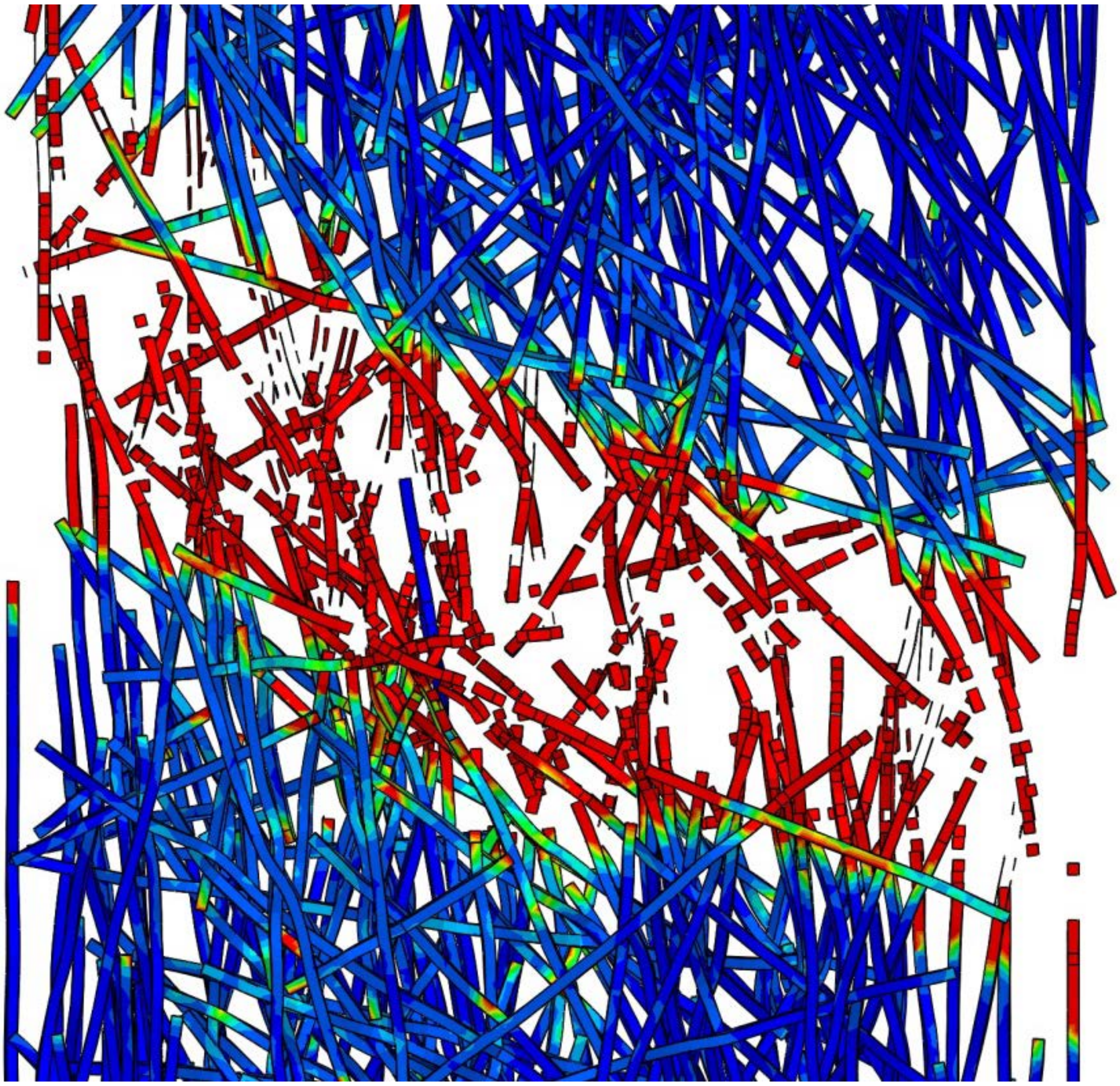
8th KMM-VIN Industrial Workshop

Modeling of Composite Materials and Composite Coatings

October 09-10, 2018
Freiburg, Germany

Programme and Abstracts



European Virtual Institute on Knowledge-Based Multifunctional Materials KMM-VIN AISBL
Fraunhofer-Institut für Werkstoffmechanik IWM

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Organized by

European Virtual Institute on Knowledge-Based Multifunctional Materials KMM-VIN-AISBL
Fraunhofer-Institut für Werkstoffmechanik IWM

Hosted by

Fraunhofer-Institut für Werkstoffmechanik IWM
Wöhlerstr. 11
79108 Freiburg
Germany

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Prof. Michal Basista	KMM-VIN

Local Organizing Committee

PD Dr. Jörg Hohe
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Dr. Claudio Findeisen
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About the Organizers

The **European Virtual Institute on Knowledge-based Multifunctional Materials KMM-VIN AISBL** is a self-sustainable non-profit organization which promotes and facilitates cooperative research and development activities of its Members in advanced structural and functional materials. It creates conditions for networking and conducting joint research on advanced materials and offers a mobility program for young researchers and customized courses and trainings with focus on materials for Transport, Energy and Biomedical sectors.

The **Fraunhofer Institute for Mechanics of Materials IWM** is a research and development partner for industry and public contracting bodies concerning the topics of component and systems reliability, safety, durability and functionality. The Fraunhofer IWM's »mechanics of materials« approach is used to identify weaknesses and defects in materials and components, determine their causes and develop solutions that lead to the safer use of components as well as the development of functional materials and resource efficient manufacturing processes.

Overview

The present workshop is the 8th workshop in a series of industry related meetings organized by KMM-VIN. The objectives of the meeting are to bring together leading experts from industry and academia to discuss the latest developments in the modeling of the mechanical response of composite materials and composite coatings.

Interest is directed to the interaction of the properties of composite materials with their microstructure, considering metallic, ceramic and polymeric materials. Beside multiscale simulation methods, the formulation and numerical implementation of adequate material models is addressed. A special topic is the effect of disordered and random microstructures, their impact on the effective material response and numerical methods to deal with the scatter induced by these effects.

