IUTAM Symposium on

Enhancing Material Performance by Exploiting Instabilities and Damage Evolution

BOOK OF ABSTRACTS

IUTAM SYMPOSIUM Warsaw 2022

June 5–10, 2022
Warsaw, Poland

Editors:
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ISBN 978-83-65550-35-4

DOI: 10.24423/iutam2022warsaw

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Supported by

International Union of Theoretical and Applied Mechanics

Institute of Fundamental Technological Research PAN

Texas A&M University

European Union's Horizon 2020 Research and Innovation Programme

Contents

Scope of the Symposium

Designing against structural, component and material failure involving finite deformation modes such as buckling, strain localization, shear banding, kink banding, wrinkling, crazing, void growth, and fracture is a long-standing engineering challenge. In many cases, these deformation modes emerge abruptly from uniform or nearly uniform deformation fields. Much progress has been made in solid mechanics defining conditions needed to preclude these types of failures that has provided engineers with design guidelines for safe performance. On the other hand, there are circumstances where such deformation modes can be exploited to achieve a desired engineering objective. A classic example is a thermostat based on a curved metal strip that buckles with a change in temperature to make or break an electric circuit. Recently, there has been broad interest in exploiting instabilities and damage evolution to enhance performance in a wide variety of contexts. Examples include techniques to control buckling and delamination to design sophisticated three-dimensional meso-structures with novel functionalities, and proposals to enhance the fracture toughness of materials by controlling the distribution of weak interfaces in brittle solids and by controlling the distribution of void nucleating defects in ductile solids. Furthermore, hierarchical metamaterials with tunable properties have been created by mimicking the microstructure-property relations in materials at the structural scale to engineer complex deformation modes.

Many more ways to exploit instabilities and damage evolution to engineer and enhance material properties, functionalities and performance remain to be understood and developed. The symposium "Enhancing Material Performance by Exploiting Instabilities and Damage Evolution" aims at gathering mechanicians who are exploring the advantages of introducing and controlling complex deformation modes into material systems at different scales of observation to enhance their properties, functionalities and performance. The participants will present their recent experimental, theoretical and computational works aimed at achieving this goal. The symposium will also feature presentations and discussions on the impact of advancement in manufacturing, characterization and computational techniques on our capabilities to improve the understanding, control and exploitation of instabilities and damage evolution to enhance material performance.

Katarzyna Kowalczyk-Gajewska
Ankit Srivastava
Chair and Co-chair of IUTAM Symposium in Warsaw

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Symposium Website

iutam2022warsaw.ippt.pan.pl

Symposium Venue

The IUTAM Symposium will be held at the Institute of Fundamental Technological Research Polish Academy of Sciences (IPPT PAN) in Warsaw, Poland.
The IPPT building is located at the Ochota Campus, Pawińskiego 5B
ippt.pan.pl

Social Events

Monday, June 6, 17:30

Welcome Reception
Lobby of the IPPT building

Tuesday, June 7, 19:00

Symposium Dinner
Vistula Boulevards of Jan Karski
Restaurant Barka Warszawska Dzień i Noc
barkawarszawska.pl

Thursday, June 9, 18:30

Museum Tour and Banquet Dinner
Kotlownia of Polish Vodka Museum
Koneser Centre of Praga district, Plac Konesera 1
muzeumpolskiejwodki.pl

Programme Overview

Sunday June 5, 2022	Monday June 6, 2022	Tuesday June 7, 2022	Wednesday June 8, 2022	Thursday June 9, 2022	Friday June 10, 2022
Open day		8:30–9:30 Breakfast	8:30–9:30 Breakfast	8:30–9:30 Breakfast	Open day
	9:00–11:00 Registration	9:30–11:15 Session 04	9:30–11:15 Session 08	9:30–11:15 Session 12	
	11:00–11:35 Opening Session	Coffee Break	Coffee Break	Coffee Break	
	11:35–12:45 Session 01	11:35–12:45 Session 05	11:35–12:45 Session 09	11:35–12:45 Session 13	
	12:45–14:00 Lunch	12:45–14:00 Lunch	12:45–14:00 Lunch	12:45–14:00 Lunch	
	14:00–15:10 Session 02	14:00–15:10 Session 06	14:00–15:10 Session 10	14:00–15:10 Session 14	
	Coffee Break	Coffee Break	Coffee Break	Coffee Break	
	15:30–17:15 Session 03	15:30–16:40 Session 07	15:30–16:40 Session 11	15:30–16:40 Session 15	
	17:30–20:00 Poster Session and Welcome Reception	19:00 Symposium Dinner*		18:30–23:00 Museum Tour and Banquet Dinner*	

The registration desk will be open in the lobby of the IPPT building.
All sessions will be in room Aula on the second floor of the IPPT.
*not included in the student fee.

Detailed Technical Programme

Monday, June 6, 2022

9:00–11:00	Registration Coffee will be served from 10:00
11:00–11:35	Opening Session
	11:35–12:45 Session 01 **Chair: J.A. Rodríguez-Martínez**
11:35–12:10	**G. Subhash** and A.A. Cheenady – Shock-Induced Spallation in Monocrystalline Boron Carbide
12:10–12:45	**S.M. Keralavarma** – Constitutive Effects on Failure by Strain Localization in Ductile Materials
12:45–14:00	Lunch
	14:00–15:10 Session 02 **Chair: B. Revil-Baudard**
14:00–14:35	B. Schroeders, T. Oudes, O. Rokoš, **R. Peerlings**, M. Geers, O. Faltus, M. Horák, M. Doškář, M. Jirásek and J. Zeman – Harnessing Microscale Buckling Instabilities to Control Macroscale Stiffness
14:35–15:10	P. Taylor, J. Londono, **P.B. Woelke** and J.W. Hutchinson – Investigation of Effect of Plate Thickness on Ductility for Engineering Applications
15:10–15:30	Coffee Break
	15:30–17:15 Session 03 **Chair: K.L. Nielsen**
15:30–16:05	M. Rezaee-Hajidehi, P. Sadowski and **S. Stupkiewicz** – Phase-Field Model for Spatially Resolved Deformation Twinning Coupled with Crystal Plasticity
16:05–16:40	N. Hosseini, J.C. Nieto-Fuentes, M. Dakshinamurthy, J.A. Rodríguez-Martínez and **G. Vadillo** – The Effect of Material Orientation on Void Growth
16:40–17:15	**O. Cazacu** and B. Revil-Baudard – Size of the Plastic Zone Near a Crack: New Exact Solutions
17:30–20:00	Poster Session and Welcome Reception

Monday, June 6, 2022

Poster Session	
17:30–20:00 IPPT building lobby	**J. Dobrzański**, K. Wojtacki and S. Stupkiewicz – Lamination-Based Efficient Treatment of Weak Discontinuities for Non-Conforming Finite-Element Meshes
	V.P. Dubey, M. Kopec and Z.L. Kowalewski – The Effect of Predeformation History Under Complex Loading on the Yield Surface Evolution of Titanium Alloy: An Experimental Investigation
	K. Frydrych and S. Papanikolaou – Structure-Based Optimization of Crystal Plasticity Parameters in Metals and Alloys
	M. Majewski, M. Wichrowski, P. Hołobut and K. Kowalczyk-Gajewska – Micromechanical and Numerical Analysis of Shape and Packing Effects in Elastic-Plastic Particulate Composites
	S. Musiał, M. Maj, L. Urbański and M. Nowak – Field Analysis of Energy Conversion During Plastic Deformation Process
	M. Nabavian Kalat, M. Staszczak, Y. Ziai, L. Urbański and E. Pieczyska – Effect of Shape Recovery and Cyclic Loading on the Evolution of Micro-Cracks in Shape Memory Polymers
	M. Rezaee-Hajidehi, K. Tůma and S. Stupkiewicz – Stress-Induced Martensitic Transformation in Shape Memory Alloys During Nano-Indentation: Insights From Phase-Field Simulations
	M. Ryś, S. Stupkiewicz and H. Petryk – Gradient-Enhanced Crystal Plasticity Model with Micropolar Regularization: Prediction of the Indentation Size Effects
	S. Virupakshi, K. Frydrych and K. Kowalczyk-Gajewska – Effect of Boundary Conditions and Crystallographic Orientation on the Cylindrical Void Growth in FCC Single Crystals Using CPFEM

Tuesday, June 7, 2022

8:30–9:30	Breakfast
	9:30–11:15 Session 04 **Chair: R. Zhao**
9:30–10:05	**C. Combescure** – Prediction of Instabilities in Periodic Architected Materials to Actively Modify Wave Propagation Properties
10:05–10:40	**J.J. Rimoli** and J.A. Kraus – Discontinuous Compression Structures: From Tensegrity Planetary Landers to High-Performing Metamaterials
10:40–11:15	**A.F. Arrieta** – Multistable Metastructures From Local Bistable Units: Actuation Simplification and Information Processing
11:15–11:35	Coffee Break
	11:35–12:45 Session 05 **Chair: C. Czarnota**
11:35–12:10	**T. Cohen** – Nonlinear Inclusion Theory with Application to the Growth and Morphogenesis of a Confined Body
12:10–12:45	**W. Sumelka** and P. Stempin – On Selected Space-Fractional Structural Models
12:45–14:00	Lunch
	14:00–15:10 Session 06 **Chair: N. Lu**
14:00–14:35	**V.S. Deshpande** – Micro-Architected Solids: Does Toughness Characterise Fracture?
14:35–15:10	**S. Gaitanaros** – Strength and Toughness of Lattice Materials
15:10–15:30	Coffee Break
	15:30–16:40 Session 07 **Chair: R. Peerlings**
15:30–16:05	**A.A. Benzerga** – On the Effects of the Third Stress Invariant in Ductile Failure
16:05–16:40	**H. Petryk** – Path Instability Criterion for Non-Potential Problems in Rate-Independent Plasticity

19:00	Symposium Dinner*

*not included in the student fee.

