. W. Ogden, Hard-magnetic soft magnetoelastic materials: Energy considerations, *International Journal of Solids and Structures*, 294:112789, 2024.

[2] R. Zhao, Y. Kim, S. A. Chester, P. Sharma, and X. Zhao, Mechanics of hard-magnetic soft materials, *Journal of the Mechanics and Physics of Solids*, 124:244–263, 2019.

A Physical State-Dependent Model for Semicrystalline Polymers: Modeling the Transition from Elasto-Plasticity to Viscous Flow

Sandra Köhler[1*], André Hüllmann[2], Prativa Giri[2], André Leonhardt[1], Andreas Seefried[2], Till Clausmeyer[1], Birgit Awiszus[1]

[1] Professorship Forming Technology, Institute of Machine Tools and Production Processes, Chemnitz University of Technology, 09107 Chemnitz, Germany

[2] Professorship of Polymer Technology, Institute of Material Handling and Plastics, Chemnitz University of Technology, 09107 Chemnitz, Germany

[*] *Presenting author*

This paper presents a multi-regime framework designed to capture the complex thermomechanical behavior of high-density polyethylene (PE-HD) across the melting transition. Assuming a homogeneous, isotropic material and volume constancy (incompressibility), the proposed approach integrates non-linear elasto-plastic hardening for the solid state and viscous behavior for the molten state into a unified numerical environment. The mathematical core of the model relies on a temperature-dependent state transition criterion based on the melting temperature T_m. The governing equations are partitioned as follows: (1) An elasto-plastic formulation utilizing the Hensel-Spittel law – traditionally employed for metallic materials – is adapted to describe the solid state flow behavior of the polymer. Flow curves are derived from temperature-controlled flat compression tests, accounting for thermal softening and strain hardening. (2) A viscous model based on the rate-power-law, where the constitutive relations are informed by oscillatory rheometry and converted using the Cox-Merz rule to define the rate-dependent viscosity. A comprehensive material card was developed, incorporating additional experimentally determined temperature-dependent thermal properties (heat capacity, thermal conductivity). A key aspect of this work is the implementation through a user-defined subroutine into the commercial FE software Simufact Forming. This enables a seamless numerical transition at the solid-liquid interface, which is critical for solving the underlying moving boundary problem. The model's predictive capability is validated through a dual approach: accuracy is verified via flat compression tests and measurement of the melt layer thickness in a heating experiment, which is tracked using tactile penetration depth analysis and embedded thermocouples. The results demonstrate that the proposed framework accurately predicts the material behavior across the melting transition.

Acknowledgements. The authors thank the German Research Foundation (DFG) for funding of the project "Analysis of melt flow in thick-walled heated element butt welded thermoplastic joints by FE simulation" (project numbers: AW 6/43-1, GE 627/21-1, grant number 529312191).

Keywords. hot plate butt welding, FE simulation, thermomechanical coupling, high-density polyethylene (HDPE), temperature-dependent material model, thermomechanical simulation, polymer welding

An Internal Variable Approach to Model Relaxation Processes Near the Glass Transition Regime of Amorphous Thermoplastics

Frederik Hille[1]*, Johannes Keursten[1], Sabine Enders[2], Thomas Böhlke[1]

[1] Karlsruhe Institute of Technology (KIT) - Institute of Engineering Mechanics

[2] Karlsruhe Institute of Technology (KIT) - Institute of Technical Thermodynamics and Refrigeration

* *Presenting author*

When predicting the material behavior of thermoplastic materials for a wide range of temperatures, it is important to incorporate the influence of their distinct glass transition regime. In this context, there are two phenomena to highlight. First, there is a significant difference in their material properties, such as the stiffness, above and below the glass transition temperature. Secondly, there is a noticeable process and rate dependency in the material behavior in the glass transition regime, i.e., viscoelasticity in the mechanical case [1]. However, such relaxation phenomena can also be observed for caloric quantities, such as the heat capacity, which depend on the temperature rate in the vicinity of the glass transition temperature. In the case of heating processes even a non-monotonic change with respect to the temperature can be observed.

In this contribution, we give an introduction to an internal variable approach to model caloric relaxation processes, similar to the works of Lion et al. [3] and Keursten et al. [2]. Based on the standard linear solid model, analogies to classical viscoelasticity can be drawn. This allows us to derive clear restrictions on the introduced material parameters to ensure thermodynamic consistency. Additionally, the influence of energetic and dissipative effects can be separated. The predictive capabilities of the model will be investigated using exemplary experimental data. By measuring the heat capacity in a DSC experiment, the presented model gives access to the evolution of the internal variable. Special focus will be put on the determination of the relaxation time, in particular with respect to different rate dependencies.

Keywords. glass transition, enthalpy relaxation, thermodynamical consistency

References

[1] U. W. Gedde, M. S. Hedenqvist, M. Johansson, L. Berglund, and J. Wohlert, *Fundamental Polymer Science*, Graduate Texts in Physics. Springer Nature Switzerland, Cham, 2025.

[2] J. Keursten, S. Enders, and T. Böhlke, Constitutive theory and simulation of entropy and enthalpy relaxation in the glass transition regime, *Advanced Structured Materials*, 238, 2025.

[3] A. Lion, C. Mittermeier, and M. Johlitz, Heat capacities and volumetric changes in the glass transition range: a constitutive approach based on the standard linear solid, *Continuum Mechanics and Thermodynamics*, 29, 2017.