Specific topics include

- multi-scale modelling of materials,
- multi-physics modelling,
- mean field approaches,
- design of materials,
- development of advanced constitutive models,
- implementation of new material models in finite element software,
- stochastic aspects in material modelling,
- experimental methods for parameter identification for advanced material models,
- application of advanced material models in structural simulation.

The industrial fields mainly addressed by the workshop are the automotive and transport sectors, the aerospace industry and the energy sector, but also include aspects from other fields, especially all fields of lightweight construction. By this means, a fruitful interaction and exchange of ideas from different technological sectors, all related to advances in the modelling of composite materials will be achieved.

The workshop comprises four keynote lectures covering aspects of polymer matrix, ceramic matrix and cellular materials, including both, the academic and the industrial points of view. The keynote lectures are complemented by 22 contributed presentations covering the entire field of composite material design options, multiscale simulation, advanced material models and their implementation as well as advanced experimental techniques for parameter identification for complex materials.

Workshop Programme

	October 09, 2018 - day 1	
12:00 - 13:00	coffee (foyer to rooms A1.19 and A1.20)	
	room A1.20: plenary session (chair: J. Hohe)	
13:00 - 13:30	welcome address	
13:30 - 14:10	keynote J. Albinger, A.K. Weiß, M. Wolff (MT Aerospace AG) Development of a differential composite booster case including a structural bonding	
14:10 - 14:40	coffee break (foyer to rooms A1.19 and A1.20)	
	room A1.20: material models and effective properties (chair: J. Albinger)	room A1.19: experimental methods for advanced models (chair: A. Jung)
14:40 - 15:00	J. Bold: Composite simulation: a new type of material model and failure criteria?	K. Tschöke, T. Gaul, B. Weihnacht, L. Schubert: Modelling composites for structural health monitoring systems using acoustic ultrasonic methods
15:00 - 15:20	L. Faksa, W. Daves, W. Ecker, T. Kaltenbrunner, C. Czettl: Modeling of the residual stress evolution in coated cemented-carbide tools during manufacturing	M. Schober, Z.M. Abdul Hamid, S. Fliegener, P. Gumbsch, J. Hohe: Characterization of fiber-matrix interface strength using micro tensile experiments
15:20 - 15:40	Z.M. Abdul Hamid, M. Gall, J. Hohe: A material model for fatigue degradation and damage in composite materials	W. Węglewski, M. Basista, M. Krajewski, K. Bochenek: An unusual grain size effect in measurements of thermal residual stress in alumina-chromium composites – explanation by modelling
15:40 - 16:00	W. Bielski, R. Wojnar: Conductivity of a two-dimensional two-component structure	J. Lienhard, F. Huberth, P. Stadtmüller, B. Ragupathi: High strain rate micro testing on long glass fiber reinforced thermoplastics
16:00 - 16:20	M. Pletz, S.G. Nagaraja, C. Schuecker: Constitutive modelling of anisotropic plasticity with application to fiber-reinforced composites	O. Saburow, F. Henning: Damage and viscoelasticity of SMC Materials: testing, modelling and parametrization
16:20 - 16:40	F. Welschinger, J. Köbler, H. Andrä, R. Müller, M. Schneider, S. Staub: Efficient multiscale methods for viscoelasticity and fatigue of short fiber-reinforced polymers	A. Jackstadt, W.V. Liebig, S. Galkin, V. Sessner , K.A. Weidenmann, L. Kärger: A multi-scale approach for the virtual characterization of transversely isotropic viscoelastic materials in the frequency domain
16:40 - 17:10	coffee break (foyer to rooms A1.19 and A1.20)	
	room A1.20: plenary session (chair: J. Hohe)	
17:10 - 17:50	keynote A. Jung, S. Diebels (Universität des Saarlandes) Multi-scale characterisation and modelling of cellular materials	
	downtown: evening program	
19:00 - 20:00	guided city walk meeting point: Historisches Kaufhaus, Münsterplatz 24	
20:00 - 23:00	conference dinner at Heiliggeist Stüble, Münsterplatz 15	

October 10, 2018 - day 2		
	room A1.20: plenary session (chair: M. Basista)	
08:30 - 09:10	keynote I. Vladimirov, A. Fischersworring-Bunk (MTU Aero Engines AG) Material and structural modelling aspects of fiber-reinforced ceramic materials in aircraft engines	
09:10 - 09:40	coffee break (foyer to rooms A1.19 and A1.20)	
	room A1.20: multiscale analysis and scale-bridging (chair: E. Baranger)	room A1.19: mean field approaches and effective properties (chair: I. Vladimirov)
09:40 - 10:00	S. Nosewicz, J. Rojek, K. Wawrzyk, P. Kowalczyk, G. Maciejewski, M. Maździarz: Multiscale modeling of sintering process of mixture of two-phase powder	P. Sadowski, K. Kowalczyk-Gajewska, S. Stupkiewicz: Efficient and robust incremental Mori-Tanaka scheme for finite-element modeling of elasto-plastic composites
10:00 - 10:20	V. Wittner, C. Morin, C. Hellmich: Hierarchical elastoplasticity of bone	P. Lenz, R. Mahnken: Damage simulation of fibre reinforced composites using mean-field homogenization methods
10:20 - 10:40	F.A. Gilabert Villegas: Modelling different scales and challenges of composite material research at Ghent University	F. Dillenberger, S. Kolling, J. Schneider: An approach for the mechanical modelling of short fibre reinforced thermoplastics (SFRTP)
10:40 - 11:00	C. Beckmann, J. Hohe: Probabilistic multiscale analysis of foam core sandwich structures	L. Parashkevova, L. Drenchev: A new variant of differential effective medium theory for mechanical properties assessments of as-cast light alloys
11:00 - 11:20	B. Coto: Molecular modelling of interfacial properties of epoxy matrix reinforced with functionalized carbon nanotubes	A. Hashibon, N. Adamovic, G. Goldberg, P. Asinari, K. Hermansson, D. Hristova-Bogaerds, R. Koopmans, T. Verbrugge, E. Wimmer: The European Materials Modelling Council EMMC
11:20 - 11:50	coffee break (foyer to rooms A1.19 and A1.20)	
	room A1.20: plenary session (chair: M. Basista)	
11:50 - 12:30	keynote E. Baranger (LMT Cachan) Strategies to enrich macroscopic models, application to ceramic matrix composites	
12:30 - 12:45	concluding remarks	
12:45 - 14:00	lunch buffet (foyer to rooms A1.19 and A1.20)	

