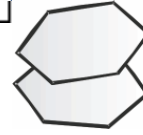Universität Karlsruhe (TH)
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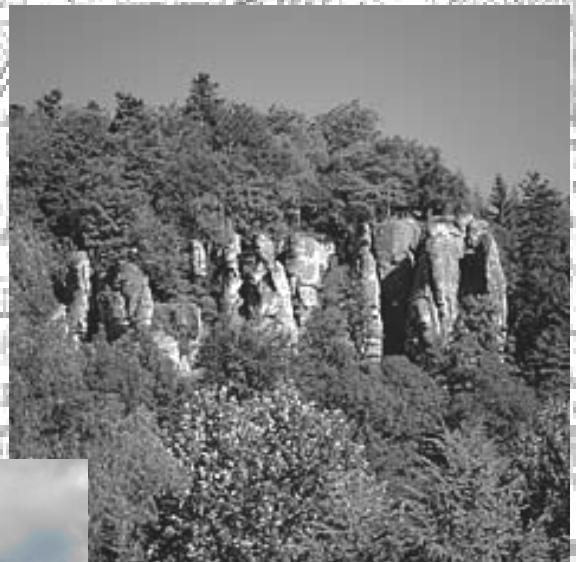
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International Workshop „Research in Mechanics of Composites 2006"

November 26-29, 2006
Bad Herrenalb, Germany

DIE FRIDERICIANA

Bad Herrenalb

Karlsruhe

Deutsche
Forschungsgemeinschaft
DFG

Monday, 27th of November 06

9:40-11:10 Room SR 6
Chair: I. Tsukrov, J. Zarka

9:40-10:05 Ch. Zhang, X.W. Gao, J. Sladek, V. Sladek
"Fracture analysis of functionally graded materials by a BEM"

10:10-10:35 L. Lacinski
"Modeling of heat conduction in functionally graded laminates"

10:40-11:05 W. Wagner
"Finite element simulation of skin-stiffener debonding in curved fiber-reinforced shell structures"

9:40-11:10 Room SR 7
Chair: M. Dauge, Z. Yosibash

9:40-10:05 W.L. Wendland, R. Duduchava, S. Nazarov
"Dual singular functions for a crack problem in isotropic elastic media"

10:10-10:35 D. Knees, A. Miehlke
"Energy release rate for cracks in finite-strain elasticity"

10:40-11:05 R. Duduchava, T. Buchukuri, O. Chkadua
"Crack-type boundary value problems of electro-elasticity"

11:10-11:30 COFFEE BREAK

11:30-12:30, Room SR 6
Chair: Ch. Zhang, A. N. Galybin

11:30-11:55 H.A, Mang, K. Hofstetter, Ch. Hellmich, J. Eberhardsteiner
"Estimating the boundary of the elastic regime for the biological composite wood from failure mechanisms at the nanoscale"

12:00-12:25 A.M. Sändig, W. Geis
"Asymptotic models for piezoelectric stack actuators with thin metal inclusions"

11:30-12:30, Room SR 7
Chair: R. Duduchava, E. Schnack

11:30-11:55 Y. Lapusta
"Micromechanics of compressive strength of fiber composites"

12:00-12:25 J. Sladek, V. Sladek, Ch. Zhang
"Local integral equations for crack problems in FGMs by a meshless method"

12:30-14:00 LUNCH BREAK

Monday, 27th of November 06

14:00-16:00, Room SR 6
Chair: H. Mang, Y. Lapusta

14:00-14:25 F.G. Rammerstorfer, <u>D. Pahr</u>, T. Daxner
"Micro- and meso-instabilities in structured composite materials and material compounds"

14:30-14:55 <u>H.J. Böhm</u>, S. Nogales, H.E. Pettermann
"Comparisons of Mori-Tanaka and unit cell predictions for the thermoelastic and thermal conduction behavior of discontinously reinforced composites"

15:00-15:25 I. Tsukrov
"Micromechanical modeling of composites using compliance contribution tensor"

15:30-15:55 R. Piat
" Hierarchical models of chemical infiltrated carbon/carbon composites "

14:00-16:00, Room SR 7
Chair: A. Wanner, D. Koch

14:00-14:25 O. Deutschmann, <u>A. Li</u>, K. Norinaga
"Modeling and simulation of materials synthesis: chemical vapor deposition and infiltration of pyrolytic carbon"

14:30-14:55 D. Gerthsen, <u>B. Reznik</u>
"Failure mechanisms in carbon-fiber/carbon-matrix composites"

15:00-15:25 <u>B. Reznik</u>, D. Gerthsen
"Atomic scale behavior of crack bridging in carbon fiber felts infiltrated with pyrolytic carbon"

15:30-15:55 <u>M. Guellali</u>, R. Oberacker, M.J. Hoffmann
"Influence of heat treatment on microstructure and mechanical properties of CVI-CFC composites with medium and highly textured pyrocarbon matrices"

16:00-16:30 COFFEE BREAK

16:30-18:00, Room SR 6
Chair: A.-M. Sändig, H.J. Böhm

16:30-16:55 <u>W.H. Müller,</u> T. Hauck
"Simple methods for the durability assessment of microelectronic solders"

17:00-17:25 <u>A. Ekhlakov,</u> E. Schnack
"Molecular dynamics model of the texture formation due to pyrolytic carbon deposition"

17:30-17:55 <u>S. Wilmanns,</u> R. Mahnken
"Simulation of asymmetric effects for shape memory alloys"

16:30-18:00, Room SR 7
Chair: A. Bussiba, B. Reznik

16:30-16:55 A. Wanner
"Load partitioning in multidirectionally fibre reinforced metal matrix composites"

17:00-17:25 <u>J.-M. Gebert,</u> A. Wanner, R. Piat. E. Schnack
"Three-dimensional analysis of crack propagation in notched carbon/carbon specimens"

17:30-17:55 <u>R. Ermel,</u> T. Beck, E. Kerscher
"Fibre-matrix interface properties of a c/c composite"

18:00 Discussion

18:30 DINNER

Tuesday, 28th of November 06

8:30-10:30 Room SR 6
Chair: E. Schnack, W. Becker

8:30-8:55 J. Zarka, H. Karaouni
"Intelligent optimal design of complex systems

9:00-9:25 A.N. Galybin
"An inverse problem of elastostatics
in mechanics of composites"

9:30-9:55 R. Tsotsova, E. Schnack
"Non-destructive reconstruction of delamination
regions in layered CFRP-composites"

8:30-10:30 Room SR 7
Chair: Z. Yosibash, L. Lacinski

8:30-8:55 T. Hauck, I. Schmadlak
"Interface fracture in copper/low k interconnects"

9:00-9:25 M. Thomas
"Energy release rate for a mode-III interface crack
in a compound of materials of p- Laplacian type"

9:30-9:55 M. Dauge, S. Tordeux, G. Vial
"Selfsimilar perturbation near a corner:
matching and multiscale expansions"

10:00-10:30 COFFEE BREAK

10:30-12:00, Room SR 6
Chair: W. Dreyer, E. Wierzbicki

10:30-10:55 T. Wallmersperger, B. Kröplin and D.J. Leo
" Electro-mechanical transport in ionoc polymer-metal
composites "

11:00-11:25 D.V. Georgievskii
"Simulation of deformation processes in weakly
nonhomogeneous medium (including composites)"

11:30-11:55 A. Grigorenko, Ya. Grigorenko, S. Yaremchenko
"Investigation of mechanical behaviour of anisotropic
Inhomogeneous shells with
complex shape on basis of spline-approximation"

12:00-12:25 C.Hager, S. Hüeber, B. Wohlmuth
"Stable dynamics approach for contact
problems based on quadrature formulas"

10:30-12:00, Room SR 7
Chair: W.L. Wendland, B. Kröplin

10:30-10:55 Z. Yosibash
"Edge singular solutions in anisotropic materials
and multi-material interfaces"

11:00-11:25 D. Leguillon, R. Piat
"Crack growth in a porous materials"

**11:30-11:55 R. Piat, D. Leguillon, F. Fritzen, M. Röser,
P. Magyesi,, Z. Yoshibash**
"Two-dimensional studies on crack propagation
in porous brittle media subject to mode I loading"

12:00-12:25 W. Becker, J. Hebel
"Numerical analysis of brittle crack initiation
at stress concentrations in composites"

12:00-12:30 Discussion

12:30-14:00 LUNCH BREAK

Tuesday, 28th of November 06

14:30-16:00, Room 1
Chair: A. Grigorenko, DV. Georgievskii

14:30-14:55 W. Dreyer
"On the role of non-convex energy functions in thermodynamics"

15:00-15:25 A. Avey (Sofiyev), O. Aksogan, E. Schnack, M. Avcar
" The stability of a three-layered composite conical shell containing a FGM layer subjected to external pressure"

15:30-15:55 T.-A. Langhoff, E. Schnack
"Restrictions to the energy density in energetic models of carbon fibre reinforced carbon"

14:00-16:00, Room 2
Chair: H.J. Böhm, J. Zarka

14:00-14:25 E. Schnack, A. Dimitrov, T.-A. Langhoff
"Numerical study of singularities in carbon based composites"

14:30-14:55 G.M. Kobelkov, S.V. Polyakov
"Comparison of methods for numerical solution of the theory of elasticity equations"

15:00-15:25 Th. Seelig
"Computational modeling of deformation and failure mechanisms in thermoplastic microlayer composites"

15:30-15:55 J. Utzinger, A. Menzel, E. Kuhl, P. Steinmann
"Computational modeling of laminar welded hybrid lightweight structures"

16:00-16:30 COFFEE BREAK

16:30-17:00 Chair K. Schulte Room SR 7
Public Lecture: D. Gerthsen
" Towards tailored carbon-carbon comosites: Structure and properties of pyrolytic carbon"

17:00-18:00, Room SR 7
Chair: E. Schnack, T.-A. Langhoff

17:00-17:25 J.N. Reddy, R.A. Arciniega
"Nonlinear analysis of composite and FGM shell structures"

17:30 Discussion

19:00 CONGRESS DINNER

Wednesday , 29th of November 06

9:00-9:25 Chair E. Schnack Room SR 7
Public Lecture: J.N.Reddy
"FORTY YEARS OF SIGNIFICANT DEVELOPMENTS IN MECHANICS
OF COMPOSITE MATERIALS AND STRUCTURES"

9:30-10:30 Room SR 6 **Chair: E.V. Glushkov, N.V. Glushkova**	**9:30-10:30 Room SR 7** **Chair: M. Schulte, M. Guellali,**
9:30-9:55 K. Schulte, F. Gehrig **"Damage and failure in fibre reinforced composites"**	**9:30-9.55 D. Koch** **"Ceramic fibre composites: experimental analysis** **and modeling of mechanical properties"**
10:00-10:25 R. Mahnken **"On the simulation of strength difference** **for adhesive materials"**	**10:00-10:25 I. Koke, F. Ferber, R. Mahnken,** **H. Funke, W.H. Müller** **"3D photogrammetric analysis of** **handmade glass fibre-reinforced composites"**

10:30-10:50 COFFEE BREAK

10:50-11:50 Room SR 6 **Chair: R. Mahnken, J.N. Reddy**	**10:50-11:50 Room SR 7** **Chair: B. Reznik, D. Koch**
10:50-11:15 E.V. Glushkov, N.V. Glushkova, E.V. Kirillova **"A laminate element method for the elastodynamic** **analysis of damaged layered composite"** **11:20-11:45 N.V. Glushkova, E.V. Glushkov,** **M.V. Golub, O.V. Kvasha** **"Mode selection, wave trapping and energy** **localization in layered structures with defects"**	**10:50-11:15 A. Bussiba, M. Kupiec,** **S. Ifergane, R. Piat. E. Schnack** **"Damage evolution and fracture events sequence** **in various composites by acoustic emission technique"** **11:20-11:45 M. Guellali, R. Oberacker, M.J. Hoffmann** **"Influence of heat treatment on microstructure and** **mechanical and physical properties** **of different pyrocarbons"**

11:50-12:00 DISCUSSION, CLOSING

12:00-14:00 LUNCH BREAK

ABSTRACTS

International Workshop

„Research in Mechanics of Composites 2006"

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NUMERICAL ANALYSIS OF BRITTLE CRACK INITIATION AT STRESS CONCENTRATIONS IN COMPOSITES

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Being potential locations for failure initiation, stress concentrations need to be treated with considerable effort in structural assessment. Especially for composites, sophisticated failure models capable of predicting important effects resulting from the complex stress and deformation state are required. Recently, hybrid crack initiation criteria (see [1]) utilising the concept of finite fracture mechanics (see [2]) have been proposed for the evaluation of such situations. By taking into account the stress field in the uncracked body as well as the energy balance for the spontaneous formation of cracks with a finite length, a wide range of regular and singular stress fields can be evaluated. In this study, a direct numerical approach (see [3]) is shown being implemented in a finite element procedure. Regular and singular stress concentrations under thermomechanical loading are analysed, applying a hybrid failure criterion in a discretised manner. For an increase in numerical efficiency, the scaled boundary finite element method (see [4]) is utilised. In this semi-analytical method, the number of spatial dimensions is reduced by one. Furthermore, order and mode of the stress concentration are readily available from the formulation. Additionally, an efficient solution scheme for the resulting nonlinear optimisation problem for the failure load is shown. Finally, the significance of generalised stress intensity factors is discussed.