Glass Transition of Polymers from a Thermodynamic Point of View

Sabine Enders[1*], Eric Bahne[2], Luis Salamon[2], Thomas Böhlke[3]
[1] KIT
[2] KIT, Technical Thermodynamics, Karlsruhe, Germany
[3] KIT, Technical Mechanics, Karlsruhe, Germany
[*] *Presenting author*

The physical properties of materials change dramatically at the glass transition. The glass transition can in principle be considered from the mechanical or from the thermodynamic point of view. In this contribution, we will focus on the thermodynamic point of view. The Generalized Entropy Theory (GET), originally developed by Freed and coworkers [1], relates the glass transition to the entropy density of the considered material. The glass transition temperature is defined with respect to the structure relaxation time, which must exceed 100 seconds. For mixtures, the GET allows the consideration of local fluctuations. The GET enables us to predict the glass transition temperature if the entropy density can be calculated. For this purpose, a thermodynamic equation of state based on statistical mechanics of the molecules can be used. One example is the lattice theory, developed by Sanchez-Lacombe (SL) [2]. This theory requires for every kind of molecule three pure-component parameters which can be adjusted to experimental data related to the pressure-volume temperature behavior in the amorphous state. In the case of mixtures, combining rules must be applied. After the parameterization of the SL, different thermodynamic quantities, including density, entropy as well as phase diagrams, can be calculated. We use the SL within the GET for the calculation of glass transition temperatures of pure polymers and polymer blends. The application of this framework permits the calculation of the glass transition of polymers as a function of molecular weight and pressure. In the case of polymer blends, the glass transition temperature can be predicted as a function of the blend composition. We will discuss this phenomenon for miscible blends (Polyisoprene + Polybutadiene, Polystyrene + Polyphenylenether) and for blends showing demixing behavior (Polystyrene + Poly(vinyl methyl ether)). In the case of copolymers (Poly(styrene co acrylonitrile)), the glass transition can be calculated as a function of the chemical composition. Additionally, the impact of small molecules, for instance softener or humidity, on the glass transition can be studied. The predictions will be compared with experimental data taken from the literature.

Acknowledgements. We thank the German Science Foundation for financial support of SUSGEL.

Keywords. glass transition, thermodynamics, polymer, polymer blends

References

[1] J. Dudowicz, K. F. Freed, and J. F. Douglas, Generalized entropy theory of polymer glass formation, In *Advances in Chemical Physics*, volume 137, pages 125–222. Wiley, 2007, ISBN 9780470238080, doi: 10.1002/9780470238080.ch3.

[2] I. C. Sanchez and R. H. Lacombe, Statistical thermodynamics of polymer solutions, *Macromolecules*, 11 (6):1145–1156, 1978, ISSN 1520-5835, doi: 10.1021/ma60066a017.

Modeling Functionally Graded 4D Printed Shape Memory Polymers

Henrik Hembrock[1*], Heiko Andrae[1], Kerim Temme[2], Theodor Galambos[2], Thorsten Pretsch[2], Ralf Müller[3]

[1] Fraunhofer ITWM
[2] Fraunhofer IAP
[3] TU Darmstadt

[*] *Presenting author*

A functionally graded material is characterized by spatially varying properties that depend on position within the structure. In addition to unit cell designs incorporating material gradients, shape memory materials can be exploited by locally programming their shape recovery behavior through controlled adjustment of the printing parameters in a fused filament fabrication (FFF) process.
Predicting the resulting shape change and establishing a link between print parameters and the effective material properties has been addressed in the literature. However, the definition of suitable design parameters that can serve as targets for optimization has not yet been fully realized. Additional challenges arise when attempting to connect the G-code to a predictive simulation capable of capturing the directional properties induced by the printing process.
This work presents a methodology to experimentally characterize the recoverable strain of 4D-printed structures without requiring a full thermal simulation of the printing process. The approach is based on beam theory and curvature measurements, using a strain ansatz to describe the pre-activated state of the material. The measured curvature is interpreted as the outcome of a strain gradient introduced during printing. Furthermore, the simulation is coupled directly with the G-code, enabling access to directional and process-induced information.
Using this framework, a 4D unit cell design can be developed and the shape change behavior can be subjected to homogenization, thereby extending a multiscale optimization framework to enable the design of functionally graded materials manufactured via 4D printing.

Acknowledgements. Fraunhofer CPM

Keywords. 4D printing, shape memory polymer, material behavior, functionally graded material, recovery strain, G-code

A Thermo-Mechanical Particle Finite Element Method for Unified Fluid-Solid Formulation: Application to Phase Change and Metal Additive Manufacturing

Dorian Bogucki[1], Martin Lacroix[1], Simon Février[1], Luc Papeleux[1], Romain Boman[1], Jean-Philippe Ponthot[1]*

[1] Liège University

* *Presenting author*

Metal Additive Manufacturing (MAM) processes are characterized by highly localized heat inputs, steep thermal gradients, rapid phase transitions, and evolving interfaces. Numerical simulation of MAM processes is particularly challenging due to the multi-physics nature of these phenomena. The aim of this contribution, is to present a single robust numerical framework based on the Particle Finite Element Method (PFEM) capable of simulating a wide range of 2D and 3D applications in both fluid and solid mechanics, including fluid-structure interaction, phase change and MAM. Our original contribution lies in the combination and adaptation of state-of-the-art developments from the PFEM literature, including fluid-solid coupling, second-order accurate time integration schemes, advanced remeshing techniques, phase transformation models and laser-material interaction. Our PFEM formulation is unified and monolithic since the same conservation equations (momentum balance, mass conservation and heat equations) and nodal unknowns (velocity, pressure and temperature) are used in a single global system of equations to solve the fluid and solid parts.

Solid materials are represented using a thermo-elastic-viscoplastic model (hypoelastic formulation) while fluid materials are represented using a general non-Newtonian fluid model. A phase transformation model allowing continuity of the deviatoric stresses across the whole mushy zone is presented. To properly model the thermo-mechanical couplings, an expression of the thermal expansion coefficient including a pressure-dependent term, which is usually not taken into account, is derived. Moreover, the generalized-α time integration scheme is adapted to our unified formulation.