Wednesday, June 8, 2022

8:30–9:30	Breakfast
	9:30–11:15 Session 08 **Chair: C. Combescure**
9:30–10:05	**N. Lu** – Poking and Bulging of 2D Crystals
10:05–10:40	**R. Zhao** – Functional Buckling and Folding of Ring Origami
10:40–11:15	**S. Basu** – Sensitivity of Very Soft Solids to Stimuli and Surface Effects
11:15–11:35	Coffee Break
	11:35–12:45 Session 09 **Chair: T. Cohen**
11:35–12:10	**W.A. Curtin** – Exploiting the Randomness of High Entropy Alloys
12:10–12:45	**M.J. Demkowicz** – The Effect of Hydrogen on Localized Plasticity and Crack Initiation in Nickel-Base Alloy 725
12:45–14:00	Lunch
	14:00–15:10 Session 10 **Chair: S.M. Keralavarma**
14:00–14:35	J. Xie and **K. Ravi-Chandar** – Exploration of Ductile Failure Processes in an Aluminum Alloy Through X-Ray CT Scan and Microscopy
14:35–15:10	**M. Radovic** and A. Srivastava – Enhancing Damage Tolerance and Crack Healing in Ceramics by Kinking: The Case of MAX Phases
15:10–15:30	Coffee Break
	15:30–16:40 Session 11 **Chair: A.F. Arrieta**
15:30–16:05	**W.J. Meng**, X. Zhang, B. Zhang, A.C. Meng, R. Namakian, D. Moldovan and K.L. Nielsen – Understanding Mechanical Integrity of Metal/Ceramic Interfacial Regions and Mechanical Response of Plastic Deformation at the Micro/Meso Scales
16:05–16:40	**S. Osovski** and S. Tsopanidis – Extracting Grain Boundary Toughness from Macro-Scale Experiments

Thursday, June 9, 2022

8:30–9:30	Breakfast
	9:30–11:15 Session 12 **Chair: S. Stupkiewicz**
9:30–10:05	**S. Forest**, J.-M. Scherer, V. Phalke and J. Besson – Grain Boundaries as Barriers Against Shear Banding and Crack Propagation in Ductile Polycrystals: A Gradient Crystal Plasticity Approach
10:05–10:40	**K.L. Nielsen**, J.E. Simon, R.G. Andersen and C. Tekoglu – Plate Bending: Localization and Fracture Triggered by Heterogeneities
10:40–11:15	**J.A. Rodríguez-Martínez** – The Effect of Actual Porous Microstructure on the Formation of Dynamic Necks, Adiabatic Shear Bands and Plastic Shock Waves
11:15–11:35	Coffee Break
	11:35–12:45 Session 13 **Chair: S. Gaitanaros**
11:35–12:10	**C.F. Niordson** – On Effects of Void Clustering on Yield Surfaces
12:10–12:45	E. Chiu, **A. Needleman**, S. Osovski and A. Srivastava – Mitigating Spall Fracture of Ductile Materials by Introducing Porosity
12:45–14:00	Lunch
	14:00–15:10 Session 14 **Chair: S. Basu**
14:00–14:35	**C. Czarnota**, A. Molinari and S. Mercier – Steady Shock Wave in Porous Metals: Visous & Micro-Inertia Effects Interplay
14:35–15:10	**B. Revil-Baudard** – Multi-Scale Modeling of Energetic Materials Under High Strain Rate Loadings
15:10–15:30	Coffee Break
	15:30–16:40 Session 15 **Chair: G. Vadillo**
15:30–16:05	**K. Kowalczyk-Gajewska** and S. Virupakshi – Evolution of Lattice Orientation Heterogeneity in HCP Single Crystals Due to Void Growth
16:05–16:40	**A. Srivastava** – Defects, Crack Path and Crack Growth Resistance

18:30–23:00	Museum Tour and Banquet Dinner*

*not included in the student fee.

ABSTRACTS

Multistable Metastructures from Local Bistable Units: Actuation Simplification and Information Processing

A.F. Arrieta

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Metamaterials aim to disrupt materials design by engineering unit cells geometry and their connectivity to realize unconventional properties. In particular, mechanical metamaterials exploit nonlinear geometrical effects at the unit cell scale to obtain rare mechanics including, negative Poisson's ratio materials [1], strong wave propagation anisotropy [2,3], high energy absorption [4,5] and reconfigurable metastructures [6–8]. We explore metamaterials and metastructures that leverage local bistability to display global stiffness adaptation [9], extreme shape reconfiguration, and intrinsic mechanologic [8]. Specifically, we exploit dome-shaped bistable units, the bistability of which depends only on their geometry, to enable a geometrically scalable and constitutive material independent route to design mechanical metamaterials. Notably, designing the unit cell connectivity allows for introducing extreme mechanical hysteresis from purely elastic interactions resulting in strong order dependence between the loading (i.e., inversion sequence of domes) and final metastructural state (i.e., global property) [10]. This implies breaking the one-to-one relationship between local unit cell state and global effective property found in conventional assemblies of bistable units [4,11]. This results in our metastructures displaying multiple possible states for a distinct microstructural distribution, a phenomenon called hierarchical multistability [8,10,12]. We leverage the order dependence to realize underactuated multistable robotics. Furthermore, we leverage the nonlinear mechanics to demonstrate information processing intrinsic to these metastructures. This provides a route to realizing mechanical systems with embodied intelligence purely from elastic, and thus reversible, interactions.

References

[1] Lakes, R.S., Adv. Mater. 5, 293–296 (1993).
[2] Liang, B., Guo, X.S., Tu, J., Zhang, D., Cheng, J.C., Nat. Mater. 9, 989–992 (2010).
[3] Nadkarni, N., Arrieta, A.F., Chong, C., Kochmann, D.M., Daraio, C., Phys. Rev. Lett. 116, 244501 (2016).
[4] Restrepo, D., Mankame, N.D., Zavattieri, P.D., Extreme Mech. Lett. 4, 52–60 (2015).
[5] Shan, S., Kang, S.H., Raney, J.R., Wang, P., Fang, L., Candido, F., Lewis, J.A., Bertoldi, K., Adv. Mater. 27, 4296–4301 (2015).
[6] Seffen, K.A., Scr. Mater. 55, 411–414 (2006).
[7] Waitukaitis, S., Menaut, R. , Chen, B.G.G., Van Hecke, M., Phys. Rev. Lett. 114, 2–6 (2015).
[8] Faber, J.A., Udani, J.P., Riley, K.S., Studart, A.R., Arrieta, A.F., Adv. Sci. 7, 2001955 (2020).
[9] Udani, J.P., Arrieta, A.F., Extreme Mech. Lett. 42, 101081 (2021).
[10] Udani, J.P., Arrieta, A.F., Under review, 2021 Jun 2. http://arxiv.org/abs/2106.01535
[11] Haghpanah, B., Salari-Sharif, L., Pourrajab, P., Hopkins, J., Valdevit, L., Adv. Mater. 28, 8065 (2016).
[12] Seffen, K.A. , Scr. Mater. 56, 417–20 (2007).

Sensitivity of Very Soft Solids to Stimuli and Surface Effects

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Ambient electro-magnetic fields, even when very strong, are not enough to deform stiff solids. Similarly, elasticity of the surface, distinct from that of the bulk, is also not a significant concern when the bulk is stiff. However, for soft materials with stiffnesses ranging from a few tens of kPa to an MPa, both of these issues can have considerable effects on their deformation behaviour.

Soft solid membranes with high electrical permittivity and breakdown strength, when placed in sufficiently strong electric fields, can undergo sudden buckling-like instabilities. These instabilities are generally accompanied by large inhomogeneous deformations, are induced in a non-contact manner and, if controlled well, can be reversed without causing electrical breakdown.

Similarly, internally pressurised thin and soft cylindrical tubes with a strong electric field applied across the thickness exhibits a multitude of possibilities, including homogeneous deformation, inhomogeneous bifurcation, snap-through instabilities and propagation of axisymmetric bulges. There are notable efforts to harness these possibilities towards technologically useful ends.

Effects of surface stresses on small liquid volumes has been studied extensively for over a century. Surface stresses on a liquid surface are isotropic and depend on only one measurable scalar material property, namely, the surface energy. Effects of surface stresses in stiff solids may assume some importance at nanoscales.

There is growing experimental evidence that, deformation of soft solids, even on length scales of the order of tens of microns are affected strongly by surface stresses that are large and dependent on surface strains. As a consequence, soft solid structures can alter their behaviour from being ‘solid like’ to ‘liquid like’ with deformation. In fact, counter-intuitively, soft solids, when reinforced with small liquid inclusions, can become stiffer than the matrix material, thanks to surface stresses at the liquid-solid boundaries. Again, controlling surface properties in soft solids provide a route to design materials with somewhat tunable overall properties.

On the Effects of the Third Stress Invariant in Ductile Failure

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There has been immense interest over the last two decades in the effect of the third stress invariant in ductile failure. However, current understanding of the effect, apparent or intrinsic, lacks fundamental grounding. A key element is to apportion the effect of induced anisotropy, which seems unavoidable under many circumstances. This is the case, for example, under shear loading. Notwithstanding this difficulty, the influence of the third stress invariant can be divided into a minor effect and a major effect, at least in materials failing by a microscopic process of void growth to coalescence. The minor effect is on void growth. The major effect is on void coalescence, or more generally on the transition between a mesoscopically homogeneous process of yielding to inhomogeneous yielding. Because the latter involves "yield systems", which microscopically refer to bands of voids, the effective behavior and corresponding damage evolution are extremely sensitive to not only the resolved shear stress on such yield systems but also to the resolved normal stress. It is this combination of resolved normal and shear stresses that renders an emergent behavior that is dependent upon all three stress invariants in an ideally isotropic version of the theory. In this talk, the conceptual elements of a theory of inhomogeneous yielding are first laid out, then applied to analyze Lode effects in ductile failure including (i) failure under extreme shear loading; (ii) failure under combined shear and tension; (iii) a focused analysis of Lode effects using the isotropic theory; (iv) comparison with predictions based on classical strain localization theory.