References

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COMPARISONS OF MORI–TANAKA AND UNIT CELL PREDICTIONS FOR THE THERMOELASTIC AND THERMAL CONDUCTION BEHAVIOR OF DISCONTINUOUSLY REINFORCED COMPOSITES

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A number of methods for modeling the thermomechanical and thermophysical behaviors of composites have been developed over the past 50 years. Two important groups of such modeling strategies are Mean Field methods, which pose low computational requirements, and numerically based Periodic Microfield approaches, which can provide more detailed results at significantly higher modeling cost.

At present, the most flexible and most commonly used Mean Field models are Mori–Tanaka methods [1], which in their "classical" form describe composites reinforced by aligned ellipsoidal reinforcements of equal shape but different size and which for two-phase materials coincide with one of the Hashin–Shtrikman bounds [2]. "Extended" Mori–Tanaka theories can also be used to study materials with non-aligned and/or coated reinforcements, but may lead to non-physical results in certain situations [3]. The most powerful Periodic Microfield approaches at present are multi-particle unit cell models, in which periodic arrangements of reinforcements are studied that follow prescribed (typically uniform) position and, where applicable, orientation statistics [4, 5].

Predictions for the linear thermoelastic and thermal conduction responses of composites reinforced by randomly oriented short fibers, by planar randomly oriented short fibers and by randomly oriented tetrakaidekahedral particles were obtained. The latter case includes interfacial thermal conductances, which are handled by the Replacement Conductivity approach [6]. Comparisons are carried out in terms of both the overall responses and the averages of "flux-like" quantities (stresses, strains, temperature gradients, heat fluxes) in individual fibers or particles. Surprisingly good agreement between the predictions of the two modeling approaches is found.

References

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DAMAGE EVOLUTION AND FRACTURE EVENTS SEQUENCE IN VARIOUS COMPOSITES BY ACOUSTIC EMISSION TECHNIQUE

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Quantitative damage evolution and elucidation of fracture micro-mechanisms in composite materials are still long term goals. In the last years efforts in this field have been directed in two different but complementary directions. One approach is related to the development of damage models, usually based on micromechanics [1]. On this basis, they predict the stiffness changes in composite materials due to cracking and have confirmed the calculated change in the longitudinal Young`s modulus due to transverse cracks. Improved models which employ mathematical expressions to describe damage evolution, predict changes in the initial material symmetry caused by damage, as well as the stiffness changes for all probable crack patterns. The second approach is the application of non-destructive techniques for the characterization of damage and fracture mechanisms in composite materials. Of these methods Acoustic Emission (AE) [2] is a powerful tool due to the link between AE and fracture mechanics.

In the current study, AE data was analyzed, using parameters such as AE event count, cumulative event count, rise time, duration time and amplitude. In addition, a more advanced analysis based on Fast and Short Fourier Transforms [3] was applied. The frequencies of AE signals have been obtained and correlated with various failure modes such as fiber break down, de-bonding and matrix cracking.

Tests were carried out on three composite materials, a fiber-metal laminate GLARE 2 (lay-up sequence of three layers of 2024-T3 Aluminum alloy and two pre-preg layers of R-glass fibers in an epoxy matrix), a graphite/epoxy with lay-up of 0°/90° and infiltrated carbon fiber felt. Their mechanical behaviors were characterized by tensile test using a uniform flat specimen in longitudinal and transverse fiber orientations. Strain and AE signals were monitored vs. load simultaneously, using computerized systems. Optical and scanning microcopies were utilized for macro and micro fracture modes classification.

The correlation of AE signals with fracture mode classification leads to identification of the damage mechanisms controlling fracture and damage evolution in the tested composites. In addition, our results indicate a similarity between the damage profile obtained by models based on micromechanics (crack density vs. strain) and AE cumulative counts vs. strain. These results encourage further work for characterization of damage sequence and degree by AE method for structural integrity evaluation.

References

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SELFSIMILAR PERTURBATION NEAR A CORNER: MATCHING AND MULTISCALE EXPANSIONS

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As a model for problems involving self-similar singular perturbation, we consider the Laplace-Dirichlet equation:

$$\text{Find } u_\varepsilon \in H_0^1(\omega_\varepsilon) \text{ such that } -\Delta u_\varepsilon = f \text{ in } \omega_\varepsilon,$$

and investigate the behavior of u_ε as $\varepsilon \to 0$. Here the domain ω_ε has an ε-perturbation near the (corner) point O:
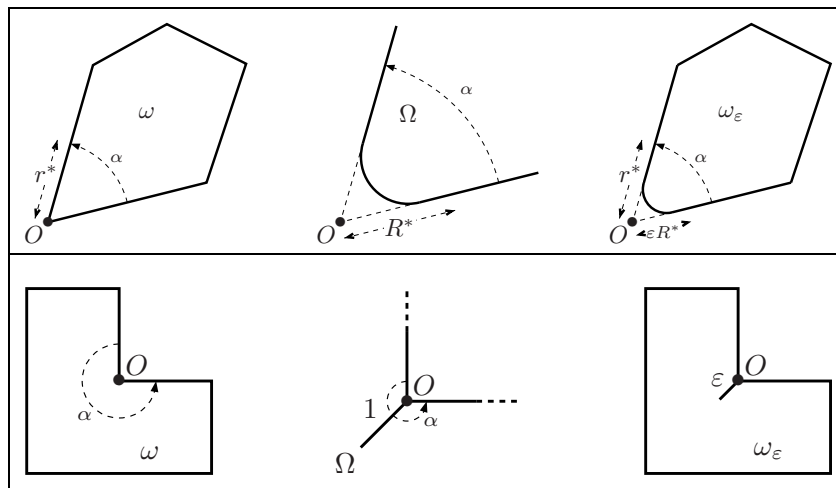
Figure 1: Two examples of domain ω_ε, with limit domain ω and perturbing pattern Ω.

The transition region between perturbed and unperturbed regions is part of a cone K of opening α. The ε-expansion of u_ε is governed by Laplace-Dirichlet singularities $r^{k\lambda} \sin k\theta\lambda$, with $\lambda = \frac{\pi}{\alpha}$.

The multiscale expansion, cf [2], of u_ε involves terms $\varepsilon^{k\lambda}v^k(x)$ with a "rapid" cut-off $\chi(\frac{x}{\varepsilon})$ near O and rapid variable terms $\varepsilon^{k\lambda}V^k(\frac{x}{\varepsilon})$ with a slow cut-off $\psi(x)$ far from O. Terms $v^k(x)$ and $V^k(X)$ are solutions of variational problems on ω and Ω, respectively. We compare these terms with those obtained by the matched asymptotics method, cf [1]. The latter, $u^k(x)$ and $U^k(\frac{x}{\varepsilon})$, belong to larger spaces: $u^k(x)$ is unbounded as $x \to 0$ and $U^k(X)$ is unbounded as $X \to \infty$.

We will discuss the existence of similar expansions for elasticity problems and composites (small isolated holes, small isolated inclusions, etc...)

References

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ON THE ROLE OF NON-CONVEX ENERGY FUNCTIONS
IN THERMODYNAMICS

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In this lecture we discuss causes for the appearance of non-convex energy functions in various problems of thermodynamics. Examples from the areas of phase transitions and of nonlinear elasticity serve to illustrate consequences and implication when non-convex energy functions are involved.

The dynamics of phase transitions is controlled by a competition of two different tendencies, concerning energy and entropy. According to the energy law, processes are driven so that there results a decrease of energy, whereas the entropy law favours processes that lead to an increase of entropy. Which one of both mechanisms dominates depends on the temperature and on the boundary conditions for the case at hand. The resulting available free energy with energetic and entropic contributions may be convex or non-convex.

For example, the entropy of mixtures like alloys, is mostly given by a convex function, whereas the energy may be either convex or concave. If the latter case is met, there exists a certain temperature region where the resultant available free energy is represented by a non-convex function. In this case non-convexity turns out to be a property of the considered material. Furthermore, we will use this example to illustrate the role of a convexification that is based on the so called Maxwell construction, [1], [2].

The next example concerns a rubber material, whose available free energy is given according to Mooney and Rivlin. We consider three examples to demonstrate that non-convexity may be due to the geometric shape of the specimen and/or due to the loading conditions. To this end we study (i) the deformation of a squared rubber plate under biaxial loading, (ii) the inflation of a spherical rubber ballon, and (iii) inflation of a cylindrical balloon, the both under various loading conditions. All these cases start from the same Mooney - Rivlin energy function, however, in the various cases, there result convex as well as non-convex energy functions, [3], [4].

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CRACK-TYPE BOUNDARY VALUE PROBLEMS OF ELECTRO-ELASTICITY

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Mathematical models of piezoelectric (electro-elastic) bodies and relevant boundary value problems have been studied with sufficient completeness (cf. W. Nowacki [5], Y. E. Pak [6], R. A. Toupin [7] etc.). Of special interest is the case where the considered body contains cracks or cuts with an edge having a dihedral angle 2π (the cuspidal edge). In that case the presence of an electric field influences essentially the pattern of stress distribution near the cut or crack edge (see Y. E. Pak).

We present a survey of fundamental research concerning solvability of classical boundary value problems of statics for a three-dimensional bounded homogeneous anisotropic piezoelectric body with a crack. The corresponding basic differential equation is a 4×4 dissipative system of order 2. Applying the potential method and the theory of pseudodifferential equations on manifolds with boundary the existence and the uniqueness of solutions of the above mentioned problems in different function spaces are proved (for the technique cf. [2, 3, 4]). Complete asymptotic expansion of solutions near the crack edge is obtained and the cases indicated when the logarithms eliminate from the entire asymptotic.

The results are refined for particular cases, e.g., for crystals with cubic symmetry.

Further results on fundamental research of composite materials (e.g., piezoelectric ceramics with metallic inclusions, taking into account a thermal effect) will be reported.

The results are partly published in [1].

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MOLECULAR DYNAMICS MODEL OF THE TEXTURE FORMATION DUE TO PYROLYTIC CARBON DEPOSTION

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The mechanical behaviour of isotropic carbon reinforced carbon fiber (CFC) composites obtained by chemical vapour infiltration not only remains controversial but strongly depends on the formation and evolution of material's nano- and micro structure during the production process [1]. Although, the experiments shows that the intrinsic deformation behaviour of this kind carbon based composites is strongly influenced by the textural degree of material, little is known about the exact character of this influence.

We assume that the texture is described by the distribution of orientations of so called turbostratic domains [1] which can be observed on the nanometer scale. We use molecular dynamics (MD) simulation that is performed on the base of the macroscopic phase-field diffuse-interface model [2] in order to elucidate the texture formation and evolution in the solid carbon phase. The polyaromatic hydrocarbon molecules are assumed as discotic particles. The molecular systems governed by an anisotropic potential (GAY-BERNE) and an empirical multi-body deposition potential.