All three conservation equations are discretized and integrated using the same scheme and a single set of integration parameters. The problem is solved using the finite element method within the Lagrangian framework and large deformations of fluids and solids are addressed using a remeshing procedure, which is the underlying principle of the PFEM. The proposed formulation is extensively verified using simple benchmarks from the literature and it is then applied to more complex problems to show the capabilities of the method in the context of MAM.

Keywords. additive manufacturing, LPBF, phase change, unified fluid-solid material model, particle finite element method

Asymmetric Plasticity in Additively Manufactured 316L Stainless Steel BCC Lattice Architecture

Ignacio Ríos[1*], Seidou Abdul Herrim[2], Anne Marie Habraken[3], Anne Mertens[2], Laurent Duchêne[3], Víctor Tuninetti[1]

[1] Department of Mechanical Engineering, Universidad de La Frontera, Temuco 4811230, Chile
[2] Department A&M, University of Liège, 4000 Liège, Belgium
[3] Department ArGEnCo-MSM, University of Liège, 4000 Liège, Belgium

[*] *Presenting author*

The macroscopic elastoplastic response of cellular solids is fundamentally governed by complex deformation kinematics that vary across disparate loading paths, presenting a significant challenge for the predictive modeling of architected materials. This inherent asymmetry, identified as a primary limiting factor in the predictive modeling of cellular metamaterials [2], underscores the urgent requirement for a physically based constitutive model integrated into a non-symmetric constitutive framework to establish a high-fidelity homogenized model.
Uniaxial experimental characterization of 316L stainless steel body-centered cubic architectures reveals a distinct bifurcation in behavior where compressive regimes are dominated by bending-driven progressive cell collapse and stable stress plateaus, while tensile loading triggers localized plastic instabilities and premature ductility exhaustion.
High-fidelity finite element simulations explicitly incorporating the lattice topology demonstrate that this non-symmetric response originates from the micromechanical distribution of stress and strain at the unit-cell level and the onset of internal structural instabilities.
The demonstrated inability of conventional symmetric constitutive models to capture these effects highlights that such frameworks are physically inadequate for describing the mechanical evolution of these complex materials. Consequently, this work provides the necessary experimental and numerical evidence to support advanced homogenized frameworks capable of capturing localized strut buckling and plastic hinge formation for accurate predictions under multiaxial loading conditions.

Keywords. asymmetric plasticity, laser powder bed fusion, 316L stainless steel, BCC lattice architecture, architected materials, constitutive modelling, deformation kinematics, localized instabilities

References

[1] X. Lijun, L. Yinan, Y. Zhu, L. Runzhi, Y. Meng, and S. Weidong, Tension-compression asymmetry in triply periodic minimal surface lattice structures, *Thin-Walled Structures*, 220:114351, 2026, doi: 10.1016/j.tws.2025.114351.

[2] V. Tuninetti, S. Narayan, I. Ríos, B. Menacer, R. Valle, M. Al-lehaibi, M. U. Kaisan, J. Samuel, A. Oñate, G. Pincheira, A. Mertens, L. Duchêne, and C. Garrido, Biomimetic lattice structures design and manufacturing for high stress, deformation, and energy absorption performance, *Biomimetics*, 10(7):458, 2025, doi: 10.3390/biomimetics10070458.

Material-Aware Topology and Filament Path Optimization for Additive Manufacturing of Continuous Fiber-Reinforced Polymers

Bruno Musil[1]*

[1] University of the Bundeswehr, Institute of Lightweight Engineering, 85579 Neubiberg, Germany

* *Presenting author*

Additive manufacturing of fiber-reinforced composites via material extrusion enables the production of structurally optimized, anisotropic components tailored to specific load conditions. A key challenge, however, is that conventional topology optimization methods do not incorporate filament paths, and existing approaches for filament path planning often fail to efficiently support the structural function of already optimized geometries.
To address these limitations, this work presents two contributions. First, a staggered optimization approach is introduced that couples two level-set methods to optimize topology and filament paths simultaneously, ensuring performance and manufacturability. Second, a hybrid three-step framework is proposed to generate fabrication-ready filament paths that align closely with local principal stress directions. The effectiveness of these methods is demonstrated on two-dimensional structures, where the optimized filament layouts achieve superior compliance compared to state-of-the-art approaches.
Practical feasibility is further validated through multi-material 3D printing with variable-width deposition, which effectively eliminates gaps and preserves the intended mechanical performance. These results demonstrate the framework's capability to bridge the gap between theoretical design optimality and real-world manufacturing constraints, providing a robust pathway for producing high-performance composite components via additive manufacturing.

Keywords. additive manufacturing, optimization, composites

References

[1] V. Murugan, G. Alaimo, S. Marconi, P. Z. Berke, T. J. Massart, and F. Auricchio, Filament path optimization of fused filament fabricated parts incorporating the effect of pre-fusion densities, *International Journal of Solids and Structures*, 254-255:111916, 2022, ISSN 0020-7683, doi: 10.1016/j.ijsolstr.2022.111916.

[2] B. Musil and P. Höfer, Simulation of anisotropic behaviour in additively manufactured structures using a curvilinear coordinate based finite element formulation, *European Journal of Mechanics - A/Solids*, 111: 105501, 2025, ISSN 0997-7538, doi: 10.1016/j.euromechsol.2024.105501.

Programmable Anisotropy From Inflation Patterns in Pressurized Cellular Solids

Paul Lacorre[1*], Louison Fiore[2], Jean-Marc Linares[2], Loïc Tadrist[2]

[1] Czech Technical University in Prague
[2] Aix Marseille Université

[*] *Presenting author*

Plants are able to move rapidly (Venus flytrap, Mimosa Pudica). Instead of muscles, they use an organ composed of thousands of cells, called the pulvinus. These cells can absorb or release water to dilate or shrink, also affecting the stiffness of the tissue. We draw inspiration from this biological design, which achieves resilience through redundancy, by manufacturing and characterizing a pressurized cellular solid made of silicon with cubic cavities. Nonlinear finite element simulations show that, as the empty cells get pressurized, the mechanical behavior evolves from orthotropic to other programmable anisotropic stiffnesses and Poisson's ratios. The homogenized mechanical properties that result from the same device with different pressure patterns are studied exhaustively for patterns of size 2x2, 3x3 and 4x4 cells to extrapolate design rules. With the help of miniaturization techniques, this prototype of programmable pneumatic actuator will find applications in soft robotics.