Size of the Plastic Zone Near a Crack: New Exact Solutions

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Experimental data indicates that fracture is preceded by some plastic deformation in the vicinity of the crack tip. In this talk, we present new analytical results which show that the extent of this plastic zone depends on both the shear and uniaxial yield stress of the material. This new correlation was established based on a new exact solution for the elastic stresses in the vicinity of a central crack embedded in a thin plate subjected to remote uniaxial tension. Unlike the classical Westergaard stress distribution, this exact stress field is not axisymmetric in the crack plane. Using this exact elastic stress field, it becomes possible to assess the influence of the particularities of the material yielding on the extent of the plastic zone near the crack. Analysis is done considering yielding governed by the von Mises, Tresca, and Drucker yield criterion, respectively. It is demonstrated that the ratio between the yield stresses in uniaxial tension and pure shear has a great influence on the size of the plastic zone around the crack. Specifically, the larger this ratio the larger is the plastic zone. Moreover, we derive new analytic relations between the length of the plastic zone, measured from the crack tip in the crack plane, and the external applied load for the case when yielding is governed by the von Mises and Tresca criterion, respectively.

Nonlinear Inclusion Theory with Application to the Growth and Morphogenesis of a Confined Body

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One of the most celebrated contributions to the study of the mechanical behavior of materials is due to J.D. Eshelby, who in the late 50s revolutionized our understanding of the elastic stress and strain fields due to an ellipsoidal inclusion/inhomogeneity that undergoes a transformation of shape and size. While Eshelby's work laid the foundation for significant advancements in various fields, including fracture mechanics, theory of phase transitions, and homogenization methods, its extension into the range of large deformations, and to situations in which the material can actively reorganize in response to the finite transformation strain, is in a nascent state. Beyond the theoretical difficulties imposed by highly nonlinear material response, a major hindrance has been the absence of experimental observations that can elucidate the intricacies that arise in this regime. In this talk, I will present our attempts to address this limitation; using the growth of embedded bacterial colonies as a case study, our theoretical model considers various growth scenarios and employs two different and complimentary methods – a minimal analytical model and finite element computations – to obtain approximate equilibrium solutions. A particular emphasis is put on determining the natural growth path of an inclusion that optimizes its shape in response to the confinement, and the onset of damage in the matrix, which together explain the observed behavior of biofilms. Beyond bacterial biofilms, this work sheds light on the role of mechanics in determining the morphogenesis pathways of confined growing bodies and thus applies to a broad range of phenomena that are ubiquitous in both natural and engineered material systems.

Prediction of Instabilities in Periodic Architected Materials to Actively Modify Wave Propagation Properties

C. Combescure

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Modern engineering challenges have pushed forward the use of architectured materials and called for a new branch of material science to be explored. These special materials exhibit unconventional properties directly linked to their geometry. While instabilities tend to be avoided when working with conventional materials, they may be beneficial for triggering pattern changes in the structure which generate novel properties in the deformed configuration. In particular, Shan et al. 2014 have demonstrated a significant change in wave propagation properties on the various deformed configurations appearing on a hexagonal tiling of circular holes in an elastomeric material. This presentation will propose a method, based on symmetry group theory, to predict instabilities appearing in periodic architected materials. Examples will be presented on hexagonal honeycombs are they are well documented in the litterature with both experimental and numerical results. They will then be extended to triangular honeycombs to prove the method extensive applicability.

References

Shan, S., Kang, S.H., Wang, P., Qu, C., Shian, S., Chen, E.R. and Bertoldi, K., Harnessing multiple folding mechanisms in soft periodic structures for tunable control of elastic waves, *Adv. Funct. Mater.* 24(31), 4935–4942 (2014).

Exploiting the Randomness of High Entropy Alloys

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High Entropy Alloys (HEAs) are many-component, non-dilute random alloys such as the fcc CoCrFeMnNi alloy and the bcc MoNbTaVW. These alloys have one or more impressive mechanical properties, such as exceptional low temperature toughness or very high temperature strength. HEA properties are controlled by the interaction of crystalline defects (dislocations, cracks) with the fluctuating chemical environment created by the random distribution of atoms on the crystalline lattice. Since the compositional space of possible alloys is immense – millions of possible compositions – it is essential to understand the mechanical behavior theoretical so as to enable computationally-guided discovery of new high-performance alloys. Here, we discuss the general new features of defects in random atomic environments and present predictive theories for alloy yield stress versus composition. The theories are used to guide discovery of new multi-performant (high strength retention, low density, acceptable ductility) alloys in the refractory bcc Hf-Ti-Zr-V-Nb-Ta-Cr-Mo-W family.

Steady Shock Wave in Porous Metals: Visous & Micro-Inertia Effects Interplay

C. Czarnota, A. Molinari and S. Mercier

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The response of porous materials under shockwave is of ongoing interest for various industrial and military applications (dynamic compaction of powders, design of blast mitigation devices, collision processes in the solar system, ...). In addition, due to the development of additive manufacturing, the design of materials containing voids is a possible way to create lightweight materials with high energy dissipation properties, to prevent in-structure electronic components or human bodies from strong acceleration forces.

We analyze here steady shockwaves formed in porous metals during planar impact experiments. We consider a population of spherical voids, with same initial radius, isotropically distributed inside a viscoplastic metallic matrix. At low shock pressure, the shock layer is mostly dependent upon the matrix rate sensitivity while for large shock stresses, the structuring of the shock layer is mostly due to micro-inertia effects (induced by radial accelerations in the vicinity of collapsing pores). Two rate sensitivities of different natures are therefore involved into the problem: i) one originating from viscous rate sensitivity of the matrix surrounding voids and ii) one brought by micro-inertia effects from the dynamic void collapse and local acceleration of material particles [2].

We characterize here the material response within the shock by a scaling law that extends to porous metals the Swegle and Grady law [1] proposed for dense metals. This relationship links the stress jump across the shock to the intensity of plastic strain rate within the shock layer. Two regimes are distinguished: (i) the first regime is representative of the viscous response of the matrix material, (ii) the second is dominated by micro-inertia effects with an important influence of the pore size [3]. The latter appears to be quite beneficial since it is conducive to a shock mitigation by attenuating the level of strain rate and of acceleration sustained by material particles.

References

[1] Czarnota, C., Molinari, A., Mercier, S., The structure of steady shock waves in porous metals, *J. Mech. Phys. Solids* 107, 204–228 (2017).
[2] Swegle, J. W., Grady, D. E., *J. Appl. Phys.* 58, 692–701 (1985).
[3] Czarnota, C., Molinari, A., Mercier, S., Steady shock waves in porous metals: Viscosity and micro-inertia effects, *Int. J. Plast.* 135, 102816 (2020).

The Effect of Hydrogen on Localized Plasticity and Crack Initiation in Nickel-Base Alloy 725

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We investigate the effect of absorbed hydrogen (H) on localized plasticity and crack initiation in nickel-base alloy 725. This study is based on *in situ* tensile testing in a scanning electron microscope (SEM) and surface plasticity characterization using digital image correlation (DIC). We find that H has no effect on the degree of localized plastic flow, neither enhancing nor reducing it. Moreover, localized plasticity is neither necessary nor sufficient for H-induced crack initiation: cracks do not initiate in locations of highest localized plasticity and many cracks initiate in areas with no apparent localized plasticity. Indeed, as H content increases, more cracks initiate without any nearby localized plasticity. Our findings militate against hydrogen enhanced localized plasticity (HELP) hypothesis of hydrogen embrittlement in alloy 725.

Micro-Architected Solids: Does Toughness Characterise Fracture?

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Rapid progress in additive manufacturing methods has led to the creation of a new class of architected metamaterials that comprise of a network of struts resembling a periodic truss structure. The mechanical performance these materials is ultimately limited by their tolerance to damage and defects. Yet, manufacturing limitations has meant that experimental investigations of the toughness of these materials have remained elusive. Using architected material specimens comprising nearly a million unit-cells we show that not only is stress intensity factor, as used in conventional elastic fracture mechanics, insufficient to characterise fracture in these architected materials but also that conventional fracture testing protocols are inadequate. Via a combination of numerical calculations and asymptotic analyses we extend the ideas of fracture mechanics to architected materials and thereby develop a design and test protocol for their structural failure.

Grain Boundaries as Barriers Against Shear Banding and Crack Propagation in Ductile Polycrystals: A Gradient Crystal Plasticity Approach

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A strain gradient crystal plasticity model involving the gradient of cumulative plastic slip, was recently developed for finite elastoviscoplastic deformations [1]. It was then applied to the simulation of adiabatic shear banding (ASB) in single and polycrystals [2]. The gradient model ensures mesh-independent strain localization simulations and also introduces a grain size-dependent material response. It is demonstrated that grain boundaries can act as barriers against the propagation of ASB depending on the misorientation between deforming grains. Strain localization is followed by ductile damage and cracking. Void growth is simulated by means of a compressible crystal plasticity model proposed in [3] and complemented by coalescence mechanisms in [4]. This provides a modeling framework for the simulation of crack initiation and propagation in ductile single and polycrystals. Grain boundaries are regarded as barriers against the propagation of intra-granular cracks, as shown in the case of laminate microstructures. The proposed simulation approach can then be used to develop grain boundary engineering for enhanced ductility of metallic alloys.