Meeting Point for Guided City Tour
and
Location of Conference Dinner

Meeting point for guided city tour:
in front of Historisches Kaufhaus (historic warehouse)
Münsterplatz 24

Conference dinner:
Restaurant Heiliggeist Stüble
Münsterplatz 15

Abstracts

Keynote Lectures

Development of a differential composite booster case including a structural bonding

Jürgen Albinger, Anna-Katharina Weiß, Marina Wolff

MT Aerospace AG
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The increasing number of competitors in the heavy launcher business leads to a demand on cost effective, reliable and high-performance launcher systems. A possibility to realise these goals is the application of enhanced technologies in combination with automated manufacturing and control processes.

For these reasons MT Aerospace AG develops carbon composite casings for solid rocket motors (SRM) in differential design, where the two cylindrical skirts are joined with the pressure vessel by a thick-walled elastomeric structural bonding. Beside the key technology structural bonding another key technology is used, a resin infusion of thick-walled monolithic composites – up to 30 [mm] – in combination with dry fibre winding and dry fibre placement.

The presentation focuses on the design, the verification and the validation by test of the structural bonding. This structural bonding is called shear-ply and has the function to reduce the internal loads between the skirts and pressure vessel. Based on the technical requirements and the affecting design loads on the booster case, the resulting three-dimensional internal load condition between skirts and pressure vessel is investigated considering different shear-ply stiffnesses. Followed by the selection and the material characterization of the most promising adhesive, the hyper-elastic material law and a damage initiation criterion is defined for the shear-ply. Finally, the integrity of the structural bonding is demonstrated by tests on scaled and full-scale level.

Multi-scale characterisation and modelling of cellular materials

Anne Jung, Stefan Diebels

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Metal foams are cellular materials with structural features resembling to lightweight load-bearing materials such as bones. Their high stiffness-to-weight-ratio coupled with their long flat stress-strain response make them ideal candidates as energy absorbers. Their macroscopic properties are strongly influenced by both the mechanical behaviour of single pores at the mesoscopic level and the struts and their structure at the microscopic length-scale based on a strong structure-property relationship.

Hybrid foams are open-cell foams consisting of an aluminium or polyurethane substrate foam coated with nanocrystalline nickel, which strengthens the struts leading to significantly improved global properties such as a tenfold energy absorption capacity compared to pure aluminium foams. The mechanical properties of the hybrid foams can be tailored by the coating thickness and coating properties, which make Ni/Al or Ni/PU hybrid foams a multifunctional material. Whereas macroscopic mechanical characterisation is widespread, micromechanical characterisation and assessment of parameters on single struts or single pores is very limited. Micromechanical characterisation of individual struts is very challenging but an emerging field of research.

The present contribution deals with the structural and mechanical characterisation of open-cell foams and hybrid foams of different pore size on individual struts, individual pores and macroscopic specimens as well as with the modelling, simulation and parameter identification. Micro tensile and micro bending tests were performed on individual struts to determine the micro material properties by parameter identification using inverse calculations. All experimental tests were coupled with an analysis of local strains using digital image correlation. Furthermore, the mesomechanical deformation behaviour is characterised by tensile and compression experiments on individual pores. Finally, macroscopic yield surfaces for macroscopic foams were experimentally excessed by a combination of compression, tension, torsion and torsion tests with superimposed loads. A simplified continuum mechanical modelling approach including parameter identification was used to simulate the yield surfaces.

Material and structural modelling aspects of fiber-reinforced ceramic materials in aircraft engines

Ivaylo Vladimirov, Andreas Fischersworring-Bunk

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The presentation discusses modelling techniques for the description of Ceramic Matrix Composites (CMC) in the context of the aerospace industry. This class of continuous fiber-reinforced ceramic materials are characterized by high temperature capability and at the same time much lower density in comparison to state-of-the-art metallic alloys, thus making them attractive for utilization in aircraft engines. The heterogeneity and intrinsic anisotropy of the material and thermo-physical properties requires the use of appropriate constitutive models and finite element formulations to take these effects into account. The focus is first placed on the technical challenges that aircraft engines have to cope with during operation and on the corresponding requirements for the constitutive models utilized in the design of aerospace components. Next, characteristic modelling aspects for the description of heterogeneous laminates of orthotropic ceramic plies are discussed both on the Gauss-point level and the element level. The anisotropic nature of the mechanical and thermo-physical properties of CMCs is addressed and some multiscale techniques for the description of the homogenized material behaviour are discussed. In addition, the use of modal analysis in the framework of the finite element method for the identification of the orthotropic material parameters of the elasticity tensor by means of laser vibrometry test data is discussed in detail.

Strategies to enrich macroscopic models, application to ceramic matrix composites

Emmanuel Baranger

LMT Ecole Normale Supérieure Paris - Saclay
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Due to their good specific mechanical properties at high temperature, ceramic matrix composites (CMC) are promising materials for the aeronautic/aerospace industry. Some parts are already produced for that purpose either in the military domain or in the civil domain. The combination of brittle matrices with brittle fibres leads to rather complex mechanical behaviours. Indeed, different crack networks can develop depending on the microstructure of the material but also on the loading conditions bringing some ductility to the structure. In that context, sizing a part made of CMC up to failure is a great challenge that necessarily relies on physically sound models and the associated identification/validation experimental tests. On top of this, one has to add multi-physics effects associated to the durability of the material. At high temperature, a glass is formed to heal the cracks and extend the lifetime of the fibres, which suffer from subcritical crack growth.

The aim of this paper is to present a modelling strategy able to account for the different information available. The starting point is a macroscopic anisotropic damage model able to capture the different crack networks for complex multi-axial loadings. This damage model is linked to a crack opening indicator through a small structural model. From that point, it is possible to model a representative crack and the physic-chemistry living in this crack i.e. solving a flow-diffusion-reaction problem. The use of enrichments allows the evaluation of the impact of the scattering of several quantities such as crack openings or fibres’ strength on the lifetime of the material.