Acknowledgements. This work was supported by the Agence Nationale de la Recherche (Paris, France) [grant number ANR-22-CE51-0012]. Since January 2026, Paul Lacorre has received partial funding from the European Union via the ROBOPROX project (Project No. CZ.02.01.01/00/22_008/0004590) and the CTU Global Postdoc Fellowship.

Keywords. metamaterials, pneumatic cellular solids, pressure-induced stiffness, periodic homogenization, nonlinear finite element analysis

Determination of Constitutive Parameters From 3D Strain Fields

Martin Diehl[1]*  , Edgar Rios[1]

[1] KU Leuven

* *Presenting author*

Fibre-reinforced polymer composites combine a stiff and strong reinforcing fibre with a relatively compliant matrix to bind the fibres together. They are taking up a central role in lightweight solutions, as they combine a high stiffness and strength with a low density. Apart from the fibre and matrix, the fibre/matrix interface is often considered to be the third constituent. These three constituents govern the mechanical performance of composites and knowing their constitutive parameters is crucial for predictive micromechanical models. Motivated by recent advancements in digital volume correlation performed on in-situ synchrotron measurements [1], we present an approach to determine these parameters from strain fields. We leverage a fast FFT-based solver implemented in DAMASK [2] that operates on a regular grid which enables a direct takeover of experimental data. To evaluate the capabilities and limits of the approach, a sensitivity study is performed in combination with a systematic parameter study.

Keywords. composites, micromechanics

References

[1] T. Chatziathanasiou, S. E. Madi, T. Sinha, J. Soete, M. Diehl, C. Breite, M. Mehdikhani, and Y. Swolfs, Strain mapping around fibre breaks in single- and multi-fibre composites: quantifying microscale deformation and damage via digital volume correlation, *Composites Part B: Engineering*, 316:113581, ISSN 1359-8368, doi: 10.1016/j.compositesb.2026.113581.

[2] F. Roters, M. Diehl, P. Shanthraj, P. Eisenlohr, C. Reuber, S. L. Wong, T. Maiti, A. Ebrahimi, T. Hochrainer, H.-O. Fabritius, S. Nikolov, M. Friak, N. Fujita, N. Grilli, K. G. F. Janssens, N. Jia, P. J. J. Kok, D. Ma, F. Meier, E. Werner, M. Stricker, D. Weygand, and D. Raabe, Damask – the düsseldorf advanced material simulation kit for modelling multi-physics crystal plasticity, damage, and thermal phenomena from the single crystal up to the component scale, *Computational Materials Science*, 158:420–478, doi: 10.1016/j.commatsci.2018.04.030.

Modeling Microstructural Evolution in Particulate Composites under Compression: A Mean-Field Homogenization Approach

Eléonore Bourdier[1]*, Sophie Dartois[1], Rémi Cornaggia[1], Renald Brenner[1]

[1] Institut Jean le Rond d'Alembert, Sorbonne Université, CNRS, F-75005, Paris, France

* *Presenting author*

From the early strain stages, particulate composites can exhibit a nonlinear effective response even when their constituents exhibit linear behavior, due to microstructural rearrangements such as porosity reduction, reorientation, and particle shape evolution. This work proposes a constitutive multi-scale model aiming at obtaining the macroscopic response of multiphase composites (pores and inclusions) while taking into account, in an approximate manner, the evolution of their microstructure and its impact on the effective anisotropic response of said composites. For this purpose, an incremental model is developed in which the microstructural state is characterized by the volume fractions, aspect ratios, and orientation of the inclusions, whose evolution is governed by equations derived from kinematic relations and estimates of the average strain and rotation rates of each phase [3, 1]. The latter are obtained through a homogenization process using mean-field approaches such as Mori-Tanaka, Lielens, and the differential scheme ([2, 4, 5]), allowing for a computationally efficient integration of essential microstructural features. The effective response is eventually obtained via a tangential operator. The model thus developed is then applied to describe the compressive behavior of concretes with a porous matrix enriched with vegetal particles.

Keywords. homogenization, microstructure evolution, mean-field schemes

References

[1] N. Aravas and P. Ponte Castañeda, Numerical methods for porous metals with deformation-induced anisotropy, *Computer Methods in Applied Mechanics and Engineering*, 193(36-38):3767–3805, 2004, ISSN 00457825, doi: 10.1016/j.cma.2004.02.009.

[2] Y. Benveniste, A new approach to the application of Mori-Tanaka's theory in composite materials, *Mechanics of Materials*, 6:147–157, 1987, doi: 10.1016/0167-6636(87)90005-6.

[3] M. Kailasam and P. Castañeda, A general constitutive theory for linear and nonlinear particulate media with microstructure evolution, *Journal of the Mechanics and Physics of Solids*, 46(3):427–465, 1998, ISSN 00225096, doi: 10.1016/S0022-5096(97)00095-1.

[4] G. Lielens, P. Pirotte, A. Couniot, F. Dupret, and R. Keunings, Prediction of thermo-mechanical properties for compression moulded composites, *Composites Part A: Applied Science and Manufacturing*, 29(1-2): 63–70, 1998, ISSN 1359835X, doi: 10.1016/S1359-835X(97)00039-0.