References

[1] Scherer, J.M., Phalke, V., Besson, J., Forest, S., Hure, J., Tanguy, B., Lagrange multiplier based vs micromorphic gradient-enhanced rate-(in)dependent crystal plasticity modelling and simulation, *Comput. Methods Appl. Mech. Eng.* 372, 113426 (2020).
[2] Phalke, V., Forest, S., Chang, H.-J., Roos, A., Adiabatic shear banding in FCC metallic single and poly-crystals using a micromorphic crystal plasticity approach, submitted to *Mech. Mater.* (2021).
[3] Ling, C., Besson, J., Forest, S., Tanguy, B., Latourte, F., Bosso, E., An elastoviscoplastic model for porous single crystals at finite strains and its assessment based on unit cell simulations, *Int. J. Plast.* 84, 58–87 (2016).
[4] Scherer, J.-M., Besson, J., Forest, S., Hure, J., Tanguy, B., A strain gradient plasticity model of porous single crystal ductile fracture, *J. Mech. Phys. Solids* 156, 104606 (2021).

Strength and Toughness of Lattice Materials

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Recent advances in additive manufacturing have enabled the synthesis of novel cellular materials and micro-lattices with unprecedented properties. While there has been a large volume of work focusing on the nonlinear mechanics associated with the elastic instabilities and plastic collapse of these material systems, their fracture properties under compressive and tensile loads remain relatively unexamined. The design of new materials with superior combinations of strength and toughness, by manipulating material architecture, requires a strong understanding of the connection between key microstructural characteristics and fracture properties. In this talk we will discuss results of our recent efforts to analyze the strength and toughness of 2D and 3D lattice materials by integrating additive manufacturing, experiments, modeling, and theory. Experiments to failure on 3D-lattice materials are performed to measure their fracture strength under compressive and tensile loads, and establish its connection to the underlying microstructure and the properties of the parent solid. We will also present an energy-based framework to analyze the toughness of lattice materials with pre-existing cracks. The proposed approach begins by establishing the energy release rate as a function of loading condition, crack length and base material properties. The fracture energy is calculated experimentally using tensile tests to failure on cracked specimens with increasing crack-length. We then employ Griffith's criterion to predict critical macroscopic failure stress and estimate the effective toughness of each lattice. Finally, we plan to discuss novel data-based techniques that allow for a systematic analysis of both regular and irregular materials.

Constitutive Effects on Failure by Strain Localization in Ductile Materials

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Fracture in ductile materials often occurs following the localization of plastic flow in a band, such as local necking in thin sheets or shear bands under plane strain conditions. The bifurcation from diffuse to localized plastic flow occurs when the incremental constitutive response of the material satisfies an instability criterion, which is generally not satisfied for rate independent materials with a smooth yield surface and obeys the normality flow rule with positive strain hardening (Rice, 1976). Even when softening mechanisms such as micro-void growth are invoked, classical models such as the Gurson model predict unrealistically large strains to the onset of plastic instability. Here, it is shown that apparent deviations from normality can result from a change in the active yield surface in a multi-surface description of plastic flow for a porous ductile material, which leads to realistic predictions of the strains to failure as a function of the loading path. The predicted failure strains are validated by comparison with those obtained using large deformation finite element simulations of voided unit cells under both proportional and non-proportional loading conditions. When specialized to plane stress states, it is shown that the model can predict realistic shapes of the forming limit curves for thin sheets under biaxial stretching as a function of the strain hardening exponent.

References

Rice, J.R., The localization of plastic deformation, in *Theoretical and Applied Mechanics*, ed. W.T. Koiter, North-Holland Publishing Co., 207–220 (1976).

Evolution of Lattice Orientation Heterogeneity in HCP Single Crystals Due to Void Growth

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Highly anisotropic solids, like magnesium alloys are known to suffer from low ductility and fracture toughness. Better understanding of void growth failure mechanism under the condition of locally constraint plastic deformation, related to insufficient number of easy slip systems and twinning activity, may reduce limitations hindering use of hcp alloys as structural elements. Recently, the unexpected effect of twin related reorientation was found in numerical simulations of the void growth, namely a strong decrease of its evolution rate under uniaxial c-axis loading as well as the creation of twin-matrix and twin-twin boundaries leading to complex shapes of evolving cavities. Using own finite element implementation of the crystal plasticity model with twinning [1] of non-porous medium the analysis of multiple factors influencing microstructure evolution and material ductility will be performed, including overall loading scheme, local crystal orientation, initial porosity, and in particular, twinning activity. The longterm goal of this research is the formulation of homogenized elastic-viscoplastic model of porous single crystal deforming by slip and twinning, in which the micro-macro transition scheme is based on the sequential linearization method [2].

References

[1] Frydrych, K., Maj, M., Urbański, L., Kowalczyk-Gajewska, K., Twinning-induced anisotropy of mechanical response of AZ31B extruded rods, *Mater. Sci. Engng.: A* 771, 138610 (2020).
[2] Kowalczyk-Gajewska, K., Petryk, H., Sequential linearization method for viscous / elastic heterogeneous materials, *Eur. J. Mech. Solids/A* 30, 650664 (2011).

Poking and Bulging of 2D Crystals

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Recently, nano-tents and nano-bubbles formed by two-dimensional (2D) materials have seen a surge of interest because they are able to induce in-plane strain as well as strain gradient via out-of-plane deformation. Our previous work has unveiled what sets the in-plane strains in terms of the shape characteristics of nano-tents and nano-bubbles. Moreover, out-of-plane poking or bulging, also known as indentation or blister tests, are popular methods for the measurement of in-plane elasticity of thin sheets. For linear elastic sheets, a load-cubic deflection relation has been frequently assumed so that the stiffness of the sheet could be readily extracted. However, we find that recent results of indentation and bulge tests on 2D materials do not follow this relation, which can be attributed to the slippage of atomically smooth 2D materials against their supporting substrates. Besides, the interfacial slippage could cause instabilities in the sheet such as radial wrinkles in the suspended region, with finite lengths. To gain a quantitative understanding, we assume constant interfacial shear traction and study the wrinkling extent and the effective stiffness of thin sheets upon poking and bulging. We identify a single dimensionless parameter governing these mechanical responses—the sliding number—defined by comparing the sheet tension (that drives the slippage) with the interfacial traction (that resists the slippage). We discuss several useful asymptotic behaviors emerging at small and large sliding numbers. These understandings are helpful for determining when the effect of the interfacial slippage (as well as other substrate-associated subtleties) can be neglected in these tests. We could also propose a simple poking/bulging methodology immune to the complexities caused by the slippage, pretension, Poisson's ratio, substrate roughness, etc., enabling a robust and accurate measure of 2D material stiffness.

Understanding Mechanical Integrity of Metal/Ceramic Interfacial Regions and Mechanical Response of Plastic Deformation at the Micro/Meso Scales

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Recent advances in focused ion beam machining at nano-/micro-/meso- scales and in-situ instrumented mechanical testing in scanning electron microscopes offer opportunities to carry out new mechanical tests at small length scales and gain new insights into key physical factors governing mechanical response at such length scales. Here, we present two examples representative of our recent activities, enabled by applying such experimental techniques and in combination with physics-based modeling and simulations.

The first example deals with mechanical integrity of metal/ceramic interfaces. With ultra-high-vacuum vapor phase deposition, epitaxial Cu/TiN thin film bilayer and TiN/Cu/TiN thin film sandwich structures are grown. Microscale tensile loading was performed on TiN/Cu/TiN sandwich specimens. Critical tensile stresses leading to fracture were measured as a function of the Cu layer thickness, with concurrent and post-mortem observations of failure modes. Molecular dynamics simulations were performed to further understand the Cu growth process on crystalline TiN templates and provide additional physical insights into the observed tensile behavior.

The second example deals with mechanical response of metals during plastic deformation at micro- to meso- length scales. Mechanical loading experiments were performed under uniaxial compression/tension as well as combined torsion/bending. In addition to quantitative measurements of force – displacement curves, site-selective material slice extraction from deformed specimens was performed using focused ion beam machining. Electron backscatter diffraction and transmission electron microscopy examinations of deformed specimens were carried out to probe the density of accumulated geometrically necessary dislocations, in combination with strain gradient plasticity modeling and simulations.

Mitigating Spall Fracture of Ductile Materials by Introducing Porosity

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Material subjected to shock/impact loading conditions can undergo spall fracture when compressive waves reflect off interfaces and free surfaces as tensile waves. Experiments have shown that in ductile materials spall fracture is induced by the evolution of porosity, by the growth of pre-existing pores and/or the growth of newly nucleated pores. However, porosity in ductile materials also introduces plastic compressibility that can lead to energy absorption, thus mitigating spall fracture. We carry out finite element analyses to investigate the role of porosity evolution on the spall fracture of ductile materials subject to flyer plate impact loading conditions. Our results show that porosity in ductile materials can indeed, in certain circumstances, mitigate spall fracture by attenuating stress waves. Here, we focus on results relating impact velocity, initial porosity, and pore nucleation to the spall fracture of ductile materials.