From the MD simulations [3] a discrete time dependent distribution function of orientations of the turbostratic domains is obtained in account for evolution of the material texture.

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FIBRE-MATRIX INTERFACE PROPERTIES OF A CARBON/CARBON COMPOSITE

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The failure behaviour of a carbon/carbon (C/C) composite is dominated by the fibre strength and especially by the strength of fibre-matrix interface. The composite fails brittle if the bonding between fibre and matrix is too strong. A weaker fibre-matrix interface leads to a debonding of fibre and matrix and a pseudoductile failure of the composite is possible. Consequently, the analysis of fibre-matrix interface is important to understand and simulate the failure behaviour of a C/C composite. Fibre pull-out length gives a qualitative indication of fibre-matrix strength [1]. A quantitative method is the measurement of interfacial shear strength between fibre and matrix by push-out tests [2].

The fibre-matrix strength of a unidirectional C/C composite with mainly high textured matrix is investigated after heat treatment at temperatures up to 2500°C. An increase of fibre pull-out length can be recognized with increasing heat treatment temperature. Fractographic investigations with SEM show that debonding occurs only between fibre and matrix. Debonding between different textured matrix layers is not observed. Push-out tests are carried out on 100 μm thick samples using a planar indentation tip with a diameter of 5 μm. Tests on a sample heat treated at 2500°C show with 2.1 MPa a very low interfacial shear strength compared to literature [3]. The decreasing interfacial shear strength with increasing heat treatment temperature corresponds well with properties of the composite. The strength and the pseudoductility observed in tensile tests are nearly constant although fibre strength decreases pronounced with increasing heat treatment temperature [4].

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AN INVERSE PROBLEM OF ELASTOSTATICS IN MECHANICS OF COMPOSITES

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In this study we consider an inverse problem of elastostatics and its different applications appearing in mechanics of composites. These applications include investigation of spatial stress fluctuations, detection of internal cracks and other defects, identification of mechanical properties of interfaces, reconstruction of the stress-displacement relationship in narrow process zones developing ahead of crack tips and some other.

In many cases surface displacements can be monitored on a part of a stress-free boundary of an elastic composite (in general, heterogeneous). When this information is further used for stress analysis it leads to redundancy in boundary conditions on the part where displacements have been measured. To compensate this redundancy no boundary conditions are imposed on some internal boundaries such as cracks, inclusions or interfaces between dissimilar materials in a particular composite. As the result one arrives to an ill-posed boundary value problem of elasticity overspecified on a part of the entire boundary and underspecified on the rest of it. It has been found that the problem has a unique but not stable solution; see proofs in [1,2] for isotropic elastic domains.

A general approach for solving this type of problems is presented. It is based on boundary integral formulations complemented by a regularisation technique [3,4] to provide stability of solutions. Several examples are considered to illustrate effectiveness of the approach in the above-mentioned applications associated with composites.

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THREE-DIMENSIONAL ANALYSIS OF CRACK PROPAGATION IN NOTCHED CARBON/CARBON SPECIMENS

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Theoretical considerations suggest that the propagation of a macrocrack may be influenced strongly by pores pre-existing in the vicinity of the crack front [1]. Carbon/carbon composites based on fiber felts exhibit substantial residual porosity. Experimental evidence of the crack-microstructure interaction is required as a basis for developing a fracture-mechanical model for this complex class of materials.

We have developed a tomography-based method for analyzing the crack path in 3D and its interaction with pre-existing pores and cracks. Experiments were performed using a X-ray Micro-Computed Tomography (µCT) system, which is a viable tool for capturing the three dimensional structure of a heterogeneous material non-destructively [2, 3]. Notched specimens of carbon/carbon composites produced by chemical-vapor infiltration of fiber felts were loaded through fracture in four-point-bending. The internal microstructure as well as the surface contours of the specimens were characterized prior to and after the fracture experiment.

By correlating the tomograms obtained in the as-produced and fractured states it was possible to visualize the crack paths and the surrounding microstructure in three dimensions and to analyze the interaction between the crack and pre-existing pores in its vicinity.

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SIMULATION OF DEFORMATION PROCESSES IN WEAKLY NONHOMOGENEOUS MEDIUM (INCLUDING COMPOSITES)

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The formulation of the initial-boundary-value problem for nonhomogeneous medium by Eulerian description of deformation processes includes in addition an obtaining of the motion law for every Lagrangian particle along its trajectory as well as an inversion of this law. In case when the values of material functions which are present at constitutive relations of medium little differ from some known distribution (in particular, constant), the asymptotic method is applied. The notion "weakly nonhomogeneity" in the broad sense and in the narrow sense of the word are introduced.

The proposed method is approved by solving several problems of continuum mechanics. One of them is a spreading–drain of weakly nonhomogeneous thick-walled perfect plastic tube. In the capacity of non-perturbed process one chooses a quasistatic deformation of nonhomogeneous by radius tube, this nonhomogeneity may be discontinuous, i.e. the solid is supposed to be stratified composite [?]. The linearized initial-boundary-value problem is formulated in terms of perturbations and is solved analytically for the first approximation. The solution describes a connection of given nonhomogeneity and peculiarities of deformation process [?].

The second problem is a squeezing by two rigid plates of weakly nonhomogeneous by yield stress thin perfect plastic layer. In the capacity of the main process the classical Prandtl' solution for quasistatic deformation of homogeneous medium is taken.

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FAILURE MECHANISMS IN CARBON-FIBER/CARBON-MATRIX COMPOSITES

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It is well known that failure mechanisms in carbon-fiber/carbon–matrix (CFC)-composites are quite complex and depend on a variety of factors like fiber distribution and volume fraction of the fiber perform as well as fiber-matrix interaction [1]. In addition, the toughness of CFC-composites depends on the matrix texture, i.e. preferential orientation of the graphene layers with respect to the fiber surface, and the interaction of a propagating crack with the matrix and the fiber-matrix interface [2]. Using fiber performs with the same architecture, we have focused on the influence of different matrix textures on the failure mechanisms of the CFC-composites.

The matrix material was produced by chemical vapor infiltration of carbon fiber preforms. Depending on the gas phase conditions during the infiltration process, matrices with different textures can be produced ranging from low-textured to high-textured pyrolytic carbon. Three-point bending tests were carried out to analyze the mechanical properties of the material [3,4]. The defect structure after failure was studied by optical light microscopy, transmission electron microscopy and scanning electron microscopy to analyze the location of cracks from the micrometer to the nanometer scale.

CFC-composites consisting mainly of high-textured pyrolytic carbon exhibit the highest toughness. This observation is explained by a model which describes crack generation and propagation at layer–layer and fiber–matrix interfaces as well as within matrix carbon layers with different textures. Intensive cracking occurs within high-textured and less frequently in medium- and low-textured pyrolytic carbon layers. In particular, fracture does not occur directly at the fiber–matrix interface but within the low-textured matrix layer deposited on the fiber. Crack deflection in interface regions between layers with different textures, crack deflection along boundaries of columnar grains in high-textured layers and at interfaces between polyhedral nanoparticles, and finally crack bridging within high-textured lamellae are cooperative failure mechanisms contributing to the toughness enhancement.

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A LAMINATE ELEMENT METHOD FOR THE ELASTODYNAMIC ANALYSIS OF DAMAGED LAYERED COMPOSITE

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Micromechanical behavior of damaged composites subjected to dynamic loading is considered. The laminate structure of composite materials with sharply different properties of the constituting layers is a severe obstacle to simulating their dynamic behavior using finite element or finite difference methods. Sharp gradients in the solutions and their complex wave structure due to reflections and refractions at the interfaces require considerable mesh refinement leading to increased computational expenses.

To avoid these disadvantages, a novel efficient analytical-numerical tool based on expansion in terms of specially elaborated laminate elements has been developed [1]. In contrast to the conventional boundary elements relying on the fundamental solutions for an infinite homogeneous space, such elements exactly satisfy all boundary conditions at the interfaces and horizontal parts of exterior surfaces, so that only conditions at the irregularities (defects) and non-horizontal edges remain to be approximated. As a result, the laminate element method (LEM) requires a much smaller number of elements than with a conventional BEM.

The LEM computer implementation is discussed; its practical application is illustrated by numerical examples for elastodynamic behavior and stress concentration in composite components with micro-damages like cracks, volumetric inclusions, cavities and imperfect bonding conditions. The problems of traveling wave diffraction by surface or interior obstacles that arise in distant ultrasonic non-destructive testing of composite materials are also considered.

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MODE SELECTION, WAVE TRAPPING AND ENERGY LOCALIZATION IN LAYERED STRUCTURES WITH DEFECTS

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The investigation into wave excitation, propagation and diffraction in laminate structures with hidden or surface-breaking obstacles (cracks, cavities, interface imperfections) is of importance both to the development of non-destructive crack detection methods and to the assessment of a possible failure in composites due to resonance effects. To study these phenomena, we have been developing an analytically based computer model relying on wave expressions in terms of path Fourier integrals, Green's matrices for the laminate structures considered and asymptotics for body and traveling waves derived from those integrals. Regarding to QNDE, the model provides parameters for selective mode excitation and directional radiation by piezo-ceramic patch actuators [1], as well as theoretical scan-images and surface records for reflected signals with arbitrary crack's size, shape and orientation [2].

Elastodynamic behavior of damaged composites is featured by a sharp growth of amplitude and stress intensity factors at certain frequencies due to resonance wave scattering by defects in layered structures. Within the model developed the scattering resonance frequencies are spectral points of the integral operators. Numerical examples of the resonance poles trajectories in the complex frequency plane depending on crack's depth, size and inclination demonstrate a possibility of their touching to the real axis (pure real trapped modes) [3]. The wave energy trapping and localization near the obstacle under the resonance condition occurs in the form of energy vortices with high density of energy fluxes. It is accompanied by high stress concentration indicating its critical meaning for the failure analysis.

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INVESTIGATION OF MECHANICAL BEHAVIOUR OF ANISOTROPIC INHOMOGENEOUS SHELLS WITH COMPLEX SHAPE ON BASIS OF SPLINE-APPROXIMATION

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Many modern composites have as a rule inhomogeneous and anisotropic physical and mechanical properties. Plates and shells with complex shape made of inhomogeneous anisotropic materials are widely used for construction of structure elements in modern engineering. To estimate their strength under possible conditions of service operation, it is necessary to have the information about the stress-strain state and dynamic characteristics of the mechanical objects being considered. The complexity of the solution of these problems is attributed to the high order of the system, variability of the coefficients and to necessity to satisfy exactly given boundary conditions.

Currently to solve the problems of computational mathematics, mathematical physics, and mechanics, spline-functions are widely used. The present report proposes an efficient approach to solving within the framework of the classic and refined models the stress-strain problems of wide class as applied to plates and shells as well as the problems on free vibrations. In accordance with the approach the initial system of partial differential equations is reduced to one-dimensional problems by using approximation of the solution in terms of basic splines in a one coordinate. The boundary-value problems obtained and eigenvalue boundary-value problems for systems of ordinary differential high-order equations are solved by the stable numerical method of discrete ortogonalization.

The approach proposed is realized as the calculating complex of applied programs for modern computers. It allows us to solve multivariant problems of the given class for various kinds of orthotropy, geometrical characteristics of plates and shells, and loading schemes under different ways of contours fixation.

The orthotropic cylindrical shells with elliptical cross-section and variable thickness, acted upon by the load uniformly distributed along the directrix, are the subject of investigation. The stress state of shells of the given class under local loads is analyzed. In particular, the effect of change in the local load on the stress-strain state with the total load being retained is studied.

The influence of fixation conditions in the case of rectangular contours on the stress-strain state of open ellipsoidal cylindrical shells with the thickness, varied along the directrix, depending on the ellipticity degree and the parameter, characterizing the change in the thickness, is investigated [1].

The orthotropic corrugated cylindrical shells, acted upon by the uniformly distributed load, are considered. The influence of change in the thickness and corrugation frequency and amplitude on the stress-strain state of shells is studied.

The problems on free vibrations of rectangular orthotropic variable-thickness shallow shells and plates under complex boundary conditions are solved within the framework of classic and refined theories. The thickness was varied by the parabolic law. The influence of boundary conditions and law of change in the thickness of the plate on the behavior of dynamic characteristics is studied [2].