[5] A. Norris, A differential scheme for the effective moduli of composites, *Mechanics of Materials*, 4(1):1–16, 1985, doi: 10.1016/0167-6636(85)90002-X.

Multiscale Characterization and Modeling of the Thermo-Mechanical Behavior of Moso Bamboo

Lukas Speichinger[1*], Ralf Förster[2], Thomas Böhlke[1]

[1] Institute of Engineering Mechanics, Chair of Continuum Mechanics, Karlsruhe Institute of Technology (KIT)

[2] Berliner Hochschule für Technik (BHT)

[*] *Presenting author*

Bamboo is one of the fastest-growing plants and exhibits mechanical properties comparable to wood, making it a promising material for sustainable construction. Its hierarchical anatomy induces pronounced anisotropy and heterogeneity across multiple scales [3], yet comprehensive characterization and modeling of its thermo-mechanical behavior remain limited, particularly at lower scales. While previous studies have investigated the fibrous mesostructure [2] and the cellular microstructure [1] of bamboo, a deeper understanding of the macroscopic thermo-mechanical behavior is still needed.

This contribution presents a multiscale framework for modeling the thermo-mechanical behavior of Moso bamboo (*Phyllostachys edulis*) incorporating FFT-based homogenization methods. Using X-ray microtomography data [1], the cellular microstructure of bamboo is characterized, enabling the reconstruction of representative volume elements (RVE) via advanced tessellation algorithms. The statistically inhomogeneous mesostructure of the culm wall is characterized via computational image processing of cross-sectional microscopy images. According to the measured characteristics an RVE of the mesostructure can be reconstructed for any radial position within the culm wall.

To characterize the thermo-elastic behavior of bamboo, uniaxial dilatometry and tensile tests are conducted with bamboo culm wall specimens consisting of varying fiber bundle fraction. According to the observed material behavior, material models for the local constituents are derived. By fitting the multiscale model to the experimental data, not only the local material parameters are identified but also the fully anisotropic and inhomogeneous macroscopic behavior is predicted.

The proposed approach, which integrates material and microstructure modeling, enables a precise prediction of bamboo's thermo-mechanical response, thereby supporting the development of bamboo-based engineering solutions.

Keywords. Moso bamboo, thermo-mechanics, multiscale modeling, FFT-based homogenization

References

[1] X. Chen, X. Wang, L. Shang, X. Ma, C. Fang, B. Fei, H. Liu, and S. Zhang, Three-dimensional structural characterization and mechanical properties of bamboo parenchyma tissue, *Industrial Crops and Products*, 208:117833, 2024, ISSN 0926-6690, doi: 10.1016/J.INDCROP.2023.117833.

[2] P. G. Dixon and L. J. Gibson, The structure and mechanics of Moso bamboo material, *Journal of The Royal Society Interface*, 11(99):20140321, 2014, ISSN 1742-5689, 1742-5662, doi: 10.1098/rsif.2014.0321.

[3] W. Liese, *The Anatomy of Bamboo Culms*. BRILL, 1998, ISBN 978-81-86247-26-6.

Modeling the Creep Behavior of Lamellar NiAl-(Cr,Mo) Composites Using Three-Scale Homogenization

Claudius Klein[1*], Jan Vollhüter[2], Steffen Neumeier[2], Alexander Kauffmann[3], Thomas Böhlke[1]

[1] Karlsruhe Institute of Technology (KIT)
[2] Friedrich-Alexander-Universität Erlangen-Nürnberg
[3] Ruhr University Bochum

[*] *Presenting author*

The macroscopic mechanical response of composite materials depends on the properties of the constituents as well as the microstructure, i.e., the spatial arrangement of the constituents. In this talk we focus on the high temperature creep response of a eutectic NiAl-(Cr,Mo) composite [4], which forms domains (eutectic colonies) within which two metallic phases are arranged as ultrafine lamellar structures. Mesoscopic creep experiments of individual colonies showed that the minimum creep rate spans several orders of magnitude depending on the load direction relative to the lamination direction. The apparent Norton exponent also shows a strong anisotropy. Both effects are due to an inhomogeneous stress partitioning between the two phases which originates from the lamellar morphology and the high material contrast. In order to model the macroscopic mechanical response of the material system, we make use of a three-scale homogenization scheme involving two length scale bridges. For this, we describe the lamellar microstructure as a periodic rank-1 laminate [3], which allows for an efficient evaluation of the effective behavior of a single colony. To account for the interaction between different colonies, we use numerical homogenization techniques, e.g., the description of the mesostructure as a Laguerre tessellation [2] with prescribed interface orientation distribution [1] and its discretization using finite elements. After identification of the constitutive laws of the single phases, we investigate the influence of different interface orientation distributions on the macroscopic creep response.

Keywords. crystal plasticity, homogenization, high temperature, creep

References

[1] K.-I. Kanatani, Distribution of directional data and fabric tensors, *International Journal of Engineering Science*, 22(2):149–164, 1984.

[2] J. Kuhn, M. Schneider, P. Sonnweber-Ribic, and T. Böhlke, Fast methods for computing centroidal laguerre tessellations for prescribed volume fractions with applications to microstructure generation of polycrystalline materials, *Computer Methods in Applied Mechanics and Engineering*, 369:113175, 2020.

[3] G. W. Milton, *The theory of composites*. 1995.

[4] K. Titz, J. Vollhüter, P. Randelzhofer, S. Neumeier, M. Göken, B. Wahlmann, and C. Körner, Design and characterization of a novel NiAl–(Cr, Mo) eutectic alloy, *Advanced Engineering Materials*, 26(9):2302079, 2024.