Plate Bending: Localization and Fracture Triggered by Heterogeneities

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The bending fracture strain of thin ductile plates is critical to many industries as it affects formability and crashworthiness. While the micro-mechanics of void nucleation and growth to coalescence are well-known, the mechanics governing bending failure on the mesoscale is subject to detailed investigation. A recent numerical study, using the Gurson model, demonstrates fracture in thin homogeneous ductile plates, subject to bending, to develop from a surface instability on the convex side of the bent plate (the tension side). The instability develops into undulations that result from multiple shear bands emanating from the free surface. It is shown how plastic flow localization in the shear bands intensifies damage development and that a crack initiates in the dominating shear band on the free surface. Hereafter, the crack propagates into the plate under monotonic loading. However, simulating the localization process requires unrealistically high initial porosity values, and the present work focuses on the underlying reasons. Heterogeneities in the plate are, here, investigated as triggers to crack initiation and failure. The study reveals that the spatial distribution of the damaged regions has a crucial effect on ductility. The initial porosity required to initiate a crack at reasonable strain levels during bending is significantly less for a heterogeneous distribution of damaged regions than for a homogeneous porous plate.

On Effects of Void Clustering on Yield Surfaces

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The yield surface of a metal depends on porosity, but also on the void size and the spatial distribution of voids. In the present work, the emphasis is on how yield surfaces for porous metals may be quantified statistically from numerical analysis of different spatial distributions. 3D finite element analyses of a range of different void configurations are carried out based on a representative volume element with periodic boundary conditions. The statistical effects are quantified and compared to a regular FCC void distribution. For a given porosity, the standard deviation of the yield surfaces as well as the mean are determined based on 15 different realizations. Results are obtained for three different void volume fractions. It is quantified how the standard deviation of the different yield surfaces depends on porosity as well as load triaxiality. While the standard deviation is small for low stress triaxialities, T, it is significant for large triaxialities with a maximum around T=5. It is furthermore shown that the Gurson-Tvergaard model is in good agreement with the predictions for the mean of the yield surfaces, and a simple method for modeling the statistical effects in the context of the Gurson-Tvergaard model is proposed.

Extracting Grain Boundary Toughness from Macro-Scale Experiments

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Probing the fracture toughness associated with microstructural features such as grain boundaries can be a challenging task, as the sampled volume and the experimental complexity limit the statistical validity of the obtained results. In this talk, I will describe a recently developed computational framework aimed at extracting the grain-boundary toughness from meso-scale experiments. The proposed framework relies on the ability of a graph neural network to perform high accuracy predictions of the micro-scale material toughness, utilizing a limited size dataset. The merit of the proposed framework arises from the capacity to enhance its performance in different material systems with limited additional training on data obtained from experiments that do not require complex measurements. While initially developed fro crack growth along grain boundaries, the proposed method can be extended to any kind of interface. The method's efficiency is demonstrated by introducing new crack growth rules with limited datasets (200-300 interfaces) and exploring the obtained prediction accuracy.

Harnessing Microscale Buckling Instabilities to Control Macroscale Stiffness

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Mechanical metamaterials employ specifically architectured microstructures to attain effective mechanical properties of interest. Their microstructures often have mechanism-like features which operate in a coordinated, periodic pattern, and which are in many cases activated by microscopic buckling-like bifurcation. As a result, the effective stiffness of the material may be up to an order of magnitude different – usually lower – post bifurcation compared with that before the point of instability is reached. Depending on the internal buckling pattern, it may furthermore be highly anisotropic. Some designs allow multiple patterns, each with its own characteristic anisotropic stiffness. In this study we explore options to control such stiffness evolutions, by a combination of, on the one hand, carefully designed microstructures and, on the other, external stimuli such as mechanical load or constraint, (pneumatic) pressure patterns, or magnetic fields. Ideally, the external actuation is employed to 'nudge' the system into the desired pattern, which is subsequently maintained by the (mechanical) service load. We will show how much insight into the mechanics of such structures may be obtained by the classical tools of buckling analysis applied to highly idealised microstructures and combined with computational modelling of more realistic geometries. Elements of the (computational) homogenisation of the material will also be touched upon.

Path Instability Criterion for Non-Potential Problems in Rate-Independent Plasticity

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Instabilities in plastically deformed solids can manifest themselves in various ways. In general, instabilities can be of a dynamic, geometric or material type, sometimes simultaneously. They can be treated in a unified manner by referring to the energy criterion of path stability, as demonstrated in a long series of works initiated by the author in 1982. This leads to a computational approach that uses incremental energy minimization and has become more popular in the past two decades. This approach, however, is limited to the incremental problems that admit an energy-based potential.

In this lecture, the incremental energy minimization is extended to a broad class of non-potential rate-independent problems. It is based on the recently proposed [1] quasi-extremal energy principle (QEP) which can be applied when ordinary stationarity or minimum principles fail. The key point is that the minimized energy function then depends not only on the variables undergoing variations but also on an unknown solution as a parameter.

The energy criterion of path stability, built into the QEP, provides a method for selecting a solution among many alternatives. In this way, the post-critical deformation branch can be selected automatically during the computation and tracked to examine a series of successive instabilities. This is shown by examples of large deformation of a fcc metal crystal with lattice rotations and associated multiple changes of active slip-systems. Application of the QEP to gradient plasticity is also discussed.

References

[1] Petryk, H., A quasi-extremal energy principle for non-potential problems in rate-independent plasticity, *J. Mech. Phys. Solids* 136, 103691 (2020).

Enhancing Damage Tolerance and Crack Healing in Ceramics by Kinking: The Case of MAX Phases

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In the last two decades, a new class of ceramics has emerged that has challenged their typical description as materials that are hard, difficult to machine, and susceptible to damage and thermal shock. This class of 70+ members - known as the MAX phases – share common unique chemical formula $M_{n+1}AX_n$, (where n = 1, 2 or 3, M is and early transition metal, A is an mostly group 13-16 elements, and X is either C or N) and naonolayered crystal structure in which strongly bonded MX layers are interleaved by weakly bonded A layers. The main reason for growing interest in MAX phases lies in their unusual mechanical properties in general, and high damage tolerance in particular. In general, MAX phases are elastically stiff, good thermal and electrical conductors, resistant to chemical attack, and have relatively low thermal expansion coefficients, but also relatively soft and most readily machinable, thermal shock resistant and damage tolerant. Moreover, some of them – notably Ti_2AlC and Ti_3SiC_2 - are fatigue, creep, and oxidation resistant. Therefore, MAX phases are considered to be a good candidate material, especially for high temperature structural applications in extreme environments. This presentation provides an overview of the current understanding of mechanical behavior of MAX phases, with the special focused on their deformation by kinking that can be traced back to their naolaminated crystal structure. Anisotropic deformation and failure mechanisms in MAX single crystals and micropillars is discussed in more details. Furthermore, deformation and failure mechanisms below and above brittle to plastic transition temperature in MAX phases are reviewed, as well as effect of microstructure (i.e. grain size and secondary phases) on the observed mechanical behavior of polycrystalline MAX phases. Possibilities for further improvements in mechanical properties of MAX phases by tailoring their composition and microstructure are also briefly discussed in this presentation.

Exploration of Ductile Failure Processes in an Aluminum Alloy Through X-Ray CT Scan and Microscopy

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The mechanism of ductile failure in structural material has been a great interest in theoretical and applied science field. Various failure models have been proposed and their ability to predict failure is still being tested and refined over the time. In this work, we explore the failure of an aluminum alloy Al-6061-T6 through interrupted tests, x-ray tomography, microscopy and simulations.

A series of experiments containing fatigue pre-cracking, interrupted loading are performed on a compact tension specimen. Digital image correlation is used to monitor the macroscopic load-displacement response. During the interrupted testing procedure, three-dimensional X-ray computed tomography is used after each loading increment to identify the three dimensional geometry of the crack front. The specimens are scanned in slices with a 5 μm resolution and then reconstructed into a 3D model which reveals the geometry of the crack surface. Plastic strain localization is observed near the outer surface of the specimen while no internal damage or voids are detected by the x-ray at the scale of 5 μm and above. High-resolution optical and scanning electron microscopic images are coupled with x-ray images to interpret the path of the crack in the microstructure.

A numerical simulation of the fracture behavior is performed in ABAQUS with a fine mesh at level of 20μm, with a J2 plasticity model, and a triaxiality dependent strain-to-failure criterion. This model is able to reproduce the details of the crack geometry such as the formation of slant cracks in shear localized regions.

Multi-Scale Modeling of Energetic Materials Under High Strain Rate Loadings

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The generation and development of hotspots are key factors in the ignition of energetic materials (EM) under dynamic loadings. Even though the overall bulk temperature of EM is too low to ignite, the formation of hotspots causes localized ignition of EM, which determines the materials' sensitivity. In this talk is presented a new computationally efficient framework developed for predicting hotspots due to plastic dissipation at the energetic crystal scale. The novel and creative solution put forward is a new description of the energetic crystal behavior, which respects the inherent symmetry of its lattice structure and a multi-scale methodology which enables to capture the bulk behavior. Illustration of the approach is presented for PETN. Specifically, a new single crystal model with yielding accounting for the specific tetragonal crystalline symmetry of the PETN crystal was developed and identified based on available data. The new criterion predicts the dependence of the onset of irreversible deformation on the loading and its orientation. It is shown that for the PETN crystal, the directionality in yielding strongly affects the local plastic dissipation and local spikes in the temperature during dynamic loading. It is also presented a new model for ES-1 that accounts for its specificities of deformation, namely difference in response between tension and compression. We conclude with illustrations of the capabilities developed for modeling dynamic events with penetrators made of ES-1 and PETN filling.

Discontinuous Compression Structures: From Tensegrity Planetary Landers to High-Performing Metamaterials

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The term tensegrity, derived from tensional integrity, refers to a certain class of structural systems composed of bars and cables. Through adequate pre-stressing of their cable members, tensegrity structures generally become mechanically stable. A distinctive characteristic of tensegrity structures is that their connectivity graph is composed of isolated subgraphs of compression members connected to the rest of the graph strictly through tension members. Thus, we usually refer to them as discontinuous compression structures. In this work we will show a unique property of some tensegrity structures: that they remain mechanically stable even after their compression members undergo buckling and well into their post-buckling regime. We then show how this post-buckling stability can be exploited to generate discontinuous-compression metamaterials with unprecedented mechanical properties, including phase transitions in the wave propagation domain, mechanically activated switch-like anisotropic electric conductivity, and failure delocalization.