Mechanical characteristics of wide class of shall and plates made of composite materials (laminated and fiber reinforced) can be investigated due to proposed numerical method.

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INFLUENCE OF HEAT TREATMENT ON MICROSTRUCTURE AND MECHANICAL PROPERTIES OF CVI-CFC COMPOSITES WITH MEDIUM AND HIGHLY TEXTURED PYROCARBON MATRICES

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The Texture of low temperature pyrocarbons, deposited under isothermal isobaric chemical vapor infiltration (I-CVI) conditions within porous fiber performs, can be widely varied between the isotropic to the highly textured state by controlling the process parameters (e.g. gas pressure, residence time, temperature,...). From earlier studies it is known that heat treatment influence differently the microstructure of these pyrocarbon types. Aim of this study is to characterize the influence of heat treatment on the microstructure and thus on the mechanical properties of different textured pyrocarbons. Therefore X-ray diffraction measurements and mechanical tests were performed on infiltrated carbon fiber felts with either medium or highly textured pyrocarbon matrices before and after heat treatments up to 2900°C.

The results of the microstructural investigations confirm that the highly textured pyrocarbons graphitize very well while the medium textured pyrocarbons graphitze very badly. This is shown by a pronounced decrease of the interlayer spacing d_{002} and increase of the apparent layer stack height L_c with increasing heat treatment temperature in the case of the samples with highly textured pyrocarbon matrices. On the contrary, the d_{002} and L_c values of the samples with medium textured pyrocarbon matrices changed only slightly after heat treatment. The samples with LT-matrix exhibit distinct concentric cracks and the density of these cracks increases with increasing heat treatment temperature. On the contrary to the samples with HT-matrix show no cracks due to the heat treatment.

The results of the three-point bending tests carried out on samples before and after heat treatments reveal in the case of the samples with highly textured pyrocarbon matrices a distinct increase of the ductility accompanied with a Weibull flexure strength decrease with increasing heat treatment temperature. On the opposite, the samples with medium textured pyrocarbon matrices show no significant changes in the mechanical properties after heat treatment.

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INFLUENCE OF HEAT TREATMENT ON MICROSTRUCTURE AND MECHANICAL AND PHYSICAL PROPERTIES OF DIFFERENT PYROCARBONS

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The influence of heat treatment on the microstructure and properties of different pyrocarbons was characterized by X-ray diffraction, electrical conductivity measurements, thermal expansion investigations, indentation, three-point bending and tensile tests before and after heat treatment up to 3000°C.

The results of the XRD investigations reveal a pronounced decrease of the interlayer spacing (d_{002}) and increase of the apparent layer stack height (L_c) with increasing heat treatment temperature up to values respectively lower or higher than those of a moderate HOPG used as a reference sample. The mosaic spread (m_s) values of the investigated pyrocarbons decrease with increasing heat treatment temperature but remain slightly higher than those of the reference sample.

Specific resistance and thermal expansion measurements were carried out to characterize the influence of the microstructural changes (mentioned above) due to the heat treatment on the physical properties of the different pyrocarbons. The results of these tests reveal that with increasing heat treatment the values of the investigated samples converge to the values of graphite known from literature.

The results of indentation, three-point bending and tensile tests carried out on the samples before and after heat treatment reveal a distinct increase of both the Young's modulus in ab-direction and the ductility accompanied with a flexural strength decrease and tensile strength increase with increasing heat treatment temperature. The reduced modulus E* (~ Young's modulus in c-direction) as well as the indentation hardness decrease significantly after heat treatment und converge to the values measured for graphite and for the HOPG reference sample.

Fractographical investigations with SEM show a good correlation between the microstructural changes due to the heat treatment and the changes in the physical and mechanical properties of the samples.

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STABLE DYNAMIC APPROACH FOR CONTACT PROBLEMS BASED ON QUADRATURE FORMULAS

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Nonlinear frictional contact problems are still a challenging task both from the mathematical and engineering point of view. These problems are of crucial importance in various applications. In this report we consider efficient and stable numerical algorithms for dynamical contact problems. Due to friction effects and the non-penetration conditions, contact problems give rise to quasi-variational inequalities. To solve the resulting nonlinear algebraic system, we use a primal-dual active set strategy which can also be interpreted as semi-smooth Newton method. In combination with optimal multigrid methods, the inexact version of this approach can be regarded as a nonlinear multigrid method, and we end up with an efficient iterative solver.

Energy-consering time discretization methods in combination with active set approaches tend to oscillations in the Lagrange multiplier representing the contact forces. Here, we present a new approach based on quadrature formulas for the inertia term. This results in a modified mass matrix decoupling the inner displacements and the displacements on the contact boundary. Numerical results show the robustness of the scheme.

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INTERFACE FRACTURE IN COPPER/LOW K INTERCONNECTS

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This paper focuses on fracture phenomena in material interfaces between copper interconnects and interlayer dielectrics of CMOS (complementary metal-oxide semiconductor) microchips. CMOS technology is widely used for microprocessors, memory chips and application specific integrated circuits (ASIC). Its development goes along with reduction of structural dimensions of transistors and electrical interconnects on chip. Meanwhile the size of the transistor cells is measured at the nanometer length scale and the line width of the interconnects is measured at the micrometer length scale.

The interconnect system on microchip represents a very inhomogeneous structure. Copper lines are embedded into interlayer dielectrics (ILD). Thermo-elastic mismatch of these materials in addition to external mechanical loads can cause a critical stress states and device failure. Cracks occur in the interface between copper lines and dielectric material. The reduction of the fracture risk has to go along with an optimization of design and manufacturing processes. Computational stress analysis of the material interfaces and the definition of an appropriate fracture criterion are required.

A multi-scale stress analysis approach will be presented that considers the interaction between CMOS structures and microchip packaging at all relevant length scales [2]. The virtual crack closure (VCC) technique is used for computation of energy release rates for pre-existing cracks in particular material interfaces of the interconnect system [1]. Various design and process parameter are assessed with respect to the resulting fracture risk.

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ENERGY RELEASE RATE FOR CRACKS IN FINITE-STRAIN ELASTICITY

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Griffith's fracture criterion describes in a quasistatic setting whether or not a pre-existing crack in an elastic body is stationary for given external forces. In terms of the energy release rate (ERR), which is the derivative of the deformation energy of the body with respect to a virtual crack extension, this criterion reads: If the ERR is less than a specific constant, then the crack is stationary, otherwise it will grow.

In linear elasticity the ERR can be expressed e.g. by the J-integral or by stress intensity factors. Regularity results for weak solutions of the corresponding field equations are essential for the derivation of these formulas. In nonlinear elasticity similar formulas for the ERR are also given in literature. These formulas are derived assuming that the elastic fields have a certain regularity or asymptotic structure near the crack tip. In general, however, such regularity results have not been proved yet and, to our knowledge, a rigorous derivation of these formulas taking into account the known regularity of weak solutions is not done yet in the nonlinear case.

In this talk we consider geometrically nonlinear elastic models with polyconvex energy densities and prove that the ERR is well defined. Moreover, without making any assumptions on the asymptotic structure of the elastic fields, we derive rigorously two formulas for the ERR, namely the Griffith-formula, which is based on the Eshelby tensor, and the J-integral. The presented techniques are also applicable to smooth interface cracks.

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COMPARISON OF METHODS FOR NUMERICAL SOLUTION OF THE THEORY ELASTICITY EQUATIONS

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Let Ω be a 2D domain consisting of two subdomains Ω_1 and Ω_2, where Ω_i, $i = 1, 2$, are elastic mediums with different Lame coefficients. To solve numerically a boundary value problem for the system of elasticity theory equations in Ω:

$$\frac{\partial}{\partial x_j}\,\sigma_{ij}(\mathbf{u}) + f_i = 0, \quad i = 1,\,2,$$

$$\sigma_{ij}(\mathbf{u}) = 2\mu\varepsilon_{ij}(\mathbf{u}) + \delta_{ij}\lambda\mathrm{div}\,\mathbf{u}, \quad \varepsilon_{ij}(\mathbf{u}) = 0.5\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad \mathbf{u} = (u_1,\,u_2)$$

(summation over repeating indices in products is assumed), we consider and compare some numerical methods. Namely, for discretization of the domain we use two types of meshes — the ordinary triangulation and the Delaunay one. To approximate the problem on these meshes, we use the classic conforming finite elements, non-conforming finite elements and the original finite difference scheme. As for finite element approximation, we used the ordinary piece-wise linear elements and compared this approximation with the finite difference one. The comparison showed advantage of the finite difference approximation because of conservative properties of this scheme while the classic finite element approximation does not preserve "flows".

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CERAMIC FIBRE COMPOSITES: EXPERIMENTAL ANALYSIS AND MODELLING OF MECHANICAL PROPERTIES

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Ceramic fibre reinforced ceramic matrix composites (CMC) represent a class of high performance ceramics whose properties are illustrating the well known advantages of technical ceramics, however, without including their main deficit i.e. the low fracture toughness. This outstanding behaviour to combine high fracture energies with a reduced flaw sensitivity can be realized in ceramic composites if both brittle components of the composite, i.e. ceramic fibres and ceramic matrix are interacting with each other in an efficient way. For this purpose a weak interface allowing debonding between fibre and matrix is required in many CMC's (WIC-CMC) while this role of a weak and more compliant component is transferred directly to the matrix in other and more advanced CMC's (WMC-CMC).

An experimental test data base is presented for a WMC-type fibre reinforced carbon composite where all materials data required for the modelling work are derived from three experiments, i.e. tensile, shear and compressive tests. The model is applicable to quasi-static loadings of samples with varying angles between fibre and loading directions.

The model describes the materials behaviour in a macroscopic way. Inelastic deformation and materials damage processes are defined, measured and interpreted on the base of a continuum damage mechanics concept. The elastic and inelastic response is then predictable up to failure as being dependent on the angle between fibre and loading directions of the specimens. The results of these predictions are in excellent agreement with the experiments.

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3D PHOTOGRAMMETRIC ANALYSIS OF
HANDMADE GLASS FIBRE-REINFORCED COMPOSITES

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Fiber-reinforced plastics are fascinating construction materials. This is mainly because no special machines and extraordinary tools are required in order to produce a laminar structure. The making of complex geometries becomes feasible in a hobby workshop just by considering certain structural guidelines for fiber-reinforced plastics and ordinary craftsmanship.

For that reason fiber-reinforced plastics are ideal materials for building, for example, a racing car, which enables students to participate in the "Formula Student Competition" on the Hockenheimring (according to Professor Funke from the FH Dortmund). Essentially glass fabrics are used as reinforcement fibers for the hand laminated car body and keep the costs of running the vehicle small. At the Lehrstuhl für Technische Mechanik at the Universität Paderborn the mechanical characteristics of the fiber-composite structure of the racing car are experimentally obtained by means of hand-laminated samples.

With laminates of selected reinforcement fibers in an epoxy resin matrix various material parameters are experimentally determined, such as the shear or Young's modulus. For measuring laminar strain photogrammetry is applied and the results are compared with predictions from the software Tool Lami*Cens* by incorporating experimentally determined fiber percentages per volume. It is planned to create a data base of the results by means of innovative *Wiki* technologies. In this paper first results are presented.

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MODELING OF HEAT CONDUCTION
IN FUNCTIONALLY GRADED LAMINATES

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The objects of the considerations are laminates having macroscopic properties continuously varying across laminas, i.e. laminated media with functionally graded microstructure. The temperature distribution in the laminated conductor can be described by the well-known linearized Fourier heat conduction equation together with the heat flux continuity conditions on the interfaces between adjacent laminae. The coefficients in Fourier equation are non-continuous and highly-oscillating functions. It is known that aforementioned equation leads to ill conditioned and complicated computational problems. That is why some averaged mathematical models for obtaining solutions to the special problems have been formulated. The aim of this contributions is to propose a new averaged model. The main attention is focused on a description of the microstructure size effect on the overall composite behavior which plays an important role in the analysis of the near-boundary phenomena. These effects are neglected in commonly used locally homogenized models of composites. As a tool of modeling *a tolerance averaging technique* is used [1]. In the proposed model the temperature field is decomposed to an averaged temperature, temperature fluctuations generated by an averaged temperature, and temperature fluctuations related to boundary/initial conditions [2]. The mutual impact of these fields and methods of solving model equations are investigated.