A Consistent Homogenization Framework for Phase-Field Theory Based on Gurtin's Microforce Balance

Geralf Hütter[1]*, Fenil Maganbhai Lathiya[1], Vincent von Oertzen[1], Björn Kiefer[1]

[1] TU Bergakademie Freiberg, Institute of Mechanics and Fluid Dynamics, Germany

* *Presenting author*

Phase-field models are a powerful tool for simulating microstructure evolution [5], but their microscopic resolution makes the direct simulation of macroscopic components computationally prohibitive. While two-scale homogenization methods like FE^2 are well-established for mechanical problems, a rigorous framework for homogenizing the phase field and its gradient remains an open challenge. Current approaches are often limited to mechanics-only scale coupling or simple mixture rules that neglect gradient energy effects [1]. Even recent mathematically rigorous attempts, such as those using asymptotic expansion for fracture, are restricted in their scope [3], highlighting the need for a more general framework.

This work presents a thermodynamically consistent homogenization framework for coupled phase-field problems. Building upon our prior work on phase-morphology kinematics [6], we establish a rigorous kinetic scale transition rooted in Gurtin's microforce theory [2]. Via a formal two-scale expansion of the order parameter, we derive a consistent transfer of the phase field and its gradient from the micro- to the macroscale. This yields a complete set of macroscopic constitutive laws and a macroscopic evolution equation for the homogenized order parameter. The framework's predictive capabilities are demonstrated within a computational two-scale simulation. The implementation leverages a micromorphic DirectFE^2 scheme, previously established by the authors [4], to solve macroscopic boundary value problems for which the material response is directly governed by the evolution of the underlying microstructure.

Keywords. phase-field theory, computational homogenization, FE^2

References

[1] V. de Rancourt, K. Ammar, B. Appolaire, and S. Forest, Homogenization of viscoplastic constitutive laws within a phase field approach, *J. Mech. Phys. Solids*, 91:239–267, 2016.

[2] M. E. Gurtin, Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance, *Phys. D*, 92(3-4):178–192, 1996.

[3] P.-S. Ma, X.-C. Liu, X.-L. Luo, S. Li, and L.-W. Zhang, Asymptotic homogenization of phase-field fracture model: An efficient multiscale finite element framework for anisotropic fracture, *Int. J. Num. Meth. Eng.*, 125(13), 2024.

[4] A. Malik, G. Hütter, M. Abendroth, and B. Kiefer, Micromorphic FE^2 simulation of plastic deformations of foam structures, *Int. J. Mech. Sci.*, 265:108883, 2024.

[5] I. Steinbach, Phase-field models in materials science, *Modell. Simul. Mater. Sci. Eng.*, 17(7):073001, 2009.

[6] V. von Oertzen and B. Kiefer, Homogenization of phase transforming materials: The concept of phase-morphology and variable scale separations, *J. Mech. Phys. Solids*, 185:105561, 2024.

Augmented Lagrangian Treatment of Inequality Constraints in Phase-Field Modelling of Microstructure Evolution

Deepjyoti Dhar[1*], Karel Tůma[2], Jiří Kozlík[2], Stanisław Stupkiewicz[1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, Mechanics of Materials, Warsaw, Poland

[2] Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

[*] *Presenting author*

In this work, a phase-field framework is implemented to investigate the microstructure evolution in Ti-Mo systems involving the parent β phase and four ω variants [1], with particular emphasis on the high ω–ω interfacial energy, which leads to separation of ω variants by the β phase. Each phase is characterized by an order parameter constrained between 0 and 1, with all the order parameters satisfying the sum-to-unity constraint. The microstructure evolution is governed by the minimization of a global rate-potential [3], with interfacial energy contributions characterized through a double-obstacle potential [4]. To evaluate computational performance and accuracy, the numerical behavior of this formulation is benchmarked against a multi-well double-ditch potential formulation within the governing phase-field framework [2]. While the constraints can be enforced by a standard penalty formulation, modeling the high-energy ω–ω interfaces remains challenging because it requires very large penalty parameters, which lead to ill-conditioning and inefficient performance of iterative solvers. To overcome this limitation, an augmented Lagrangian framework is implemented in the form of the Uzawa algorithm, where the primal variables are solved for fixed dual variables and the dual variables are then updated systematically. The effectiveness of this approach is demonstrated through preliminary one-dimensional simulations. Subsequently, the proposed formulation is scaled to higher-dimensional simulations, emphasizing its robustness and improved convergence behavior in complex scenarios.

Keywords. microstructure evolution, constrained optimization, augmented Lagrangian method, Uzawa algorithm

References

[1] S. Banerjee and P. Mukhopadhyay, *Phase transformations: examples from titanium and zirconium alloys*, volume 12. Elsevier, 2010.

[2] J. Kozlík, K. Tůma, O. Souček, J. Dobrzański, and S. Stupkiewicz, Multiwell phase-field model for arbitrarily strong total-spreading case, *International Journal of Engineering Science*, 221:104474, 2026.

[3] C. Miehe, A multi-field incremental variational framework for gradient-extended standard dissipative solids, *Journal of the Mechanics and Physics of Solids*, 59(4):898–923, 2011.

[4] I. Steinbach, Phase-field models in materials science, *Modelling and simulation in materials science and engineering*, 17(7):073001, 2009.