The Effect of Actual Porous Microstructure on the Formation of Dynamic Necks, Adiabatic Shear Bands and Plastic Shock Waves

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We have performed a microstructurally-informed finite element analysis on the effect of actual porosity on the formation of dynamic necks, adiabatic shear bands and plastic shock waves in metallic materials subjected to high strain rates. For that purpose, we have characterized by X-ray tomography the porous microstructure of 4 different additively manufactured materials (aluminium alloy AlSi10Mg, stainless steel 316L, titanium alloy Ti6Al4V and Inconel 718L) with initial void volume fractions ranging from $\approx 0.0007\%$ to $\approx 2\%$, and pore sizes varying between ≈ 6 μm and ≈ 110 μm. The pore size distributions obtained from the tomograms have been fitted using a Log-normal statistical function, which has been used in conjunction with a Force Biased Algorithm to generate finite element models in ABAQUS/Explicit with actual distributions of voids. Four benchmark problems have been investigated: rapid radial expansion of rings, dynamic torsion of thin-walled tubes, collapse of thick-walled cylinders and dynamic cylindrical cavity expansion. The finite element results provide new insights into the role of void volume fraction, voids size and voids shape on the formation of dynamic plastic instabilities for different loading rates and stress states.

Defects, Crack Path and Crack Growth Resistance

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The strength of a material can be analyzed using the weakest link theory, which relates the probability of failure of the material as a whole to the probability of failure of each volume element within it. Consequently, attempts are made to eliminate weak links, i.e., microstructural features of low intrinsic strength, and introduce features of high intrinsic strength in a material. However, while weak links may degrade a material's strength, their effect on crack growth resistance, is not obvious. Indeed, material microstructure, more often than not, affects strength and crack growth resistance in different ways. Herein, we explore multiple possibilities of enhancing materials' crack growth resistance by deliberately introducing weak links into the materials' microstructures. In one example, we attempt to engineer the crack path and increase the crack growth resistance by adding or removing weak particles that guide the crack. In another example, we investigate the possibility of achieving high fracture toughness by the design of lightweight (density below water) metallic micro-architectured materials that comprise hexagonal array of holes in plates. Finally, we demonstrate that the intergranular crack growth resistance of a polycrystal that contains exclusively high toughness grain boundaries is suboptimal and its crack growth resistance can be increased by introducing a minority fraction of weak grain boundaries.

Phase-Field Model for Spatially Resolved Deformation Twinning Coupled with Crystal Plasticity

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Deformation twinning is classically treated as a simple shear that occurs on well-defined crystallographic twinning systems. Here we propose to treat twinning as a displacive transformation, resembling a phase transformation, such that the transformation from the parent matrix to a twin deformation variant occurs through a stretch followed by a rotation. The respective finite-deformation kinematics is then introduced in the sharp- and diffuse-interface frameworks and includes a consistent description of twinning-induced reorientation of crystal lattice and slip systems. This kinematics is also a convenient framework for developing a phase-field model of coupled twinning and crystal plasticity. The phase-field model is developed within the incremental energy minimization approach. The resulting incremental minimization problem is non-smooth due to the rate-independent dissipation terms and bound constraints enforced on the order parameter describing the diffuse twin boundaries. A micromorphic regularization is thus applied to facilitate finite-element implementation of the model, in particular, to efficiently treat the non-smooth terms in the incremental potential. Spatially resolved evolution of twin microstructure is studied for an HCP magnesium alloy, for which a two-dimensional computational model is developed that includes one twin deformation variant, i.e., two conjugate twining systems, and three effective slip systems (one basal and two pyramidal slip systems).

Shock-Induced Spallation in Monocrystalline Boron Carbide

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Traditional molecular dynamics (MD) shock simulations to investigate spallation characteristics of materials are computationally expensive as they require a compressive pulse to be generated and propagated in a domain, followed by its reflection to a tensile pulse. We propose an efficient MD-based method to cause spallation by propagating two tensile shock fronts of equal amplitude from opposite ends of a domain and meet at the center. We investigated the spallation characteristics of monocrystalline boron carbide along the [111] orientation (along the three-atom chain) and at 90° to [111]. In both cases, boron carbide exhibited a linear-elastic axial stress-strain response up to the yield stress followed by non-linear behavior that differed significantly in the two crystal orientations. Along [111], post-yield softening was noted followed by an almost perfectly plastic response. In contrast, a post-yield hardening was observed at 90° to [111] up to a peak stress followed by an abrupt loss of strength. Further, spallation along [111] was accompanied by micro-crack initiation normal to the loading direction while at 90° to [111], spallation was preceded by crack formation at ∼45° to the loading direction. To explain these observations, a systematic analysis of bond deformation was conducted, wherein the average strain experienced by each of the 41 bonds in a unit cell of boron carbide was estimated as a function of simulation time. This enabled identification of bonds which experience the highest strains (and damage) when loaded along a given orientation, thus pointing towards plausible explanations for the aforementioned stark differences in mechanical response.

On Selected Space-Fractional Structural Models

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The considerations are concentrated on the mathematical modelling of structural elements undergoing a strong scale effect. The property of the matter that it mechanical properties depend on specimen dimension will be included by utilising fractional calculus, through the Riesz-Caputo fractional derivative. Space-fractional Euler–Bernoulli and Timoshenko beams as well as space-fractional Kirchhoff-Love plates will be discussed. Theoretical considerations will be contrasted with experimental results for static and dynamic cases together with the effects of the functionally graded material. The fundamental result is that for a single set of material parameters, the elaborated models can mimic the scale effect for both static and dynamic cases, which is sometimes not true for competitive formulations.

References

Sumelka, W., Thermoelasticity in the framework of the fractional continuum mechanics. *J. Therm. Stresses* 37(6), 678–706 (2014).
Szajek, K., Sumelka, W., Discrete mass-spring structure identification in nonlocal continuum space-fractional model. *Eur. Phys. J. Plus*, 134(9), 448 (2019).
Stempin, P., Sumelka, W., Space-fractional Euler-Bernoulli beam model - theory and identification for silver nanobeam bending. *Int. J. Mech. Sci.*, 186, 105902 (2020).
Stempin, P., Sumelka, W. Dynamics of space-fractional Euler–Bernoulli and Timoshenko beams. *Materials*, 14(8), 1817 (2021).
Stempin, P., Sumelka, W., Formulation and experimental validation of space-fractional Timoshenko beam model with functionally graded materials effects. *Comput. Mech.* 68(3), 697–708 (2021).

The Effect of Material Orientation on Void Growth

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In this work, we have brought to light the effect of material orientation on void growth. For that purpose, we have performed finite element calculations using a cubic unit-cell model with a spherical void at its center and subjected to periodic boundary conditions. The behavior of the material is described with an elastic isotropic, plastic orthotropic constitutive model with yielding defined by Yld2004-18p criterion (Barlat et al., 2005). We have used the multi-point constraint subroutine developed by Dakshinamurthy et al. (2021) to enforce constant values of macroscopic stress triaxiality T and Lode parameter L in calculations. We have carried out simulations using a novel strategy which consists of including angular misalignments within the range ($0 \leq \theta \leq 90$), so that one loading direction is parallel to one of the symmetry axes of the material, and θ is the angle formed between the other two loading directions and the second and third orthotropy axes. The finite element calculations have shown that the misalignment between loading and material axes makes the void and the faces of the unit-cell to rotate and twist during loading. Moreover, the main contribution of this work is the identification of an intermediate value of the angle for which the growth rate of the void reaches an extreme value (minimum or maximum), so that the numerical results indicate that material orientation and angular misalignment can be strategically exploited to control void growth, and thus promote or delay localization and fracture of anisotropic metal products.

References

Barlat, F., Aretz, H., Yoon, J. W., Karabin, M. E., Brem, J. C. and Dick, R. E., Linear transfomation-based anisotropic yield functions, *Int. J. Plast.* 21(5), 1009–1039 (2005).
Dakshinamurthy, M., Kowalczyk-Gajewska, K., Vadillo, G., Influence of crystallographic orientation on the void growth at the grain boundaries in bi-crystals, *Int. J. Solids Struct.* 212, 61–79 (2021).

Investigation of Effect of Plate Thickness on Ductility for Engineering Applications

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The main focus of this talk is on the effect of metal plate thickness on failure strain measured outside the localized area of deformation. The study is motivated by the need to improve a puncture resistance of rail tank cars carrying hazardous materials. Full scale experiments and detailed simulations of tank car puncture have been conducted, allowing development of multiple concepts improving the puncture resistance. In terms of performance, one of the most effective solutions involves increasing the tank car shell thickness. However, this concept is based on the assumption that increasing the thickness of the shell does not lead to any significant loss of ductility. To investigate this assumption, a series of detailed numerical simulations of plates ranging in thickness from 1.4 to 25.4 mm has been conducted using the micro-mechanics based Gurson material model. The Gurson model parameters were selected based on the prior study of fundamental differences in ductile plate failure under bending vs. tension. The same element size, motivated by the void spacing for the tank car steel, was used for all thicknesses. The simulated plate specimens with varying thickness were subjected to both plane strain tension and plane strain bending loading conditions. Preliminary results indicate that increasing the plate thickness leads to significant loss of ductility in bending and a minor increase of ductility in tension. These results are consequential not just for tank car puncture resistance, but a wide range of other engineering applications.