Finally, we determine the usability range of the proposed model in relation to the space varying distribution of macroscopic material properties. The pertinent analysis will be restricted to a sequence of benchmark problems. These problems will be solved in the framework of proposed model and compared with the numerical solutions obtained in the framework of Fourier model.

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RESTRICTIONS TO THE ENERGY DENSITY IN ENERGETIC MODELS OF CARBON FIBRE REINFORCED CARBON

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In many composites phase transitions occur as a consequence of thermomechanical loading changing the microstructure and also the macroscopic properties. Energetic models have been developed for a wide range of problems in many of which the energy functionals are no longer convex (see e.g. [1]). Recently the notion of Γ-convergence in connection with problems of homogenisation for multi-scale materials has been used in engineering [2]. For rate independent problems incremental variational formulations have been proposed [3].

In this contribution, an energetic model for carbon fibre reinforced carbon is proposed to describe the macroscopic material properties of carbon fibre reinforced carbon [4]. For this composite, phase transitions between regions of different texture of the carbon matrix have been observed on nanoscale as well as columnar microstructures on microscale [5]. In such non-convex situations, interfacial contributions serve for relaxing the total energy. Proposals for the interface energy are made based on interface observations by transmission electron microscopy [6]. Within this framework, several restrictions on the energy functional especially are discussed here.

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MICROMECHANICS OF COMPRESSIVE STRENGTH OF FIBER COMPOSITES

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Microbuckling is an important strength limiting factor for fiber composites. The first models of the phenomenon were 2D. They considered the fibers and matrix as a system of layers [1]. Since that time, a variety of approaches to studying this phenomenon have been proposed. The majority of them are two-dimensional. However, the stress-strain state in fiber composites at the micro-level of scale is essentially three-dimensional. A 3D approach, proposed in [2], treated a double-periodic array of fibers in an infinite matrix and considered the fibers and matrix separately in a linearized formulation. Detailed information on compressive failure mechanisms can be found e.g. in [3], [4], and, on presently existing 3D linearized models of microbuckling, in [5]. In this talk, some recent developments in modeling of compressive failure at the micro-level of scale are discussed. Since it is advantageous to employ 3D approaches to get micromechanically founded solutions, we reduce the consideration to 3D problems. Special attention is given to models and solutions permitting a strict estimation of some typical micro-interactions, interface and surface effects during microbuckling in composites. Problem formulation is proposed. It considers a composite at the micro-level of scale and includes fibers, matrix, interfaces and possible free surfaces and defects. The problem is solved without smearing out these components or reducing the problem to a 2D case. The fiber-matrix interfaces are considered as surfaces, responsible for the correct stress transfer in 3D. Calculations are executed for some periodic distributions of fibers in a matrix. Examples are given of several idealized interface situations. Simple material models are applied separately to the matrix and to the fibers to describe their mechanical behavior. These are a perfect fiber-matrix bonding and a sliding contact without normal displacement discontinuity. In the latter case the fibers are supported by the matrix only by normal forces, shear forces being neglected. The mathematical formulation and the solution procedure are extended to three-phase and multi-phase materials. Critical loads and characteristics of the microbuckling modes are calculated for the considered examples of fiber-matrix systems. We show that these modes depend significantly on the mechanical properties of all composite constituents, microstructure parameters, the quality of the fiber-matrix interfaces, and on the presence of defects and free surfaces.

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CRACK GROWTH IN A POROUS MATERIAL

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The random distribution of pores in location, size and shape makes the fracture of porous materials a difficult problem and a quite sparse literature exists in the domain [1-3]. We address herein a simplified model of porous material as can be obtained for instance in ceramics by introducing organic or polymer particles like corn starch or polyamide prior to the sintering step [4]. Resulting spherical pores are almost regularly located with a homogeneous distribution in size. A fracture criterion involving both toughness and tensile strength [5] allows studying the competition between, on the one hand the blunting effect due to the pores, resulting in an apparent toughness improvement, and on the other hand the weakening effect caused by an increasing volume fraction of pores. This rough 2D model based upon a matched asymptotic procedure agrees satisfactorily with experiments on porous ceramics.

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MODELLING AND SIMULATION OF MATERIALS SYNTHESIS: CHEMICAL VAPOR DEPOSITION AND INFILTRATION OF PYROLYTIC CARBON

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Abstract: Numerical simulation of materials synthesis based on detailed models for the chemical kinetics and transport processes is expected to support development and optimization of production processes. Exemplarily, chemical vapor deposition and infiltration of pyrolytic carbon for the production of carbon fiber reinforced carbon is studied by recently developed modeling approaches and computational tools. First, the development of a gas phase reaction mechanism of chemical vapor deposition (CVD) of carbon from unsaturated light hydrocarbons (CH_4, C_2H_4, C_2H_2, and C_3H_6) is presented. The mechanism consisting of 757 reactions among 230 species is based on existing information on elementary reactions and evaluated by comparison of numerically predicted and experimentally determined product composition for more than 40 stable gas phase compounds in a CVD flow reactor. The reactor was operated at widely varying conditions: 800-1100 °C and 2-15 kPa. Experimentally observed pressure and temperature effects on the species profiles as function of residence time are well predicted. Second, a model and computer code is presented for the numerical simulation of chemical vapor infiltration (CVI) carbon for the production of carbon fiber reinforced carbon. The chemistry model is based on a multi-step reaction scheme for pyrocarbon deposition, derived from the elementary mechanism, and a hydrogen inhibition model of pyrocarbon growth. This chemical model is implemented in transient 2D simulations of chemical vapor infiltration. The coupled models for mass transport (convection and diffusion), chemical vapor deposition and surface growth, gas-phase and surface chemical reactions are numerically solved by a FEM approach. Three sets of experiments were exemplarily simulated with inlet flows of 20 kPa CH_4, 20 kPa CH_4 with 4 kPa H_2, and 20 kPa CH_4 with 10 kPa H_2, all at a temperature of 1095°C. The continuous infiltration, pyrolysis, and deposition of methane and its consecutively formed C_xH_y products lead to temporarily and spatially varying species concentrations and porosity inside the carbon felt. The predicted density distribution agrees well with experimental data.

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ON THE SIMULATION OF STRENGTH DIFFERENCE
FOR ADHESIVE MATERIALS

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Adhesion has gained increased application in recent years for the bonding process in several industrial fields, such as the branches of automotive industry, the aeroplane construction and the building industry. The advantages of adhesion materials over conventional bonding processes are the economical aspect, automation and its capability for tight seams. The experimental investigation of certain adhesive materials reveals elastic strains, plastic strains and hardening, respectively. Furthermore the different loading cases of tension, compression of torsion show a pronounced strength difference effect. For simulation of these phenomena a yield function dependent on the first and second basic invariants of the related stress tensor in the framework of elasto-plasticity is used. A plastic potential with the same mathematical structure is introduced to formulate the evolution equation for the inelastic strains. Furthermore thermodynamic consistency of the model equations is considered, thus rendering some restrictions on the material parameters. For evolution of the strain like internal variable two cases are considered, and the consequences on the thermodynamic consistency and the numerical implementation are extensively discussed. In a further part of the presentation the extension to large strains is outlined. Two examples are presented. The first example demonstrates the capability of the model equations to simulate the yield strength difference between tension and torsion for the adhesive material Betamate 1496. A second example investigates the deformation evolution of a compact tension specimen with an adhesive zone.

ESTIMATING THE BOUNDARY OF THE ELASTIC REGIME FOR THE BIOLOGICAL COMPOSITE WOOD FROM FAILURE MECHANISMS AT THE NANOSCALE

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The strength of wood is highly anisotropic. This anisotropy stems from the intrinsic structural hierarchy of the material: In all species, wood is composed of cells which are hollow tubes oriented in the stem direction. The cell wall consists of stiff cellulose fibrils with crystalline cores and amorphous surfaces. They are embedded in a soft polymer matrix composed of hemicellulose, lignin, extractives, and water. The elementary constituents of the wood cell wall exhibit tissue-independent stiffness and strength properties. The orientation of cellulose fibrils and tubular holes and the spatial gradation of porosity lead to the anisotropy and the inhomogeneity of the macroscopic material behavior.

These universal morphological patterns were recently quantified in a multiscale homogenization scheme [1] allowing for prediction of the tissue-dependent (macroscopic) elastic properties of wood from its composition (volume fractions of elementary constituents and lumen/vessel porosities). As regards tissue-specific anisotropic strength properties, experimental investigations have shown that (macroscopic) failure of wood is initiated by shear failure of lignin in the wood cell wall [2]. Corresponding local strain peaks in lignin are estimated through quadratic averages [3] over the strains in material phases representing microstructural entities such as the cell wall or the elementary constituents. This gives access to prediction of tissue-dependent (macroscopic) failure surfaces for arbitrary deviations between principal material and loading directions.

Material validation is based on two independent sets of experimental data: Tissue-dependent stiffness and strength values predicted by the micromechanics model ('model output') on the basis of tissue-independent stiffness and strength properties of the universal constituents of wood (experimental set I) for tissue-specific composition data (experimental set IIa, 'model input') are compared to corresponding experimentally determined stiffness and strength values (experimental set IIb). Macroscopic stress states predicted from local shear failure of lignin agree very well with results from uniaxial and biaxial strength tests across a variety of wood species and tissues [4]. This confirms the paramount role of lignin as the strength-determining component of wood.

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SIMPLE METHODS FOR THE DURABILITY
ASSESSMENT OF MICROELECTRONIC SOLDERS

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Due to the extremely small size of modern microelectronic packages it becomes extremely important to take the *graininess and associated heterogeneity* of their solder joints (lead-containing as well as lead-free) into account whenever durability and reliability questions are concerned. It is for that reason that various *miniature experiments* are performed [1-3] in order to reveal temperature dependent mechanical properties of solders, such as Young's modulus, plastic as well as viscoplastic (creep) parameters. Due to its way of measurement (specimen size effect) this data will indirectly contain some "homogenized" information on the local solder structure.

This paper starts with an overview on current experiments and presents extracts from a thermo-mechanical database which has recently been compiled from the literature as well as ongoing publicly funded research work for various, technologically important solders. This data, in particular, Young's modulus and creep laws will then be applied to deformation studies as follows. First, we consider a slender beam that is clamped at its ends, made of solder and subjected to various military as well as automative temperature cycles. Based on the aforementioned material data we study the resulting stress-strain hysteresis in order to obtain some information on the dissipated energy. Particular emphasis is given to the influence of the choice of the stress-free reference temperature as well as to ratchetting. This information is then used in context with simple reliability equations of the Coffin-Manson type for durability and reliability predictions. Second, the same procedure is applied to a slender beam which is clamped at one end and subjected to a suitable tensile as well as compressive deformation at the other.

The results of these 1D investigations are finally compared to more elaborate FE-studies of three-dimensional microelectronic components that have been soldered to a PC-board. The objective is to support the FE-reliability predictions made for these objects by a simplified analysis.

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TWO-DIMENSIONAL STUDIES ON CRACK PROPAGATION IN POROUS BRITTLE MEDIA SUBJECT TO MODE I LOADING

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The failure criterion proposed in [1, 2] is enhanced herein to study crack propagation in porous specimens subject to 4-point bending configurations. In the first step we investigated realistic carbon-carbon composite specimens [3, 4] with pores. Finite element models with pores reconstructed from experimental micrographs of the surface were investigated. Results of the numerical study are compared with experimental observations. During these studies new questions were posed, namely, what is the influence of the dimensions of the pores and their positions around the crack-tip on the crack increment size and direction. To understand these phenomenological aspects a finite element study was performed on cracks propagating in an idealized porous media (circular shaped pores) taking into account the influence of porosity and pores distribution on crack propagation.