Modeling of Phase Transitions during Hydride Formation in Palladium-Hydrogen Systems

Johannes Gisy[1]* , Magdalena Seiler[2], Stefan Wagner[2], Astrid Pundt[2], Thomas Böhlke[1]

[1] Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics, Chair of Continuum Mechanics

[2] Karlsruhe Institute of Technology (KIT), Institute for Applied Materials, Materials Science and Engineering

* *Presenting author*

Thin metal films are exposed to hydrogen (H) such that hydride formation and phase stability can be investigated. The hydride-forming metal, i.e., palladium (Pd), is sputtered on an inert substrate. Due to the H-induced lattice expansion of the adhered film, stresses arise, and the composite structure bends. Depending on the stress state, the H concentration and the temperature, hydride formation is possible or suppressed [2]. However, inelastic deformations alter the phase stability for a fixed temperature. Experimental studies by Colla et al. [1] investigate the creep behavior of thin Pd films, revealing a rate dependency of the plastic flow. To support these investigations, a Finite-Element (FE) model to represent physically, but also geometrically, the composite structure is needed. A chemo--mechanical model for the thin film accounting for H diffusion and inelastic deformation is introduced. The focus is on the chemo-mechanical coupling as hydride formation in the PdH system at room temperature depends strongly on the plastic deformations [2]. The diffusion model fully couples the chemical and mechanical constitutive response following [4] and [3]. The chemical potential depends on the mechanical stress state which impacts the phase stability during hydride formation. However, only the hydrostatic stresses contribute to the chemical potential while plasticity coupling is solely due to geometrical constraints. Thus, the thickness's contrast and its influence on the stress state needs to be studied. Current results regarding the role of phase formations on the stress evolution as well as a comparison between model and experimental measurements will be presented.

Keywords. chemo-mechanical coupling, visco-plasticity, phase transitions

References

[1] M. S. Colla *et al.*, Dislocation-mediated relaxation in nanograined columnar palladium films revealed by on-chip time-resolved HRTEM testing, *Nature Communications*, 6(1), 2015, doi: 10.1038/ncomms6922.

[2] A. Dyck, T. Böhlke, A. Pundt, and S. Wagner, Phase transformation in the palladium hydrogen system: Effects of boundary conditions on phase stabilities, *Scripta Materialia*, 247:116117, 2024, doi: 10.1016/j.scriptamat.2024.116117.

[3] A. Dyck *et al.*, Hydride formation in open thin film metal hydrogen systems: Cahn–Hilliard-type phase-field simulations coupled to elasto-plastic deformations, *Mechanics of Materials*, 203:105258, 2025, doi: 10.1016/j.mechmat.2025.105258.

[4] J. Gisy, A. Dyck, and T. Böhlke, A numerical study on the physical couplings of a geometrically linear thermo-chemo-mechanical model, *International Journal of Solids and Structures*, 309:113162, 2025, doi: 10.1016/j.ijsolstr.2024.113162.

Finite Element Analysis of Residual Stress Field Formed in Bimaterial GaN/AlGaN Substrates

Paweł Dłużewski[1]*, Piotr Tauzowski[2]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, ul. Pawińskiego 5B, 02-106 Warszawa, PL

[2] Institute of Fundamental Technological Research, Polish Academy of Sciences

* *Presenting author*

The last years have brought about a large development of blue light emitting laser diodes made in GaN based multilayers. The indium-rich InGaN layers deposited on GaN substrate can segregate into islands (quantum dots).
In this paper we analyse the residual stress field in a bimaterial GaN/AlGaN substrate prepared for epitaxial growth of InGaN layers. The stress field is analysed by solving a series of nonlinear finite-element boundary-value-problems [1, 2] considered for anisotropic chemo-hyperelastic material. The main source of residual stresses formed in the substrate yields from the chemo-elastic coupling (Vegard's law). The planar homogeneity of such obtained residual stress field is perturbed by the knurling-like pattern conducted on the reverse side of the substrate (on the opposite side to the epitaxial growth surface). Different finite strain measures, different sets of third-order elastic constants as well as different spatial distribution of GaN and $Al_xGa_{1-x}N$ layers in the substrate are considered in this analysis. We show how strongly the resultant pattern of stress field formed in the area of epitaxial growth depends on the assumed chemical composition, elastic model and geometrical parameters.
With respect to the wanted form of the stress-strain distribution, we consider this problem in terms of the topological optimisation of a chemo-elastic boundary-value-problem. The optimisation procedure performs a design space exploration over the geometry and chemical composition of finite element mesh. The design variables are the GaN layer thickness and the chemical composition profile. For each design instance, a full 3D hexahedral FE mesh of the multi-layer tile geometry (GaN + AlGaN layers with rounded notches) is generated, the composition distribution is assigned layer-by-layer via linear interpolation onto mesh nodes, and the weighted chemo-elastic problem is solved. After all evaluations, the best and worst designs are identified based on the minimum and maximum values of the objective function, and are subsequently visualised and exported to FEAP input files for high-fidelity verification.

Keywords. crystal growth, hyperelasticity, residual stress fields, optimisation of chemical composition

References

[1] P. Dłużewski, T. D. Young, G. Dimitakopulos, and P. Komninou, Continuum and atomistic modeling of the mixed straight dislocation, *International Journal for Multiscale Computational Engineering*, 8(3):331–342, 2010.

[2] G. Jurczak and P. Dłużewski, Finite element modelling of nonlinear piezoelectricity in wurtzite GaN/AlN quantum dots, *Computational Materials Science*, 111:197–202, 2016.

Do We Need Complex Constitutive Models to Simulate the Concrete Gap Test?

Petr Havlásek[1*], Milan Jirásek[1]

[1] Czech Technical University in Prague

[*] *Presenting author*

The gap test [3] is a recently introduced non-trivial experiment designed to evaluate the effect of crack-parallel stresses on the tensile strength and fracture energy of materials and to benchmark constitutive models for concrete, as suggested by its conceptual author, Z.P. Bažant.
Although the setup resembles a three-point bending test of a notched beam, the defining difference is the initial preloading stage. In this stage, the central part of the specimen is vertically compressed, and this load is maintained during the subsequent bending phase. Experimental data indicate that low-magnitude preloading has a favorable effect on the bending response, whereas higher magnitudes lead to a significant reduction in strength.
Preliminary results from our recent numerical study [2] suggested that structural effects present in the experiment may outweigh the impact of the constitutive model behavior under complex multiaxial stress states. Those simulations, performed in the OOFEM platform [4], employed the CDPM2 damage-plasticity model for concrete failure by Grassl and coworkers [1], calibrated on conventional three-point bending tests across three specimen sizes to ensure the size effect was captured correctly.
This contribution compares the response obtained with the sophisticated CDPM2 model with that of a simple isotropic damage model featuring exponential softening and a smoothed Rankine expression for the equivalent strain. The responses are compared to the entire experimental dataset, consisting of three specimen sizes and three levels of preloading. Finally, we investigate whether modifying the dimensions of the preloading plates can diminish the parasitic structural effects observed in the original setup.