Functional Buckling and Folding of Ring Origami

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In this talk, the concept of ring origami folding mechanism will be introduced as a strategy for deployable/foldable structures. Different ring shapes including circle, ellipse, triangle, rectangle, hexagon, and other polygons will be discussed. By rationally designing the geometrical properties the ring, such as cross-section geometry, aspect ratio, and radius of rounded corners, the rings with different geometry can trigger buckling-induced snapping and self-guided folding under either bending or twisting load. The ring folds into a three-fold ring structure and the stable folded configuration can be as small as 12% of the initial envelope area of the ring. Through finite-element analysis, snap-folding behaviors of the single ring with different geometries are studied for ring origami assemblies for functional foldable structures. Geometric parameters' effects on the foldability, stability, and the packing ratio are investigated and are validated experimentally. With different rings as basic building blocks, the folding of ring origami assemblies is further experimentally demonstrated, showing significant packing ratios. The ring origami is further integrated with 3D printable flexible circuits to design foldable and wearable devices. It is envisioned that the reported snap-folding of origami rings will provide alternative strategies to design foldable/deployable structures and devices with reliable self-guided deformation and large area change.

POSTERS

Lamination-Based Efficient Treatment of Weak Discontinuities for Non-Conforming Finite-Element Meshes

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

References

[1] Kabel, M., Merkert, D., Schneider, M., Use of composite voxels in FFT-based homogenization, *Comput. Methods Appl. Mech. Eng.* 294, 168–188 (2015).

The Effect of Predeformation History Under Complex Loading on the Yield Surface Evolution of Titanium Alloy: An Experimental Investigation

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The main goal of this work was to describe the evolution of the yield surface using an experimental investigation dealing with the pre-deformation effects executed by the axial tension and proportional cyclic torsion on tubular specimens. The analysis of material behavior beyond the yield point was supported by the concept of yield surface, in which the description of the initial and subsequent yield surfaces receives special emphasis. The yield surface has been determined by the technique of sequential probes of the single specimen along 17 different strain-controlled paths in the plane stress state. It was found, that for the defined plastic offset strain, as-received specimen exhibits anisotropic behavior that could have resulted from the metal production process or the specimen manufacturing process. Furthermore, the yield surface size of pre-deformed specimen was reduced in all directions, except of that representing axial tension.

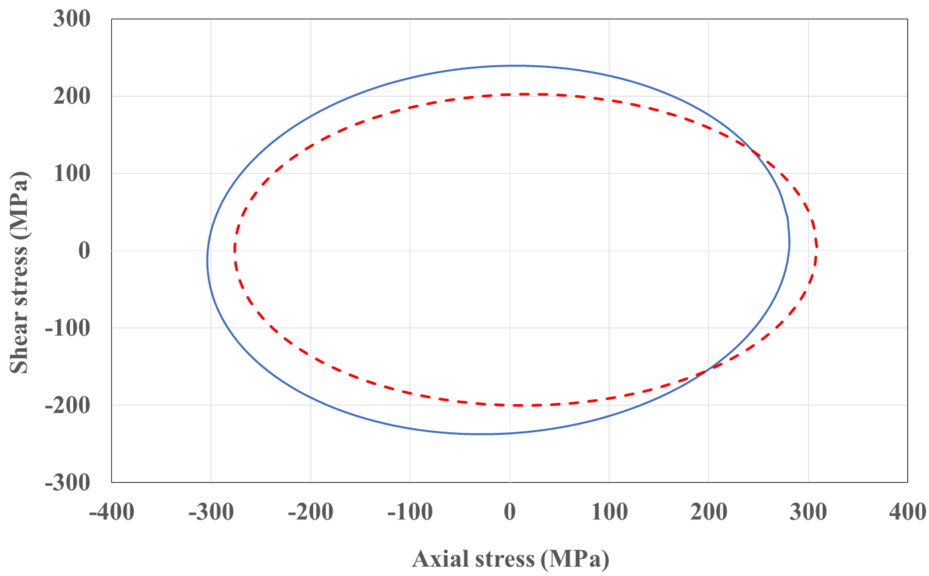

Figure 1: Yield surfaces (1×10^{-4} offset strain) for the pure titanium in as-received state (blue continuous line) and in the pre-deformed state due to simultaneous monotonic axial tension up to permanent strain equal to 1% and proportional cyclic torsion of strain amplitude $\pm 0.4\%$ at 0.5 Hz frequency (red broken line).

Acknowledgment: This work was supported by NCN project No. 2019/35/B/ST8/03151, entitled "Yield Surface Identification of Functional Materials and Its Evolution Reflecting Deformation History under Complex Loadings".

Structure-Based Optimization of Crystal Plasticity Parameters in Metals and Alloys

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The crystal plasticity (CP) theory enables to include the microstructural information about the plastic deformation mechanisms (such as dislocation slip, deformation twinning or martensitic transformation) in a continuum mechanics setting. A crucial aspect of the CP modelling is proper calibration of the parameters. This task is often carried out in an automatic fashion using various optimization techniques such as gradient optimization, Levenberg-Marquardt method, Bayesian optimization or particle swarm optimization. However, the evolutionary algorithms (EAs) seem to be the most commonly applied approach in this context. Their prevalence stems from many advantages such as easy understanding and implementation, compatibility with discontinuous objective function, good performance even when many parameters are to be optimized at the same time and ability to escape local minima. The poster presentation will first present the author's experience with EA parameter optimization of polycrystalline metals and alloys using Eshelby solution-based self-consistent mean-field models, cf. [1, 2]. Then, the recently developed optimization of CP parameters based on the results of crystal plasticity finite element method (CPFEM) simulations of instrumented indentation will be shown. In particular, the recent results will highlight the efficiency of using the minimization of the difference between load-penetration curves or surface topographies as the objective function.

References

[1] Girard, G., Frydrych, K., Kowalczyk-Gajewska, K., Martiny, M., Mercier, S., Cyclic response of electrodeposited copper films. Experiments and elastic-viscoplastic mean-field modeling, *Mech. Mater.* 153, 103685 (2021).
[2] Frydrych, K., Jarzębska, A., Virupakshi, S., Kowalczyk-Gajewska, K., Bieda, M., Chulist, R., Skorupska, M., Schell, N., Sztwiernia, K., Texture-based optimization of crystal plasticity parameters: Application to zinc and its alloy, *Metall. Mater. Trans. A* 52, 3257–3273 (2021).

Micromechanical and Numerical Analysis of Shape and Packing Effects in Elastic-Plastic Particulate Composites

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The combined effect of reinforcement shape and packing on the macroscopic behaviour of particulate composites is presented. The proposed semi-analytical modelling method combines the Replacement Mori-Tanaka scheme and the analytical Morphologically Representative Pattern approach. The concentration tensors of non-ellipsoidal inhomogeneities are found numerically using simple simulations of a single particle. The extension to the regime of non-linear material behaviour is performed by employing the incremental linearization of the material response in two variants: tangent and secant, depending on the definition of the current stiffness tensor. The metal matrix is assumed to be a ductile material with linear elasticity and the Huber-von Mises yield function with the associated flow rule. The inclusion phase is considered to be a linearly elastic material with parameters relevant to a ceramic. The results are compared with the outcomes of numerical simulations and predictions of the classical mean-field models based on the Eshelby solution, e.g., the Mori-Tanaka model or the Self-Consistent scheme. The statistical volume elements have randomly placed inclusions with a selected shape. Five shapes of inhomogeneities are selected for the analysis: a sphere, a prolate ellipsoid, a sphere with cavities, an oblate spheroid with a cavity as well as an inhomogeneity created by three prolate spheroids crossing at right angles. It is found that the proposed modification of the Morphologically Representative Pattern approach can be used as an alternative to computational homogenization in the case of elastic-plastic composites with different shapes and packings of particles.

Field Analysis of Energy Conversion During Plastic Deformation Process

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The paper presents field analysis of energy conversion process during uniaxial tension of the 310S austenitic steel. A new experimental approach which enables to determine energy balance components is proposed. The distribution of plastic work was determined based on the displacement field obtained using digital image correlation (DIC) technique and the previously developed DIC-based stress determination method [1]. In the present study, the constitutive model has been extended of the influence of strain rate and plastic anisotropy. The plastic anisotropy is described by the yield function introduced by Barlat and Liam [2]. On the other hand, the method of obtaining distribution of energy dissipated as heat combines temperature field measurements, coupled DIC and infrared thermography (IRT) analysis and also transient heat conduction equation [3]. The field analysis of the contributions of all the terms in the equation is performed with respect to the various process durations. The approach takes into account the thermoelastic effect and the heat exchange with the surroundings due to the heat convection and radiation. As a measure of the energy conversion the energy storage rate Z (defined as the ratio of the stored energy increment to the plastic work increment) was used. Just before the end of the process the Z value decreases significantly and becomes close to 0 or even negative, which means that the material loses its ability to store the energy. The microstructure investigation based on the electron backscatter diffraction (EBSD) analysis for subsequent stages of the process showed that material's microstructure evolves towards two dominant texture components.

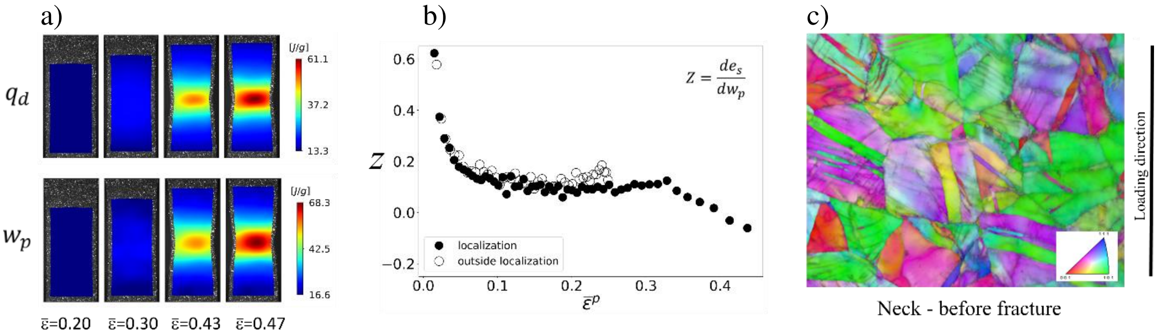

Figure 1: The evolutions of the q_d and w_p a), the energy storage rate b) and corresponding orientation map in necking area c).