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HIERARCHICAL MODELS OF CHEMICAL INFILTRATED CARBON/CARBON COMPOSITES

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In the last years there has been an increasing interest in the multi-scale mechanics of the materials, i.e. in predicting the macroscopic constitutive response on the basis of the underlying microstructure. At each level of structural hierarchy, one may model the material as a continuum, and the representative volume element problem can be formulated in terms of standard equilibrium and boundary conditions. The overall physical behaviour of these micro-heterogeneous materials depends strongly on the shape, size, orientation, properties and spatial distribution of their microconstituents [1]. For prediction of the macroscopic behaviour of such materials the multi-scale homogenization techniques were developed.

As an example of such investigation we develop the hierarchical material model of the chemical vapour infiltrated carbon fiber composites (CFCs) with a unidirectional or random distribution of fibers. We embed fibers into matrix using the procedure described in [2] for unidirectional fibers and [3] for infiltrated felt. After that we homogenizie the material and introduce the pores using a numerical conformal mapping technique for unidirectional composite [2] and an approximation of irregular 3D pores by equivalent ellipsoids in the case of infiltrated felt [3].

The approach based on hierarchical structural modeling can be used to theoretically predict the mechanical parameters of CFCs with different microstructure and to develop virtual materials with prescribed mechanical properties.

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MICRO- AND MESO-INSTABILITIES IN STRUCTURED COMPOSITE MATERIALS AND MATERIAL COMPOUNDS

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Light-weight materials frequently exhibit very special micro- and meso-structures, such as sandwiches composed of thin layers of homogeneous or composite materials, and core materials which also show some microstructure as, e.g., honeycombs and closed or open cell foams. In order to calculate the load carrying capacity of structures made of such materials and material compounds not only strength and stability consideration on the structural level but also on the meso and micro-level must be taken into account. For instance, stability loss occurring at length scales which are several orders of magnitude smaller than the size of the structural part can be the starting point of failure of the complete structure. Typical materials instabilities, i.e. instabilities on the level of the material's microstructure, are buckling of struts and cell walls of polymer or metallic foams [1] or crushing phenomena in honeycomb cores of sandwich plates or shells. Such phenomena are treated in terms of micro-instabilities. Typical kinds of meso-instabilities are localizations in the form of bands of buckled foam cells leading to phenomena similar to material instabilities such as the formation of necks or shear bands by plastic localization in polycrystalline materials.

Wrinkling of face layers of sandwich plates under macroscopic in-plane loading or bending is studied as a particular form of "meso-instabilities" of lightweight material compounds. A semi-analytical-numerical approach has been developed [2] which is able to take various anisotropy effects into account. Although wrinkling starts as a bifurcation process with a distinct periodic eigenfunction, the post-critical behavior shows the formation of single localized folds being the result of crushing of the microstructure of the core.

In sandwiches with honeycomb cores and very thin faces a special kind of meso-instability, namely face layer dimpling, can be observed, too. It is shown by computational means that this kind of mesoscopic structural instability represents an interactive buckling of cell walls and face sheets.

The computational models on the micro- and on the meso-level are based on unit-cell concepts [3], well known from the field of micromechanics of materials.

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NONLINEAR ANALYSIS OF COMPOSITE AND FGM SHELL STRUCTURES

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In solid mechanics and structural mechanics the development of accurate shell theories has been one of the most important research activities. Finite element models of hear deformable plate and shell theories plagued with shear, membrane, and thickness locking phenomena [1-3]. Therefore, it is important to develop a consistent shell theory and associated finite element model that is both accurate and robust (i.e., does not suffer from any type of locking).

In this lecture, a finite element computational model for the nonlinear analysis of shell structures consisting of laminated shells or through-thickness functionally graded shells is presented. A tensor-based finite element formulation is presented to describe the mathematical model of a shell in a natural and simple way by using curvilinear coordinates. In addition, a family of high-order elements with Lagrangian interpolations is used to avoid membrane and shear locking and no mixed interpolations are employed. A first-order shell theory with seven parameters is derived with exact nonlinear deformations and under the framework of the Lagrangian description. This approach takes into account thickness changes and, therefore, 3D constitutive equations are utilized. Numerical simulations and comparisons of the present results with those found in the literature for typical benchmark problems involving isotropic and laminated composite plates and shells, as well as functionally graded plates and shells, are found to be excellent and show the validity of the developed finite element model. Moreover, the simplicity of this approach makes it attractive for applications in contact mechanics and damage propagation of shells.

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ATOMIC SCALE BEHAVIOR OF CRACK BRIDGING IN CARBON FIBER FELTS INFILTRATED WITH PYROLYTIC CARBON

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The crack bridging is an important failure mechanism contributing to the toughness enhancement of carbon-carbon composites [1, 2]. The objective of this study is to study the crack bridging mechanism at the atomic scale. High-resolution scanning electron microscopy and high-resolution transmission electron microscopy coupled with electron-energy-loss spectroscopy have been used for this purpose. It is observed that the crack bridging occurs by bent graphitic lamellae. The increased flexibility of bent lamellae is associated with the atomic defects in graphene layers. It is shown that the crack bridging is typical for composites with a higher toughness [3].

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ASYMPTOTIC MODELS FOR PIEZOELECTRIC STACK ACTUATORS WITH THIN METAL INCLUSIONS

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Cofired multi-layer actuators will be considered as composites. They consist of anisotropic piezo-elastic ceramic materials with stacked parallel electrodes. They are mathematically modeled as a
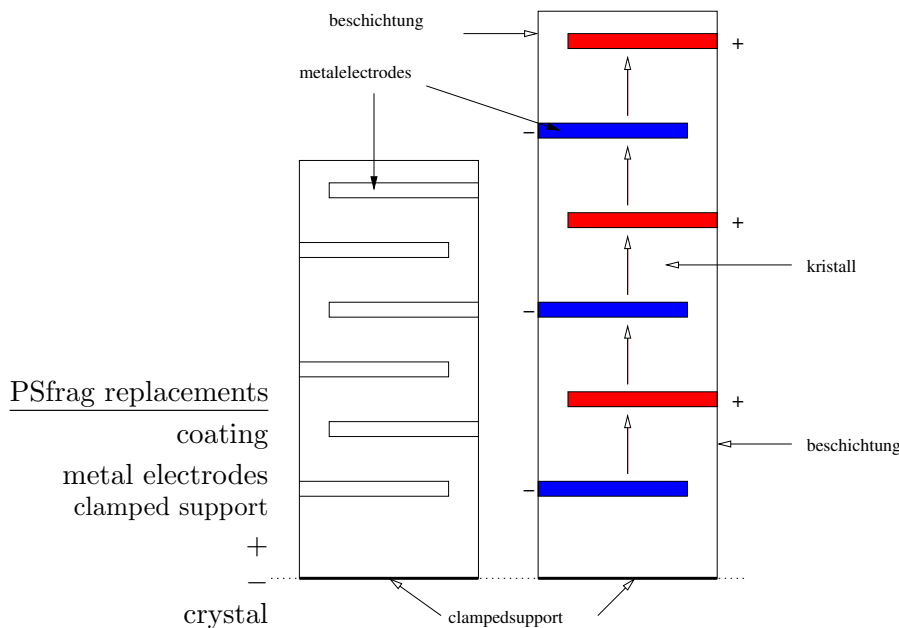

Figure 1: 2D-sketch of a MLC-type stack actuator.

quasi-static linear multi-field problem with appropriate boundary and transmission conditions [1]. The small relative thickness of the electrodes as well as the multi-field character of the problem provides difficulties in the numerical computation. Therefore, we formally derive an asymptotic model where the electrodes occur as interfaces in the ceramic domain. Depending on the material parameters of the metal (undamaged and damaged case) the resulting transmission conditions are standard, nonstandard or even imperfect [2].

It turns out, that the stack actuator can be efficiently simulated by this asymptotic model which allows to compute the mechanical and electrical fields in real devices. Furthermore, the influence of the temperature field is demonstrated numerically [3].

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NUMERICAL STUDY OF SINGULARITIES
IN CARBON BASED COMPOSITES

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One of the important issues in modern fracture mechanics is understanding and prediction of fracture in materials with 3-dimensional morphology. The major difficulty in studying fracture of these materials is that the crack propagation can not be simplified through decomposition into plane problems along the crack front edge, thus the methods of 2-dimensional linear elastic fracture mechanics aren't adapted for precise analysis in situations where the stress-intensity factor varies along the crack front or when the crack front has 3-dimensional curvilinear form. The reason for these difficulties are the *corner points* along the crack front where the elastic fields are with three dimensional nature. Typical example for such *corner* is the intersection of the crack front with the interface between two different phases like for example fiber-matrix interface in CVI-infiltrated carbon-carbon composites or an interlaminar interface between different oriented composite plies. According to the concept of weak and strong singularities, it is possible to obtain the singular exponents and thus the asymptotics for the stress intensity factor (SIF) and the strain energy release rate (SERR) in a neighbourhood of particular corner point, so that the convenient single parameter description on which fracture mechanics is based to be preserved. In this talk we propose a novel dimensional-reducing approach for computation of singular exponents (eigenvalues) at the tip of a 3-dimensional crack [1]. On the basis of Kondratievs theorem we present a Petrov-Galerkin discretization scheme for evaluation of unknown eigenvalues. Our method demonstrates very good convergence and accuracy for benchmark problems with different materials where the singular exponents and corresponding singular modes are calculated for arbitrarily-inclined crack geometries and analysis of the crack behavior according to the strength of the singularity is performed [2].

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DAMAGE AND FAILURE IN FIBRE REINFORCED COMPOSITES

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Few things last forever. It would appear that most material things that respond to their environment change their form or function with time. Our technical understanding of the relationship of the history of response to engineering properties such as strength and stiffness is yet incomplete [1]. The safety, reliability, and durability of every engineering component rests directly on our understanding of what Lord Kelvin first called 'materials response', or commonly the subjects of creep and fatigue.

Most engineering components are subjected to load and environmental histories which vary in time over the period of service. The reduction of strength and the subsequent failure of materials subjected to repeated loading has been first addressed as a fundamental problem in 1837 by Albert [2] for repeated load proof tests on mine-hoist chains made of iron. Although the subject of fatigue has attracted numerous scientists and engineers over a period of more than 150 years, it is estimated that today 90% of all cases of failure are due to fatigue. This has to do with the increasing complexity under which materials must serve their engineering purposes.

The anisotropic and heterogeneous character of the material provides composite systems with many degrees of freedom for optimum configuration of the material, but requires a high degree of know-how for design, computation, manufacturing, and life-prediction. Designing lightweight FRP components which are exposed to dynamic loads requires tools that – if high safety factors should be avoided – are able to handle the mechanical degradation process of the material.

A common approach to model the degradation process is based on the variation of an effective mechanical property of the FRP – such as stiffness – and to find a mathematical description for its change with the applied load [3]. Such a damage parameter does not directly describe physically existent damage but its effect on the considered property. Due to the phenomenological character of those macroscopic approaches the results can hardly be generalised – each specific material has to be tested extensively under well defined load conditions. The challenge of damage accumulation for macroscopic damage parameters has not yet been solved. However, macroscopic damage parameters benefit from their simple applicability and adaptability to different kinds of materials, damage mechanisms occurring, and loadings. The paper will highlight the various damage mechanisms occurring and the resulting consequences for highly loaded composite parts.

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COMPUTATIONAL MODELING OF DEFORMATION AND FAILURE MECHANISMS IN THERMOPLASTIC MICROLAYER COMPOSITES

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Amorphous thermoplastic polymers display an ambivalent and complex mechanical behavior, ranging from the ability to undergo large inelastic deformations (e.g. shear banding) to brittle failure by crazing. Typical examples are polycarbonate (PC) and styrene-acrylonitrile (SAN), where the former is known to be ductile while the latter is rather brittle.