The last part of this paper will open the discussion on the description of the mechanical response of a yarn using patterns. For that a GFEM technique is developed based on morphological and mechanical enrichment functions.

Abstracts

Contributed Lectures

Material models and effective properties

Composite Simulation: a new type of material model and failure criteria?

Jens Bold

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The numerical calculation of plates made from carbon fiber reinforced plastics under compression after impact (CAI) is the main subject of this presentation.

In a first step different failure criteria and nonlinear material theories for composite materials will be evaluated. A new material and failure model will be introduced and compared to existing ones. The new phenomenal based BOLD material law for fiber reinforced plastics is introduced and combined with the CUNTZE failure criteria for unidirectional and woven materials. Based on test results this material and failure model will be verified.

This new model was programmed as user defined material in MSC Nastran. Numerical simulation will be shown and compared to results of CAI tests. A very good conformance between the results will be shown.

First numerical simulation show that it also can be used for open-hole-tension calculations and also for other types of element test.

Modeling of the residual stress evolution in coated cemented-carbide tools during manufacturing

Lukas Faksa[1], Werner Daves[1,2], Werner Ecker[1], Thomas Kaltenbrunner[1], Christoph Czettl[3]

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In machining processes, cutting tools are exposed to extreme conditions. The occurring thermo-mechanical loading requires enhanced tool resistance tailored to the cutting conditions. A cemented-carbide substrate covered with multiple protective layers present a typical compound design for such an application. The investigated tool consists of a WC/Co substrate covered by a TiCN and an Al_2O_3 layer. During the fabrication of the compound residual stresses evolve. In order to extend the tool life it is promising to apply compressive residual stresses to the coating and/or substrate by a shot peening post-treatment. A two dimensional finite element based process model is employed to simulate the evolution of residual stresses in the different material layers taking into account the cooling from deposition temperature to ambient temperature followed by shot peening. The process model considers the substrate and the different layers as a continuum, respectively. The aim of this approach is to predict the influence of blasting parameters on the development of residual stresses distributions in coated WC/Co inserts. By means of a submodel which takes into account the actual substrate microstructure obtained from EBSD measurements it is possible to study the stress and plastic strain partitioning between the microstructural constituents. Additionally, the microstructural model provides information about the deformation mechanism of the substrate WC/Co compound.

A material model for fatigue degradation and damage in composite materials

Zalikha Murni Abdul Hamid, Monika Gall, Jörg Hohe

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Fatigue damage, degradation and failure are major concerns in the lifetime assessment of structural components. For fiber reinforced plastics, a special problem arises, consisting in a material degradation occurring in the initial stage of cyclic loading. In laminates with different fiber orientations for the individual plies, this effect may cause a considerable redistribution of stresses and strains during the lifetime of the structural component.

The objective of the present contribution is a new formulation of a fatigue degradation model describing this effect on the single-ply material level. Restricting the analysis to stiff and brittle carbon-epoxy types of composites or similar materials, the model can be defined, based on Hooke’s law. The basic linear elastic material model is enhanced by a damage formulation using three independent damage variables for the three individual spatial directions. The shear damage is described through a combination of the damage variables related to the spatial directions associated with the respective shear plane. For the individual damage variables, a power-law type damage evolution law is derived from the assumption that the damage is driven by a microplastic work, which is estimated from the elastic stresses and strains.

The model is implemented as a user-defined subroutine into a commercial finite element program and applied to an experimental data base of different uniaxial fatigue experiments on a filament wound CFRP material. The model proves to accurately predict the fatigue degradation and failure of the material. It has the special advantage that it is not only able to predict fatigue failure under cyclic loads with constant amplitudes but also accounts for more complex loading histories in a natural manner.

Conductivity of a two-dimensional two-component structure

Włodzimierz Bielski[1], Ryszard Wojnar[2]

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[2] Polish Academy of Sciences, Institute of Fundamental Research
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Two-dimensional systems deserve special attention, as it is evidenced by recent discoveries of the unique properties of the graphen sheets, and paying attention to the specific importance of two-dimensionality in biological structures. The considered problem has a broad meaning, since it deals with elliptic problems. Two-dimensional systems composed of two components are also important. If these components are in a 1: 1 ratio and are distributed in a statistically homogeneous way, their effective transport coefficients (conductivities) are given by the geometric mean of the component properties, [1-5]. We study two-dimensional systems made of anisotropic components, in peculiar chessboard-like tesselations constructed according to a fractal pattern (Sierpinski Gasket and Carpet), dissipation and percolation properties of such systems.

[1] J.B. Keller, A theorem on the conductivity of a composite medium, Journal of Mathematical Physics 5 (4) 548-549, 1964.
[2] A.M. Dykhne, Conductivity of a two-dimensional two-phase system, Soviet Physics JETP, 32(1) 63-65, 1971; in Russian: Zh. Eksp. Teor. Fiz. 59(1) 110-115, 1970.
[3] V.V. Jikov, S. M. Kozlov, O. A. Oleinik, Homogenization of differential operators and integral functionals, Springer-Verlag Berlin Heidelberg 1994.
[4] S. Mortola, S. Steffe, Homogenization of quadratic forms on fractals, 1994,
[5] I.V. Andrianov, J. Awrejcewicz, V.V. Danishevskyy, Asymptotical mechanics of composites, Modelling composites without FEM, Series: Advanced Structured Materials, vol. 77, Springer 2018.

Constitutive modelling of anisotropic plasticity with application to fiber-reinforced composites

Martin Pletz, Swaroop G. Nagaraja, Clara Schuecker

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Fiber-reinforced composites with thermoplastic or thermoset matrix materials exhibit distinct plastic deformations, particularly when loaded in shear or perpendicular to the fiber direction. For a unidirectional composite layer, tension and compression in the fiber direction cause elastic behavior only. In-plane shear, transverse shear and transverse compression show specific plastic curves. This anisotropic plastic behavior can be described either by using micromechanical models that introduce the plastic behavior in the matrix constituent using isotropic plasticity, or by homogenized, anisotropic ply-level plasticity models.