References

[1] Musiał, S., Nowak, M., Maj, M., *Arch. Civ. Mech. Eng.* 19(4), 1183–1193 (2019).
[2] Barlat, F., Lian, K., *Int. J. Plast.* 5(1), 51–66 (1989).
[3] Musiał, S., Maj, M., Urbański, L., Nowak, M., *Int. J. Solids Struct.* 238, 111411 (2022).

Effect of Shape Recovery and Cyclic Loading on the Evolution of Micro-Cracks in Shape Memory Polymers

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Shape memory polymers (SMPs) have attracted a great attention as smart materials due to their high shape recovery characteristics. The mechanically deformed SMP recovers its original shape by being exposed to an external stimulus, e.g. heat [1]. In this study, the polyurethane shape memory polymer (PU-SMP) with $T_g = 45°$C, manufactured by the *SMP Technologies Inc.*, Tokyo, Japan, was subjected to one and five loading-unloading tensile cycles at strain rate of $10^{-2}s^{-1}$ up to maximum strain of 60$\%$. The investigation was conducted on Instron 5969 testing machine at room temperature. The effect of (I) thermal shape recovery of the PU-SMP at the temperature $T_g + 20 = 65°$C and (II) number of loading-unloading cycles on the formation and healing of micro-cracks were investigated through microscopic observation by scanning electron microscope (SEM).

Detection of initiation and propagation of defects in materials and finding ways to avoid or heal them allows us to predict the behavior of the material during the service time and overcome the potential dangers of failure [2]. The results of our study proved that the mechanical deformation and shape recovery of the PU-SMP are related to the formation and healing of the micro-cracks, respectively. As demonstrated in Fig. 1, the cracks which were formed during the one loading-unloading cycle (Fig. 1a) are healed during the thermal shape recovery (Fig. 1b). Moreover, the micro-cracks which were formed during the one-cycle are also healed during five loading-unloading cycles (Fig. 1c).

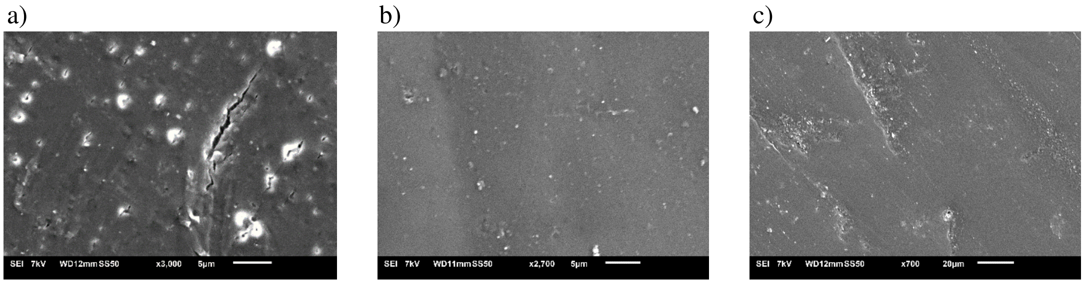

Figure 1: SEM images of PU-SMP specimen after a) one-cycle loading-unloading b) thermal shape recovery c) five-cycle loading-unloading.

Thermal shape recovery property of the PU-SMP enables the micro-cracks to be healed at the temperatures above T_g. Besides, there might be an optimum number of loading-unloading cycles in which micro-cracks formed in the PU-SMP specimen are healed.

Acknowledgments: The research has been carried out with support of the Polish National Center of Science under Grant 2017/27/B/ST8/03074.

References

[1] Pieczyska E.A., Maj M., Kowalczyk-Gajewska K., Staszczak M., Gradys A., Majewski M., Cristea M., Tobushi H. and Hayashi S., *Smart Mater. Struct.* 24(4), 045043 (2015).

[2] Awaja F., Zhang S., Tripathi M., Nikiforov A., Pugno N., *Prog. Mater Sci.* 83, 536–573 (2016).

Stress-Induced Martensitic Transformation in Shape Memory Alloys During Nano-Indentation: Insights from Phase-Field Simulations

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Instrumented micro- and nano-indentation is a powerful experimental tool for the characterization of the material behaviour at small scales. It applies also to shape memory alloys (SMAs), which have gained much popularity thanks to their interesting features of pseudoelasticity and shape memory effect. In general, when the SMA material is in the pseudoelastic state, the indentation-induced martensitic microstructure disappears during unloading, and thereby, the load–indentation depth response is the only available experimental data that can be used for material characterization. It thus seems that modeling is the primary means to examine the martensitic microstructure and can be exploited to supplement the experiment.

The phase-field method is an efficient computational tool for modeling the spatially-resolved microstructure at the continuum level. In the present study, a finite-strain phase-field model is developed for multivariant martensitic transformation. The model possesses a number of important features that enables it to provide a physically relevant description of martensitic transformation under nano-indentation. More specifically, the model is formulated in the finite-deformation framework, admits an arbitrary crystallography of phase transformation, and an arbitrary elastic anisotropy of phases (consistent with crystallographic symmetry of phases). The goal in this work is to thoroughly investigate the microstructure evolution in CuAlNi SMA during nano-indentation. In particular, the impact of the crystal orientation on the microstructure evolution and mechanical response is studied. Moreover, we show that the characteristic features of our model are crucial elements to correctly predict the microstructure.

Gradient-Enhanced Crystal Plasticity Model with Micropolar Regularization: Prediction of the Indentation Size Effects

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In recent times of miniaturization and nanotechnology, the understanding of the behavior of materials at the micro- and nano-scales has attracted attention of many theoretical and experimental studies. Despite years of efforts, there are still challenges and unsolved theoretical dilemmas. In the case of crystal plasticity (CP), it is now accepted that the response of the material at the micro scale is influenced by the geometrically necessary dislocations (GNDs) which are associated with the incompatibility of plastic (or elastic) deformation. Notwithstanding the accepted concept of GNDs and a great variety of existing CP models, 3D indentation simulations with acceptable experimental validation are still scarce in the literature.

In the current work, we present a model of gradient crystal plasticity (GCP) which is based on the 'minimal' gradient enhancement of CP that involves a natural length scale in the hardening law. In its simplest form, the internal length scale coincides with the mean free path of dislocations – the well-known length-scale in the dislocation theory of plasticity – and therefore has a direct physical meaning [1]. In the present work, the Cosserat model is employed to encompass the gradient-enhanced model in the finite element setting. It is shown that the resulting computational model is capable of predicting the indentation size effect on nominal hardness of a Cu single crystal with a satisfactory accuracy [2].

References

[1] Petryk, H., Stupkiewicz, S., A minimal gradient-enhancement of the classical continuum theory of crystal plasticity. Part I: The hardening law, *Arch. Mech.* 68, 459–485 (2016).
[2] Ryś, M., Stupkiewicz, S., Petryk, H., Micropolar regularization of crystal plasticity with the gradient-enhanced incremental hardening law, *Int. J. Plasticity* (submitted).

Effect of Boundary Conditions and Crystallographic Orientation on the Cylindrical Void Growth in FCC Single Crystals Using CPFEM

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The crystal plasticity finite element method was used to investigate cylindrical void growth and coalescence in face-centered cubic single crystals. In the finite element model, a rate-dependent crystal plasticity constitutive theory has been implemented [1].Twelve potentially active slip systems $\{111\}\langle 110\rangle$ are used to characterize plastic deformation in fcc single crystals. A 2D plane strain model with one void has been used. The effects of lattice orientation and boundary conditions on void growth are investigated. Boundary constraints were enforced in two different ways. The first is based on enforcing constant in plane stress biaxiality via a particular truss element for many defined values of the stress biaxiality ratio η [3], while the second is based on displacement controlled by imposing load biaxiality factor β. Three crystallographic orientations were examined, with the major loading direction along [100], [110], and [111].

Two loading scenarios were explored in the current study for displacement-controlled boundary conditions. One is a uniaxial loading case, while the other is a biaxial loading scenario, with varying load biaxiality factor β to investigate its impact on void evolution. When compared to biaxial loading, void evolution under uniaxial loading is greatly influenced by crystal orientation. Under biaxial loading, the influence of lattice orientation diminishes. The void expansion and coalescence are dictated by stress triaxiality and accumulated strain in such circumstances. The void growth is accelerated with larger load biaxiality factor β due to higher in plane mean stress, and the void shape is a polygon with rounded corners, as shown in [2]. The response of void evolution differs for the same β and η values. However, the response is the same for uniaxial loading and $\eta = 0$ case.

References

[1] Frydrych, K., Kowalczyk-Gajewska, K., Grain refinement in the equal channel angular pressing process: simulations using the crystal plasticity finite element method, *Modell. Simul. Mater. Sci. Eng.* 26, 065015 (2018).
[2] Srivastava, A., Needleman, A., Effect of crystal orientation on porosity evolution in a creeping single crystal, *Mech. Mater.* 90, 10–29 (2015).
[3] Ling, C., Besson, J., Forest, S., Tanguy, B., Latourte, F., Bosso, E., An elastoviscoplastic model for porous single crystals at finite strains and its assessment based on unit cell simulations, *Int. J. Plast.* 84, 58–87 (2016).

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