Subject of this presentation is the numerical simulation of the microscopic and macroscopic deformation and failure behavior of composites which consist of many alternating layers of PC and SAN. Microlayer composites of this type were experimentally studied in [1] where several aspects of the microscopic deformation mechanisms have been revealed in a qualitative manner. The present work aims at gaining some additional insight from micromechanical models and detailed finite element simulations. Therefore, the rate-dependent deformation behavior of the glassy polymers is described by an appropriate viscoplastic constitutive model [2] while the formation of crazes is treated within the framework of cohesive surfaces [3]. This approach allows to reproduce the formation of crazes in SAN and of shear bands in PC along with their network-like interaction prior to failure, as observed in tensile tests on this class of composite materials [1]. Moreover, the relation between local failure mechanisms (e.g. craze breakdown) and the macroscopic response of the composite is analyzed as well as its dependence on the composition (volume fractions of PC and SAN). Approaches to account for the absolute layer thickness by introducing an internal length scale motivated from polymer physics are also discussed and evaluated.

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LOCAL INTEGRAL EQUATIONS FOR CRACK PROBLEMS IN FGMS BY A MESHLESS METHOD

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Functionally graded materials (FGMs) can be considered as a special case of composite materials. In FGMs, the composition and the volume fraction of their constituents vary continuously with spatial coordinates. These materials have been introduced in recent years to benefit from the ideal performance of its constituents, e.g. high heat and corrosion resistances of ceramics on one side, and large mechanical strength and toughness of metals on the other side. A review on FGMs can be found in the monograph of Suresh and Mortensen [1] and the review chapter by Paulino et al. [2].

The solution of the boundary or initial boundary value problems for continuously nonhomogeneous solids requires advanced numerical methods due to the high mathematical complexity. Beside the well established finite element method (FEM), the boundary element method (BEM) provides an efficient and popular alternative to the FEM for solving certain classes of boundary or initial boundary value problems. The conventional BEM is accurate and efficient for many engineering problems. However, it requires the availability of the fundamental solutions or Green's functions to the governing equations. Material anisotropy increases the number of elastic constants in Hooke´s law, and hence makes the construction of the fundamental solutions cumbersome.

In this paper, a new computational method is presented to analyze boundary value problems in anisotropic FGMs with cracks. For general nonhomogeneous, anisotropic and linear elastic solids, elastostatic and elastodynamic fundamental solutions are, hitherto, to the best of the authors' knowledge, not available. To overcome this difficulty, a local integral equation formulation can be used for general nonhomogeneous solids ([3], [4]). The application of local integral equations (LIEs) requires the use of a domain approximation of the physical fields. Such an approach has been recently applied to problems in homogeneous, anisotropic and linear elastic solids by Sladek et al. [4]. It is extended in this paper to continuously nonhomogeneous, anisotropic and linear elastic solids. The Laplace-transform technique is applied to eliminate the time variable in the governing equations and the boundary conditions of elastodynamic problems. Several numerical examples for crack problems in nonhomogeneous orthotropic and linear elastic solids are presented and discussed.

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THE STABILITY OF A THREE-LAYERED COMPOSITE CONICAL SHELL CONTAINING A FGM LAYER SUBJECTED TO EXTERNAL PRESSURE

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ABSTRACT

Functionally graded materials (FGMs) have received considerable attention in many engineering applications since they were first reported in 1984 in Japan. FGMs are both macroscopically and microscopically heterogeneous composites, which are normally made from a mixture of ceramics and metals with continuous composition gradation from a pure ceramic on one surface to full metal on the other. This leads to gradual and smooth change in the material profile as well as the effective physical properties, making them distinguish from the conventional fiber-matrix composites and preferable in many engineering applications, especially in high temperature environments such as aerospace structures, fusion reactors and nuclear industry [1,2].

In this work, stability of a three-layered truncated conical shell containing a FGM layer subjected to external pressure is studied. The material properties of functionally graded layer are assumed to vary continuously through the thickness of the shell [2-4]. The variation of properties followed an arbitrary distribution in terms of the volume fractions of the constituents. The fundamental relations, the dynamic stability and compatibility equations of three-layered truncated conical shells containing a FGM layer are obtained. Applying Galerkin's method, these equations have been transformed to a pair of time dependent differential equation and critical external pressure and frequency parameter are obtained. The results show that the critical parameters are affected by the configurations of the constituent materials and the variation of the shell geometry. Comparing results with those in the literature validates the present analysis.

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ENERGY RELEASE RATE FOR A MODE-III INTERFACE CRACK IN A COMPOUND OF MATERIALS OF *P*-LAPLACIAN TYPE

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In this talk there will be treated a 2D domain Ω_{δ_0} consisting of two nonlinear, hyperelastic materials located in the subdomains Ω_1 and Ω_2. The interface between Ω_1 and Ω_2 is assumed to be a straight line and to contain a crack of the length δ_0 with expansion direction along the interface, see fig. 1. Mode-III-loadings are applied. The boundary transmission problem for this configuration Ω_{δ_0} is supposed as follows (where $i, j \in \{1, 2\}$ in the sequel):

Find $u : \Omega_{\delta_0} \to \mathbb{R}$, with $u|_{\Omega_j} = u_j$ for given functions $f : \Omega_{\delta_0} \to \mathbb{R}$ with $f|_{\Omega_j} = f_j$, $h : \Gamma_N \to \mathbb{R}$ with $h|_{\Gamma_N \cap \partial \Omega_j} = h_j$ and $g : \Gamma_D \to \mathbb{R}$ with $g|_{\Gamma_D \cap \partial \Omega_j} = g_j$, such that:

$$-\mu_j \operatorname{div}\left((\kappa_j + |\nabla u_j|^2)^{\frac{p_j-2}{2}} \nabla u_j \right) = f_j \ \text{in} \ \Omega_j, \tag{1}$$

$$u_1 - u_2 = 0 \ \text{on} \ \Gamma_T, \tag{2}$$

$$\mu_1 (\kappa_1 + |\nabla u_1|^2)^{\frac{p_1-2}{2}} \nabla u_1 \cdot \mathbf{n}_{12} + \mu_2 (\kappa_2 + |\nabla u_2|^2)^{\frac{p_2-2}{2}} \nabla u_2 \cdot \mathbf{n}_{21} = 0 \ \text{on} \ \Gamma_T, \tag{3}$$

$$u_j = g_j \ \text{on} \ \Gamma_D \cap \partial \Omega_j, \tag{4}$$

$$\mu_j (\kappa_j + |\nabla u_j|^2)^{\frac{p_j-2}{2}} \nabla u_j \cdot \mathbf{n}_j = h_j \ \text{on} \ \Gamma_N \cap \partial \Omega_j, \tag{5}$$

$$\mu_j (\kappa_j + |\nabla u_j|^2)^{\frac{p_j-2}{2}} \nabla u_j \cdot \mathbf{n}_j = 0 \ \text{on} \ R_{\delta j}. \tag{6}$$

Here $\overline{\Omega_{\delta_0}} = \overline{\Omega_1} \cup \overline{\Omega_2}$. The parts Γ_D, Γ_N, Γ_T of the boundary denote the Dirichlet-, Neumann-, or transmission-boundary and R_{δ_j} are the crack lips, $\mathbf{n}_j$ and $\mathbf{n}_{ji}$ are outer unit normal vectors of Ω_j. $\mu_j \in (0, \infty)$, $c_j \in (0, \infty)$, $\kappa_j \in [0, 1]$ are given material constants.

In order to predict a further crack growth, the following formulation of the Griffith fracture criterion can be used: *The crack grows if the energy release rate is greater or equal a certain energy amount needed for the fracture process:*

$$ERR(\Omega_{\delta_0}) := -\left.\frac{\mathrm{d}E(\Omega_{\delta_0+\delta})}{\mathrm{d}\delta}\right|_{\delta=0} \geq \left.\frac{\mathrm{d}D(\Omega_{\delta_0+\delta})}{\mathrm{d}\delta}\right|_{\delta=0} = \mathcal{G}_c. \tag{7}$$

Thereby the energy release rate $ERR(\Omega_{\delta_0})$ is proportional to the Gâteaux derivative of the potential energy $E(\Omega_{\delta_0+\delta})$ at $\delta = 0$. The dissipative energy $D(\Omega_{\delta_0+\delta})$ only depends on the crack length and material constants, such that $\left.\frac{\mathrm{d}D(\Omega_{\delta_0+\delta})}{\mathrm{d}\delta}\right|_{\delta=0}$ coincides with the fracture toughness of the interface $\mathcal{G}_c$.

The focus of this talk lies in the presentation of explicit formulas for the energy release rate of the configuration Ω_{δ_0}, such as the Griffith formula and the J-Integral. Numerical results based on these derived formulas will be shown.
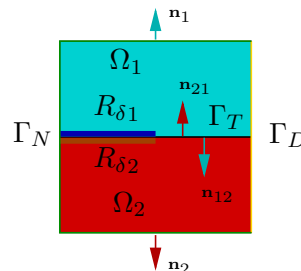

Figure 1: The considered domain

NON-DESTRUCTIVE RECONSTRUCTION OF DELAMINATION REGIONS IN LAYERED CFRP-COMPOSITES

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The purpose of this study is to propose a solution of the inverse problem dealing with determination of internal delamination regions in carbon-fibre reinforced plastic composites(CFRP) subjected to tensile load, based on the surface measurement data.

The inverse problem that admits the determination of the crack position, topology and shape can be considered as a free-discontinuity problem with the unknown pair $(\mathbf{u}, S)$, where $\mathbf{u}$ represents the elastic displacement vector in the unfractured part of the laminate and S is the crack surface. The empirical computational algorithm AICRA, Alternating Iterative Crack Reconstruction Algorithm [1, 2], developed for a preliminary known interlaminar surface can be applied to every interface between two composite layers. To ensure the uniqueness of the inverse problem and to identify the true delamination region from the obtained solution pairs $(\mathbf{u}, S)$, we consider a functional, based on the variational formulation provided by Mumford and Shah [3]. When regarded in the context of delamination, the Mumford and Shah functional contains the bulk energy of the unfractured part of the body, the surface energy of the delamination region, and a lower order term. A variational approximation with elliptic lower semicontinuous functional via Γ-convergence [4] enables to find a local minimizer of the Mumford and Shah functional.

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MICROMECHANICAL MODELING OF COMPOSITES USING COMPLIANCE CONTRIBUTION TENSOR

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Contributions of individual inhomogeneities to the overall mechanical behavior of composite, porous or damaged materials can be characterized by their compliance or stiffness contribution tensors [1-2]. In the case of anisotropic matrix material or non-uniform orientational distribution of inhomogeneities, these tensors also determine the overall anisotropy of composites.

In this presentation we describe the micromechanical procedure to predict the overall properties of solids containing elastic fibers, rigid particles, regularly or irregularly shaped pores, and cracks. The components of the corresponding compliance contribution tensors are found either analytically or numerically. The procedure is illustrated by considering the following three material systems [2-4]:

–   porous carbon/carbon composites manufactured by chemical vapor infiltration;
–   metals containing mixed-mode plastic cracks;
–   polymers reinforced by carbon nanotubes.

In all these cases we find the complete set of material properties and establish dependence of the overall behavior on the corresponding inclusion/defect density parameters. The solutions are compared with the available experimental observations and known results of other authors.

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COMPUTATIONAL MODELLING OF LAMINAR WELDED HYBRID LIGHTWEIGHT STRUCTURES

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Using interfacial elastoplasticity [1] with Lemaitre-type damage [2], phenomenological simulations of laminar welded hybrid lightweight structures are accomplished. The applied traction-separation-law is decoupled with respect to a local orthonormal frame such that the stress-strain response is controlled independently in the normal and in the tangential direction. The talk starts with a short overview over different modern manufacturing procedures for laminar welded metal/fibre-reinforced polymer composites [3], followed by a concise outline concerning experimental and analytical techniques. Thereafter, a detailed characterization of the applied theoretical and numerical methods is highlighted. Beside comparisons with one-dimensional (integral) measurements (force-displacement-curves), two-dimensional (local) experimental data given by Electronic Speckle Pattern Interferometry (ESPI) [4] is compared with the simulation. The talk is closed by a discussion of the achieved results.