Acknowledgements. Financial support received from the Czech Science Foundation under project 25-17495S is gratefully acknowledged.

Keywords. concrete, gap test, crack-parallel stress, modeling, size effect

References

[1] P. Grassl, D. Xenos, U. Nyström, R. Rempling, and K. Gylltoft, CDPM2: A damage-plasticity approach to modelling the failure of concrete, *International Journal of Solids and Structures*, 50(24):3805–3816, 2013, ISSN 0020-7683, doi: 10.1016/j.ijsolstr.2013.07.008.

[2] M. Jirásek and C. Li, Lessons learned from simulations of the gap test, In G. Meschke, B. Pichler, and J. G. Rots, editors, *Computational Modelling of Concrete and Concrete Structures*. Taylor & Francis, 1st edition, 2026, doi: 10.1201/9781003660026-66.

[3] H. T. Nguyen, M. Pathirage, G. Cusatis, and Z. P. Bažant, Gap test of crack-parallel stress effect on quasibrittle fracture and its consequences, *Journal of Applied Mechanics*, 87(7):071012, 2020.

[4] B. Patzák and Z. Bittnar, Design of object oriented finite element code, *Advances in Engineering Software*, 32(10-11):759–767, 2001.

Localization Analysis in the Plastic Regime of Concrete Damage-Plastic Models

Michal Šmejkal[1]*

[1] CTU in Prague, Faculty of Civil Engineering

* *Presenting author*

This presentation explores the conditions for strain localization within the plastic regime of the Concrete Damage Plasticity Model (CDPM2 [1]), prior to the initiation of material damage. While localization in concrete is typically associated with the softening branch—where damage evolution leads to a loss of material stability—non-associated plasticity models can exhibit discontinuous bifurcations even during the hardening phase. This study focuses on the theoretical and numerical assessment of the localization tensor to determine the boundaries of stable plastic flow.

The analysis reveals that localization can indeed occur within the plastic regime, primarily as a consequence of the non-associated flow rule. For a given stress state and set of material parameters, the critical hardening modulus required to maintain a positive determinant of the localization (acoustic) tensor is analytically evaluated. Subsequently, the stress space is discretized to systematically evaluate this critical hardening modulus across stress states that can be reached before the onset of damage. The results demonstrate that when all other material parameters are held fixed, the hardening modulus parameter H_p must be selected within a specific admissible interval to entirely prevent localization during the loading process. Furthermore, the study investigates the sensitivity of this allowed interval for H_p to variations in the remaining material parameters, showing how certain parameter combinations restrict or altogether eliminate the stable domain.

The results provide essential guidelines for the robust calibration of CDPM2, ensuring that the model remains stable during the hardening phase and that any subsequent localization is physically representative of the damage process rather than a premature mathematical instability of the plastic formulation.

Keywords. localization analysis, damage, plasticity

References

[1] P. Grassl, D. Xenos, U. Nyström, R. Rempling, and K. Gylltoft, CDPM2: A damage-plasticity approach to modelling the failure of concrete, *International Journal of Solids and Structures*, 50(24):3805–3816, 2013.

Microstructure-Based Discrete Lattice Modeling of Interlayer Fracture in 3D-Printed Concrete

Benjamin Werner[1]*, Ron Peerlings[1], Ondřej Rokoš[1]

[1] Eindhoven University of Technology, Department of Mechanical Engineering, Eindhoven, The Netherlands

* *Presenting author*

Extrusion-based 3D-printed concrete (3DPC) is characterized by pronounced anisotropy and reduced interlayer strength due to its layer-wise manufacturing process. Recent experimental work indicates that the interlayer forms a mechanically distinct filament interfacial zone with altered particle content, local stiffness, and incomplete bonding at filament boundaries. A numerical framework must therefore account for the microstructural heterogeneity induced by printing in order to predict interlayer failure realistically.

This contribution presents a microstructure-based discrete lattice model for fracture in 3DPC. The material is represented by a regular three-dimensional X-braced truss lattice in which the cementitious matrix and aggregates are resolved explicitly. The printed interlayer is modeled as a core–filament-interfacial-zone–core arrangement with spatially varying particle volume fraction, particle size, and local stiffness. Damage and fracture are described at the bond level, allowing crack initiation, localization, and propagation to emerge naturally from the underlying heterogeneity. To capture the brittle softening response, the equilibrium problem is solved using a dissipative arc-length solver.

The main objective of the study is to identify which interlayer parameters most strongly influence tensile strength and fracture behavior. The effect of particle distribution across the filament interfacial zone is examined, including smooth profile variations motivated by experimental observations of particle depletion in the interlayer region. Additional parameters include the thickness of the interfacial zone, particle-size contrast between the filament core and interlayer, and reduced stiffness of the interfacial zone. The resulting simulations are used to compare crack paths, load–displacement response, and localization patterns for different microstructural scenarios.

The proposed framework links experimentally observed interlayer morphology to the mesoscale fracture response of 3DPC. At the same time, it serves as a basis for future multiscale extensions using the QuasiContinuum methodology, enabling efficient simulation of larger printed structures while retaining explicit microstructural resolution in critical regions.

Acknowledgements. This work was supported by the European Union through a Marie Skłodowska-Curie grant (Grant Agreement No. 101151096, starting in September 2024).

Keywords. 3D-printed concrete, interlayer fracture, discrete lattice model, material heterogeneity, damage modeling

Author index

Keyword index