This work introduces a variety of thermodynamically consistent constitutive models that can describe this plastic behavior on the ply level. The material models generally use power law hardening and three yield stresses as parameters for in-plane shear, out-of-plane shear and transverse compression. They differ in the specific formulation of flow potential and the dependency of the yield stress on hydrostatic stress using either associated or non-associated flow. The material parameters are fit to experimental data from the literature (in-plane shear and transverse compression). The obtained material models are tested for a number of biaxial load cases from literature and correspond quite well to the tested curves. Some interesting aspects regarding the applicability of associated and non-associated flow are discussed. These issues could be addressed in the future by using micromechanical models with matrix behavior that considers the physics of polymer deformation. Some preliminary micro-mechanical investigations will be shown to that end.

Efficient multiscale methods for viscoelasticity and fatigue of short fiber-reinforced polymers

F. Welschinger[1], J. Köbler[2], H. Andrä[2], R. Müller[3], M. Schneider[4], S. Staub[2]

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In order to predict the nonlinear mechanical behavior of components made of short fiber reinforced plastics (SFRP) under long term and cyclic loading, coupled process and component simulations are required. The injection molding process leads to locally varying fiber orientations within the component. This varying microstructure [1] significantly influences the viscoelastic and fatigue behavior. The interaction between the microstructure [2] and the nonlinear macroscopic properties is resolved by a coupled FFT-FEM two-scale method, where the fiber orientation tensor is obtained by analyzing µCT images or by the corresponding process simulation. The aim of this work is to reduce the numerical effort of such a multiscale method. In a first step, the highly efficient micro-scale solver FeelMath [3] for regular grids using a FFT-based pre-conditioner is presented. Afterwards, a numerical scheme based on a precomputed database trained with FeelMath simulations on the microscale and a model order reduction algorithm, is discussed. The combination of these ideas reduces the numerical effort, such that the method is applicable for industrial problems. Comparative studies of the fully coupled and reduced model document the high accuracy of this approach. The overall performance of this methodology is demonstrated by three dimensional, industrial applications.

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[2] Schneider, M. [2017]: The sequential addition and migration method to generate representative volume elements for the homogenization of short fiber reinforced plastics, Computational Mechanics, 59: 247-263.
[3] www.geodict.com

Abstracts

Contributed Lectures

Experimental methods for advanced models

Modelling composites for structural health monitoring systems using acoustic ultrasonic methods

Kilian Tschöke, Tobias Gaul, Bianca Weihnacht, Lars Schubert

Fraunhofer Institute for Ceramic Technologies and Systems IKTS
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Fibre reinforced composites are well suited for various applications, such as aerospace and automotive engineering. They are very attractive due to their high stiffness and strength to weight ratios and their corrosion resistance. However, questions of operational safety are still unsolved. The occurrence of a pre-damage caused by aging or even misuse is often responsible for shortening of life time. Impact damages for example are usually investigated by conventional ultrasonic impulse-echo techniques. These techniques are on the one hand time-consuming and on the other hand qualified service personnel is required.

Structural Health Monitoring (SHM) has the opportunity to overcome these disadvantages. The method described in this paper uses ultrasonic guided waves as a continuous or periodic automated method for the determination and monitoring of the state of the object under surveillance. Measurements are carried out by permanently installed, e.g. integrated transducers, and by the analysis of the measurement data. The proposed approach uses integrated piezoelectric transducers applying the active ultrasonic guided wave measurement technique. Guided waves are able to propagate over a large distance and they interact in the whole cross-section of a specimen and enable therefore access to areas with limited accessibility.

However, curved components or heterogeneous and anisotropic materials complicate the design of the SHM system. The enormous effort involved in development and adaptation cannot be completely covered by laboratory experiments. Therefore, the use of model-based methods is an alternative to laboratory testing, but requires appropriate simulation models. Adapted Finite Difference Methods, such as the FDTD method, or Finite Volume Methods, such as EFIT (Elastodynamic Finite Integration Technique), have been used successfully for many years for non-destructive testing. The present contribution addresses these aspects and shows approaches to adapt simulation models specifically to the requirements of Structural Health Monitoring methods based on guided waves

Characterization of fiber-matrix interface strength using micro tensile experiments

Michael Schober, Zalikha Murni Abdul Hamid, Sascha Fliegener, Peter Gumbsch, Jörg Hohe

Fraunhofer-Institut für Werkstoffmechanik IWM
Wöhlerstr. 11, 79108 Freiburg, Germany

Fiber reinforced plastics are lightweight materials featuring high stiffness and strength to weight ratios. Therefore, they are considered as promising candidate materials for the design and manufacturing of lightweight components for sustainable transportation. A vast variety of materials exists, including thermoplastic composites which can be recycled due to the reversibility of the solidification process of the matrix. Based on cellulose fibers, even natural materials can be assembled. In the integrity assessment of fiber reinforced composites, especially of the discontinuously fiber reinforced type, the integrity of the fiber and matrix interface plays an important role since the external load needs to be transferred from the matrix to the fibers over the interface.

Objective of the present contribution is to provide a robust and universal methodology to optimize the interface properties for a broad range of fiber-matrix combinations. For this purpose, different experimental techniques for the characterization of the fiber-matrix interface are established. Whereas the conventional single-fiber microbond test considering a polymer droplet stripped off a single fiber allows for a simple interpretation, it has the disadvantage that both, the polymeric matrix material and the interface are prepared for the experiment in a special manner which is different from the processing of real materials in structural application. To avoid this disadvantage and to be able to characterize the fiber-matrix interface under realistic conditions, tensile experiments on micro specimens with gauge section widths in the range between 100 μm and 200 μm are developed. The specimens are machined directly from structural components or at least from plaques manufactured by the identical process. The experiments are evaluated by a numerical simulation based on a direct model of the microstructure of the respective specimen determined by tomographic methods. Subsequently, the interface properties are determined by a reverse engineering approach.