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FINITE ELEMENT SIMULATION OF SKIN-STIFFENER DEBONDING

IN CURVED FIBER-REINFORCED SHELL STRUCTURES

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Uni-directional fiber-reinforced composite laminates are widely used in aerospace industry for a great variety of structural parts. In order to enhance the exploitation of material reserves, there is a need for the integration of progressive damage scenarios in the design phase. Due to their hazardous effects on the load-carrying capacity of composite structures, this work focusses on the simulation of skin-stringer debonding in curved fiber-reinforced composite panels. 2D and 3D finite element formulations are developed which are based on a cohesive zone approach. The constitutive law is characterized by a linear as well as an exponential softening after the onset of separation and is mainly inspired by works of DE-ANDRÉS ET AL. [2] and ORTIZ & PANDOLFI [3]. A penalty term is added to avoid the interpenetration of the crack faces. A consistent tangent will be provided allowing for robust nonlinear iteration behaviour. The damage process is history-dependent leading to an irreversible stiffness degradation in damaged zones. The FE-formulations are compared to experimental results for typical standard tests like e.g. DCB of American Society for Testing and Materials (ASTM)[1]. Furthermore more complex structures like stringer stiffened shells made of fiber reinforced composite material, often used in aerospace industry, are investigated. We compare our numerical results to experimental data from KORJAKINS ET AL. [4] at Riga Technical University (RTU) with graphite/epoxy composite IM7/8552, based on a cooperation within an EU-project. The results of the numerical simulations agree very well with the experiments which validates the application of the proposed numerical models.

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ELECTRO-MECHANICAL TRANSPORT IN IONIC POLYMER-METAL COMPOSITES

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Ionomeric polymer transducers are a class of smart material that exhibits large bending strains (>2%) but correspondingly low force output when subjected to low voltage (<4V) excitation. It is clear from experiment and theory that diffusion of ionic species within the polymer is one key point for electro-mechanical coupling.

For this reason, in this paper a computational model is presented that predicts the charge transport in ionic polymer-metal composites. In [1] it was shown that this computational approach can accurately predict the current response and charge accumulation for the case of step voltage excitation.

In this research, ionomeric polymer transducers subjected to a step change of the applied voltage as well as to a time-harmonic excitation are investigated. To describe the actuation behavior, a computational model for the transport [2] and the electro-mechanical transduction is given. The transport model is based upon a coupled chemo-electrical multi-field formulation and computes the charge density profile as well as the current flux for an applied alternating electric potential.

From this, the bending deflection of the actuator may be calculated by introducing pressure loads stemming from linear and quadratic contribution terms of the charge density. Material parameters such as permittivity and diffusion constant of the coupled chemo-electro-mechanical model are obtained by experimental investigations of the ionic polymer metal composites using step voltage inputs.

A comparison of the experimental and numerical investigations for ionomeric polymer transducers subjected to a time-harmonic exitation shows a very good correlation for both low and high frequencies at low applied voltage.

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LOAD PARTITIONING IN MULTIDIRECTIONALLY FIBER REINFORCED METAL MATRIX COMPOSITES

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A model for plastic and creep deformation of metal matrix composites multidirectionally reinforced by short ceramic fibers is proposed. The reinforcement is described by the effective stiffness tensor of a multidirectional arrangement of continuous fibers and the internal damage of the composite during creep due to fiber fragmentation is introduced by assigning a heuristic nonlinear stress-strain relationship to the fibers [1]. Based on the model, the load partitioning between matrix and fibers is computed. The macroscopic behaviour is simulated for composites exhibiting different fiber orientation distributions and different heuristic nonlinar stress-strain functions. For a 2D-random orientation distribution, a good qualitative match between simulation and experimental results is obtained for various loading situations. The evolution of deviatoric matrix stresses as monitored by neutron diffraction [2] complies also well with the theoretical results.

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DUAL SINGULAR FUNCTIONS FOR A CRACK PROBLEM IN ISOTROPIC ELASTIC MEDIA

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The solution of the elasticity equations in a three-dimensional body containing a bounded crack surface in its interior can be represented by an appropriate asymptotic expansion near to the crack front. For the representation of the corresponding stress intensity distributions along the crack front, one needs the dual singular functions. If the crack front is a straight line, it turns out that the corresponding dual singular function can be given explicitly. For their derivation one needs a combination of pseudodifferential operator techniques with the Wiener-Hopf technique applied to appropriate boundary integral equations.

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SIMULATION OF ASYMMETRIC EFFECTS FOR SHAPE MEMORY ALLOYS

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Extended experimental tests for shape memory alloys exhibit different behaviours for different loading types, such as tension, compression and shear. These observations, labelled here briefly as asymmetric effects, are reported in the literature e.g. in [1] or [2]. The paper is concerned with modelling of these effects in the framework of plasticity. To this end an additive decomposition of the flow rule is assumed into a sum of weighted stress mode related quantities. The characterization of the stress modes is obtained in the octahedral plane of the deviatoric stress space in terms of a single scalar variable, such that stress mode dependent scalar weighting functions can be constructed. Furthermore the numerical implementation into a finite element program of the resulting set of constitutive equations is outlined. For parameter identification a sequential strategy exploiting the mode decomposition and the individual loading scenarios, such as tension, compression and shear, respectively is described. Verification of the proposed methodology is succeeded for simulation of the pseudoelastic behaviour of shape memory alloys with different hardening characteristics in tension and shear.
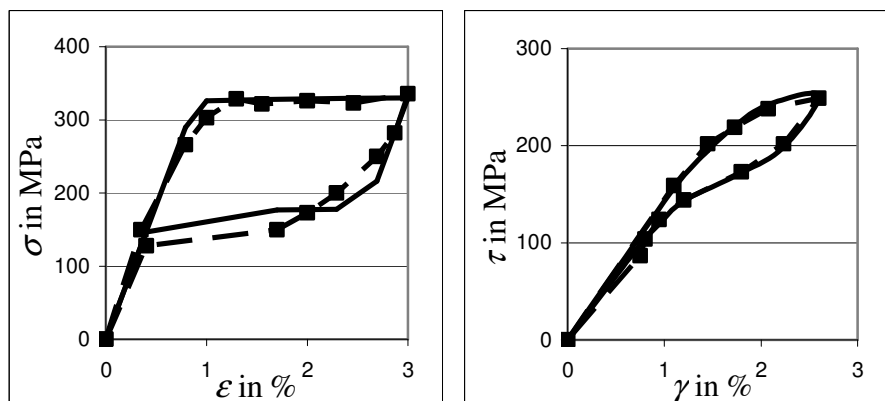
Fig.1: Pseudoelastic behaviour of Shape Memory Alloys: Comparison of experimental (symbols, from [2]) and computed (solid curves) results (a) Tension test: normal stress vs. strain (b) Shear test: shear stress vs. shear strain

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Keywords: Shape memory alloys, tension, compression, shear, asymmetry, constitutive equations, finite element simulation, parameter identification

EDGE SINGULAR SOLUTIONS IN ANISOTROPIC MATERIALS AND MULTI-MATERIAL INTERFACES

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The asymptotic solution of elasticity problems, in the vicinity of edges in 3-D isotropic and anisotropic domains is provided explicitly. It involves a sequence of eigen-pairs and their corresponding coefficients which are functions along the edge. The determination of these eigenpairs (and more importantly their shadows), and reliable computation of the coefficients (edge stress intensity functions) of the asymptotic expansion will be addressed in this talk. Special attention is devoted to anisotropic domains, and multi-material interfaces which are typical to composite materials. These are of practical engineering importance because failure theories involve them.

Recent results, on the special structure of edge-singularities, including so-called shadow eigen-functions, will be presented [1]. New methods for the computation of their characteristics will be demonstrated by numerical methods: namely the quasi-dual method for the computation of the edge stress intensity functions. These are used in conjunction with the p-FEM and numerical examples will be provided [2, 3].

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FRACTURE ANALYSIS OF FUNCTIONALLY GRADED MATERIALS BY A BEM

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ABSTRACT

Functionally graded materials (FGMs) represent a new class of composite materials designed to achieve high performance levels superior to that of homogeneous materials by combining the desirable properties of each constituent. A representative example for FGMs is the metal/ceramic FGM, which is compositionally graded from a refractory ceramic to a metal. It can incorporate incompatible functions such as the heat, wear, and corrosion resistances of ceramics and the high toughness, high strength, machinability and bonding capability of metals without severe internal thermal stresses. Due to the inherent brittle nature of ceramics, microcracks or crack-like defects may be induced during the fabrication process and under the in-service loading conditions. Hence, investigation of the fracture behavior of FGMs has received much attention in the scientific community in recent years and it is essential to the design, optimization, high-performance and prominent engineering applications of FGMs. Since analytical methods can only be successfully applied to fracture analysis of FGMs for very simple geometrical and loading conditions, numerical methods are needed in general cases. In principle, both the finite element method (FEM) and the boundary element method (BEM) can be applied for fracture analysis of cracked FGMs. Though the BEM has been successfully applied to homogeneous materials since many years, its application to FGMs is unfortunately yet very limited due the fact that the corresponding fundamental solutions or Green's functions for general FGMs are either not available or mathematically too complex. The nonhomogeneous nature of FGMs prohibits an easy construction of Green's functions for general cases.

In this paper, an efficient BEM for two-dimensional (2D) crack analysis in continuously nonhomogeneous, isotropic and linear elastic functionally graded materials (FGMs) is presented. The method uses a boundary-domain integral equation formulation. An exponential variation of Young's modulus and constant Poisson's ratio are assumed. Fundamental solutions for homogeneous, isotropic and linear elastic solids are utilized in the present BEM, which leads to a boundary-domain integral formulation due to the materials nonhomogeneity. By introducing normalized displacements, displacement gradients in the domain-integrals can be avoided. The arising domain-integrals are transformed into boundary-integrals along the global boundary by using the radial integration method developed by Gao ([1], [2]). The normalized displacements in the domain-integrals are approximated by a series of basis functions, which consist of a combination of radial basis functions and polynomials in terms of global coordinates. The present BEM is a meshless method and requires only boundary nodes and interior nodes instead of meshes. In comparison with other meshless methods, the present BEM is easy to implement and can be easily integrated into existing BEM codes for homogeneous and linear elastic solids. Numerical examples show that the present BEM is highly accurate and efficient, and it is quite robust and insensitive to the number and the distribution of used interior nodes.

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INTELLIGENT OPTIMAL DESIGN OF COMPLEX SYSTEMS

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The designers of materials and structures are often compelled to make decisions under uncertain conditions, seeking solutions to problems which do not have known solutions. These include constitutive modelling, fatigue life prediction, wear, friction, errors of numerical simulations. An approach to deal with such problems using the whole available expert knowledge, experimental data and computational tools has been developed at the Laboratoire de Mécanique des Solides of Ecole Polytechnique (Paris, France) and is now distributed by CADLM (www.cadlm.fr).

It is based on coupling the existing knowledge of experts, numerical results, and experimental data, with some special automatic learning and optimization techniques.

For this approach [1], it is necessary:

i) to build a DATABASE of examples, i.e., to obtain some experimental, an real or simulated results, where the EXPERTS indicate all variables or descriptors which are essential to the considered problem. This is, at first, done with some PRIMITIVE descriptors x. Then, the data are transformed into INTELLIGENT descriptors XX, using the existing knowledge (usually insufficient) and theories. These intelligent descriptors allow to make the fusion of data and the improvements of the automatic learnings.

The results or conclusions may be classes (good, not good, ...) or numbers.

ii) to generate the RULES using any Automatic Learning Tool. Each conclusion is explained as function (or set of rules) of some of the input intelligent descriptors, together with a known reliability or accuracy measure

and iii) to optimize at two levels (the Inverse Problems).

* Considering the intelligent descriptors as independent, it is possible to get the OPTIMAL SOLUTION satisfying the special required properties and allowing the DISCOVERY OF NEW MECHANISMS,

* Considering the intelligent descriptors linked to primitive descriptors, it is possible to obtain the optimal solution which is technologically possible.

So, not only a Practical Optimal Solution is obtained, but also the experts may learn the missing parts, may build models or theories based only on the retained intelligent descriptors and guided by the structure of the rules or relationships.

In the lecture, we shall show its application to the optimal formulation and process of a woven composite material when we have to characterize its mechanical properties (elastic and limit ones) and its electromagnetical properties while taking care of its weight and its cost and thus to reach the HIGH QUALITY AND LOW COST MATERIALS.

We shall also show the multilevel modeling and the multidisciplinary optimization of this problem.

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