An unusual grain size effect in measurements of thermal residual stress in alumina-chromium composites – explanation by modelling

W. Węglewski, M. Basista, M. Krajewski, K. Bochenek

Polish Academy of Sciences, Institute of Fundamental Technological Research
Pawińskiego 5B, 02-106 Warszawa, Poland

We present experimental measurements and numerical simulations of processing-induced thermal residual stresses (TRS) in aluminium oxide (alumina) reinforced with chromium particulates (60vol.%Al2O3/40vol.%Cr). This composite was manufactured by powder metallurgy method using two chromium powders (5 µm vs. 45 µm particle mean size), while the mean size of alumina particles (1 µm) remained unchanged in all experiments.

The average TRS in alumina were determined by two optical methods: photoluminescence piezo-spectroscopy (PLPS) and Raman spectroscopy (RS). For comparison the TRS were also measured using two diffraction methods: neutron diffraction (ND) and X-ray diffraction (XRD). The four experimental techniques have revealed a systematic size effect of chromium particles on the magnitude and sign of the average residual stress in the alumina. When the fine chromium powder (5 µm) was used the average TRS in the ceramic phase was tensile what contradicted the predictions of micromechanical models based on the Eshelby solution. When the coarser chromium powder (45 µm) was used the measured average TRS in the ceramic phase was compressive as expected.

Assuming that this unusual size effect was caused by the complex composite microstructure, which cannot be captured by the classical models of micromechanics, a plausible explanation was sought using numerical simulations based on microscopic images of the material microstructure. The effective coefficients of thermal expansion (CoE) of the two composites were computed by FEM using SEM images of the microstructure. The numerical results were compared with the experimentally measured values of CoEs. A significant effect of the composite microstructure on the CoEs was identified as a potential source of the anomalous residual stress behaviour of the composite with small Cr particles.

Acknowledgement: This research was supported by the National Science Centre (Poland) grant no. UMO-2014/15/B/ST8/04314.

High strain rate micro testing on long glass fiber reinforced thermoplastics

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Long glass fiber reinforced thermoplastics (LFT) are popular in lightweight automotive applications. The mechanical performance combined with good processability and low-cost raw materials open up LFT applications in crash relevant components. To achieve an optimum performance of these components the crash relevant material characterization of LFT is essential.

The macroscopic homogenized material behavior is a well-known. The micro mechanic of damage, especially in crash loading, is objective of extensive research. Applied macroscopic modelling of LFT needs to be improved by strain rate dependent damage criteria. Micro modelling and testing shall identify the critical parameter to describe the macroscopic damage behavior. To calibrate the micro models, microscopic tests are needed in a range of strain rates. At the Fraunhofer IWM a new micro testing rig, "DynMicro" with a wide range of testing velocities is introduced to provide experimentally information about the "micro crash behavior".

Quasi-static and dynamic tensile tests with specially prepared LFT micro specimens were conducted. High-speed video imaging with a resolution of < 3 µm brought deep insights into the damage behavior of LFT originated in the fiber matrix interface. Significant differences in the frictional interaction of fiber and matrix and a subsequent expansion of crazing was found, comparing quasi-static and dynamic tests. Supporting scanning electron micrograph (SEM) pictures after the tests gave information about the differences in interface damage and deformation depending on the testing velocity.

In combination with results from high-speed infrared measurements in macro tests, the micro tests deliver a better understanding of the thermomechanical mechanisms of the strain rate dependent damage of LFT. With these information and prepended computer tomography (CT) analysis of the fiber distribution in the gauge section of the specimens, a basis for representative strain rate dependent micro model is provided.

Damage and viscoelasticity of SMC Materials: testing, modelling and parametrization

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The material behaviour of SMC materials is characterised by viscoelasticity and damage. Both effects are present, though hard to distinguish in experiments with SMC materials. Therefore, a direct method to find the material parameters is difficult. Instead, a multi-step approach is presented by using staged cyclic testing procedures and fitting a model to the measured behaviour. The SMC material is modelled and implemented as anisotropic viscoelastic with damage and adaptable to different strain rates behaviour. Due to the resulting high amount of fitting parameters, evolutionary algorithms are utilized for parametrization. Since the model is fitted directly to experimental tests by means of fully parametrized virtual tests, the damage and viscoelasticity are both taken into account and the related damage and viscoelastic model parameters are determined simultaneously. A comparison shows good agreement of the proposed Model and the measurements.

A multi-scale approach for the virtual characterization of transversely isotropic viscoelastic materials in the frequency domain

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This paper proposes a multi-scale approach for the modelling of carbon fiber-reinforced plastics under steady-state conditions in the frequency domain. on the micro-scale, statistically representative volume elements under periodic boundary conditions are used to determine homogenized master curves for five independent Generalized Maxwell Models which represent the transversely isotropic viscoelastic behavior of unidirectionally reinforced lamina. A comparison with experimentally determined storage and loss moduli of the composite under investigation is carried out. These five master curves are transformed into independent Prony series using a least-squares optimization strategy, thus representing the lamina on the meso-scale. The proposed material model is implemented as a user-defined material model for the commercial finite element software ABAQUS and parametrized by using the previously identified Prony series coefficients. The developed user-defined material model is used to investigate the steady-state behavior of carbon fiber-reinforced polymer laminates and hybrid CFRP-elastomer-metal laminates on the macroscopic component level. The proposed method is found capable of virtually characterizing the viscoelastic behavior of carbon fiber-reinforced polymers in the frequency domain and presents a viable tool to investigate and optimize hybrid CFRP-elastomer-metal laminates with regard to steady-state behavior and vibration damping characteristics.

Abstracts

Contributed Lectures

Multiscale analysis and scale-bridging

Multiscale modeling of sintering process of mixture of two-phase powder

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Sintering is a manufacturing process in which loose or weakly bonded metal or ceramic powders are consolidated into a solid compact body by heat treatment which can be combined with mechanical pressure. Macroscopically during sintering, one can observe changes of the bulk material volume (shrinkage) and, associated with this, densification and decrease of porosity. The microstructure during sintering undergoes an evolution characterized by grain rearrangement, increase of grain compaction and formation of cohesive bonds between powder particles which occurs due to mass transport. Surface and grain boundary diffusion are normally dominant mechanisms of mass transport in sintering.

This work presents a three-scale framework for numerical modelling of sintering phenomena of two-phase mixture. The proposed approach bridges simulations performed at the atomistic, microscopic and macroscopic scales. The atomistic modelling has been carried out using the molecular dynamics (MD) to determine the diffusive parameters, which define material behavior during sintering and are used in the microscopic model of sintering. The authors' own original viscoelastic model [1] developed within the framework of the discrete element model have been used for simulation of the powder sintering process at the microscopic level. The macroscopic constitutive model is based on the assumption that the sintered material is a continuous medium. The parameters of the constitutive model are determined by simulation of sintering at the microscopic level. The model has been validated using the results of own experimental studies of pressure-sintering of $NiAl/Al_2O_3$ powder.

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Hierarchical elastoplasticity of bone

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Bone is characterized by a hierarchically organized microstructure, exhibiting universal organizational patterns, whose „dosages", however, vary between different species, organs, and anatomical locations. This complex internal structure leads to a necessity of taking into account all hierarchical components - some of which behave plastic - in order to explain the overall elastoplastic response of bone.

Methods: A multiscale continuum micromechanics model is used to predict the resistance to failure under mechanical load - the bone strength - based on the mechanical properties and volume fractions of bone's three elementary constituents: mineral, collagen and water.

The hierarchical organization of bone is considered in terms of a micromechanical six-step homogenization scheme. Within this model, the sole source of elastoplasticity lies in mutual sliding between mineral phases. While the mineral is characterized by non-associated Mohr-Coulomb elastoplasticity, the collagen fails in a brittle manner, according to a Rankine criterion. Upscaling of these processes from the nano to the macroscale was made possible by a novel iterative variant of the so-called return-map algorithm.

Results: The model is able to accurately predict the experimentally determined strength of bones of different species and anatomical locations tested in uniaxial tension and compression. Furthermore, the sequence of plastic events and the stresses and strains can be determined across all hierarchical levels, illustrating the influence of the specimen-specific bone composition, which is governed by the bone porosity and the mass density, on the overall mechanical behavior of the bone.

Modelling different scales and challenges of composite material research at Ghent University

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A general overview of the modelling activities currently performed at Ghent University will be shown. A detailed description of the latest developments in material modelling will be discussed, focusing on the main challenges and work ongoing under the context of several projects in close collaboration with the automotive industry and raw material producers. In that sense, some aspects of the so-called multiscale modelling approach will be discussed: first, the challenges of the scale-to-scale transition; second, the importance of including rate effects to cope correctly with dynamic loading; and finally, several insights on how to incorporate degradation mechanisms combined with highly-anisotropic features efficiently. Likewise, the potentialities of this approach for any kind of composite-based materials (e.g., fibre-reinforced plastics, concrete, ceramic or asphalts) will be also presented. Especial focus will be placed on the connection with the experimental tests required to obtain reliable models as well as the current limitations and further improvements.

Probabilistic multiscale analysis of foam core sandwich structures

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Solid foams are important core materials in sandwich construction combining a rather low specific weight with a high bending and torsional stiffness and strength. Further advantages are their inherent good thermal and acoustic insulation properties. On the other hand, one of the main shortcomings of solid foams as sandwich core material is their disordered random microstructure leading to a distinct scatter in the effective properties and thus uncertainties in the structural response of sandwich plates and shells.

Objective of the present contribution is the definition of a numerical scheme for prediction of the uncertainties in the structural response of sandwich plates and shells with core layers consisting of solid foams. In a first step, the effective material properties of the solid foams are determined including their uncertainty. For this purpose, a probabilistic homogenization procedure is established, based on the analysis of the mechanical response of small scale stochastic volume elements. These small scale volume elements are defined as subsets of a large scale, statistically representative volume element. As a result, the probability distributions for the effective properties and the local correlation are obtained. In a second step, these results are employed as input properties for a random field description of the material response of the solid foam on the macroscopic level. In a third step, the random field model is employed in a probabilistic numerical analysis of the sandwich structure on the macroscopic level.

In a case study, the proposed integrated computational materials engineering model is applied to the analysis of a single edge clamped sandwich beam with a foam core. Whereas the material uncertainty is found to be only of minor importance in the deformation of the beam, significant uncertainties are observed in the strength of the considered structure.

Molecular modelling of interfacial properties of epoxy matrix reinforced with functionalized carbon nanotubes

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A forcefield based molecular modelling approach is used to study the interfacial interactions of epoxy/carbon nanotube nanocomposites. The influence of the geometrical characteristics of the carbon nanotubes (CNTs), i.e. tube length, diameter and chirality, as well as the functionalization of CNTs on the interfacial interactions of the nanotube–polymer nanocomposite is analyzed by means of pull-out simulations. The combination of the molecular modelling approach with shear lag theory allows to predict the value of the shear modulus of the matrix at the interface and the effective shear transfer distance. The results show how the length of the model of CNTs used has a strong influence on the interfacial shear strength calculations while the influence of the radius and chirality is small. The methodology allows to explain the scattering of interfacial shear strength values between different studies molecular modelling studies in literature. Moreover, the results obtained for pristine nanotubes are in good quantitative agreement with the few experimental results available on literature, That indicates a change in the shear modulus of the epoxy matrix at the interface. This good agreement with experiments allows to validate the methodology to be further applied to functionalized nanotubes. In this sense, it is shown how different functional groups can improve the interfacial shear strength as functional groups changes on the electrostatic and Van der Waals interactions between the matrix and the nanotubes depending on the degree of functionalization of the CNTs.

Abstracts

Contributed Lectures

Mean field approaches and effective properties

Efficient and robust incremental Mori-Tanaka scheme for finite-element modeling of elasto-plastic composites

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The Mori-Tanaka (MT) scheme is a micromechanical mean-field model originally developed for the estimation of the effective properties of linearly elastic two-phase composites. Application of the MT model when the matrix exhibits a non-linear behavior is possible provided linearization of the constitutive law is performed. Successful finite-element implementations of the incremental MT model have already been reported in the literature. However, robustness, computational efficiency, consistent linearization, and related issues have not attracted sufficient attention yet and are discussed in this work.

Firstly, we have developed a consistent algorithmic treatment of the incremental Mori-Tanaka scheme for modeling non-linear deformation of composites. The resulting computational scheme can be classified as a doubly-nested iteration-subiteration scheme. Satisfactory efficiency has been achieved thanks to consistent linearization of the macroscopic response predicted by the finite-step incremental MT scheme. The automatic differentiation technique has been used for exact linearization at each level so that the quadratic convergence rate of the multi-level Newton method has been obtained.

Secondly, we have found that, for a finite strain increment, the incremental Mori-Tanaka scheme leads to a discontinuity in the response at the instant of the elastic-to-plastic transition in the matrix. The magnitude of the related stress jump depends on the strain increment and also on material properties and volume fractions of the phases. This undesirable feature, not commented in the literature so far, imposes a severe constraint on the maximum strain increment that can effectively be used in large-scale finite-element computations. An enhanced scheme has thus been developed that is characterized by a continuous response. As a result, a computationally efficient and robust micromechanical constitutive model suitable for large-scale finite-element computations is obtained. Its performance is illustrated by three-dimensional FE simulations.

Damage simulation of fibre reinforced composites using mean-field homogenization methods

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A mean-field homogenization framework for constitutive multiscale (meso-macro) modelling including material failure of three distinct linear elastic material phases is presented in this work. Within this framework it is possible to compute the macroscopic mechanical behaviour of fibre reinforced materials based on the constitutive models of the constituents. The three phases are unidirectional fibres surrounded by an interface, which is surrounded by a matrix material. Different mean-field homogenization methods are used to determine the effective properties for example the Mori-Tanaka scheme [4], the Self-Consistent method [3] and the interaction direct derivative [5], a more recently published method. For homogenization of the three phase composite we use the two-level recursive scheme from [2]. The fibre and interface is seen as a two-phase composite which, once homogenized, plays the role of a homogeneous inclusion for the matrix material.

A distinction is made between four different failure modes namely matrix failure, fibre failure, matrix-fibre interface failure and a simultaneous failure of the matrix and the fibre called matrix-fibre failure. For matrix failure a critical yield stress is decisive in the matrix. The fibre failure is caused by a high normal stress in direction of the fibre. The shear stress between the fibre and matrix is responsible for the matrix-fibre interface failure. To simulate a crack growth, we use the element deletion method in ABAQUS implicit [1]. Representative examples demonstrate the different types of failure and the resulting crack growth in a fibre reinforced material.

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An approach for the mechanical modelling of short fibre reinforced thermoplastics (SFRTP)

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In this work a novel material modelling approach is presented for SFRTPs. A requirement for safe design is the ability to precisely predict mechanical behaviour by FE simulations. Typical examples include relevant components in automotive applications regarding crash, occupant- and pedestrian safety.

Thermoplastic materials are frequently reinforced by short glass fibres in order to enhance stiffness and strength properties. Components made of short fibre reinforced thermoplastics (SFRTP) are manufactured cost-effectively by the injection moulding process. During the moulding, complex locally inhomogeneous fibre distributions arise in the components. Therefore, SFRTP components show a varying degree of anisotropy. Moreover, the influence of the thermoplastic matrix leads to a non-linear visco-plastic SFRTP behaviour. Plastic deformation and failure depends strongly on the stress-state.

The novel material model is implemented for explicit FE-Simulations and takes into account these effects. Regarding elasticity and the initial yield surface, a micromechanical Mori-Tanaka based model is applied. A quadratic yield surface (SAMP) is introduced on matrix level and transferred into a Tsai-Wu yield surface on composite level. Non-linear behaviour is determined from a single experiment for each stress state. A simple analytical equation for the description of the non-linear deformation of SFRTPs is introduced. Based on experiments it is shown that a simple inclusion of strain rate dependency is possible.

The model allows the computation of SFRTP behaviour for arbitrary stress states and orientation distributions and the utilisation of complex yield surfaces. Computation optimization for explicit simulations is possible. The material model was validated for a self-compounded PPGF30 material regarding tension, compression and shear for different orientation distributions.

A new variant of differential effective medium theory for mechanical properties assessments of as- cast light alloys

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The presented analytical approach is aimed to evaluate the mechanical properties of multiphase alloys regarded as "in situ" multiphase composites. The materials of interest are composites with high volume fraction of phases embedded into the matrix. According to the two-steps homogenization procedure adopted the multiphase Representative Volume Element (RVE) consisting of a matrix and nf phases is equivalent to a RVE containing n pseudo grains, n>= nf . Each pseudo-grain is a two-phase composite with predominant non-matrix phase. The new size- sensitive variant of Differential Effective Medium (DEM) homogenization scheme for a two-phase composite is described in close form solutions for semispherical inclusions. Herein the variant of size-sensitive Mori- Tanaka method is postulated as an explicit homogenization scheme for the dilute inclusion problem, which has been further developed following the ideas of DEM. In this way a special dimensionless term arises being the only trace of Cosserat properties of initial matrix. This term is regarded as an internal model parameter expressing in average manner the sensitivity of the parent matrix to the presence of inclusions of particular shape and diameter.

The particular case when the inclusions and the matrix have one and the same bulk modulus is applied to model the elastic behavior of cast Mg alloys with discontinuous precipitations. The analytical solutions obtained for a composite with zero bulk modulus of inclusions are appropriate for modelling of closed sell foams of different kind. The properties predictions of the new modification of DEM are compared with classical one, with other theories and with some experimental data available.

The European Materials Modelling Council EMMC: bringing materials modelling closer to industry

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The aim of the European Materials Modelling Council (EMMC) is to establish current and forward looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. EMMC pursues objectives to bridge the gap between academic innovation and industrial application including enhancing the interaction and collaboration between all stakeholders engaged in different types of materials modelling. In this presentation a review of recent actions of the EMMC, including advances in ontologies and interoperability and materials modelling marketplaces and discuss avenues for collaboration and contributions.

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