Plenaries

Plenary 1

Particle Shape Effects in Particle Reinforced Composites

Helmut J. Böhm

Institute of Lightweight Design and Structural Biomechanics,
Vienna University of Technology, Vienna, Austria
hjb@ilsb.tuwien.ac.at

Keywords: Polyhedral particles, periodic homogenization

The majority of analytical and numerical models for the thermomechanical and thermophysical behavior of particle reinforced composites have been based on spherical or ellipsoidal inhomogeneities. The present contribution aims at expanding this envelope by studying materials consisting of a matrix reinforced by identical, randomly oriented, equiaxed, convex polyhedral particles. This is done by using the Finite Element method for evaluating the microscopic and macroscopic responses of idealized volume elements that take the form of periodic unit cells containing multiple, randomly positioned inhomogeneities embedded in a linear elastic or a thermoelastoplastic matrix. Because each of the unit cells contains only some 20 particles, the volume elements are too small to be representative of random matrix-inclusion materials. This is countered by ensemble averaging over a number of statistically equivalent phase geometries for each particle shape considered, viz., spheres, tetrahedra, cubes, octahedra and tetrakaidekahedra. Because the resulting ensemble averaged, homogenized elastic tensors deviate to some extent from the required macroscopic isotropy, the closest isotropic elasticity tensors are extracted. The evaluation of the macroscopic responses to elastoplastic loading cycles and of the microscopic stress fields are also based on the ensemble concept.

The predicted responses are compared to analogous results obtained for spherical particles and to the pertinent bounds for the macroscopic behavior. Noticeable particle shape effects are found both for the thermoelastic and the for conduction behavior. Simulations of load controlled cycles under macroscopic, uniaxial tensile and shear loading in the elastoplastic regime show a clear influence of the particle shape on the macroscopic responses, whereas hydrostatic and thermal cycles in ductile-matrix composites are hardly affected. Thermal residual stresses tend to increase particle shape effects under subsequent mechanical loading in the elastoplastic regime. The microstress fields in the matrix display a clear, but limited sensitivity to the particle shapes, and much stronger effects are predicted for the stress fields in the particles, where polyhedral inhomogeneites tend to induce marked intra-particle and inter-particle fluctuations. These effects show a clear ordering by shape, becoming more marked in the sequence spheres–tetrakaidekahedra–octahedra–cubes–tetrahedra.

Plenary 2

Metal-ceramic nanolaminates: a new paradigm in metal-ceramic composites

Y. Lingwei[1], S. Lotfian[2], J. M. Molina-Aldareguía[1], J. LLorca[1,3]

[1]IMDEA Materials Institute, 28906 Getafe, Madrid, Spain
[2]Max-Planck-Institut für Eisenforschung, 40237 Dusseldorf, Germany
[3]Department of Materials Science, Polytechnic University of Madrid, 28040 Madrid, Spain
javier.llorca@imdea.org

Keywords: Nanoscale multilayers, nanomechanics, modeling, metal-ceramic composites.

Metal-ceramic nanolaminates are two-dimensional nanocomposites made up by alternating metallic and ceramic layers with a thickness in the range 2 nm to 100 nm. They are manufactured by physical vapor deposition in the form of coating with thicknesses up to several µm and present a combination of mechanical and functional properties that a very appealing for many engineering applications. From the mechanical viewpoint, metal-ceramic nanolaminates show a dramatic increase in strength as compared to standard metal-ceramic nanocomposites. This is due as a result of strengthening of the ceramic and metallic nanolayers because of the limited flaw size in the former, the constraint induced by the ceramic on the plastic deformation of the metallic layer and the enhancement of the metal yield stress due to size effects [1-3]. Moreover, it has been recently reported an increase in both strength and toughness with decreasing layer thickness [4].

This contribution is focused in the analysis of the deformation and failure mechanisms of a model Al/SiC metal-ceramic nanolaminate by means of a combination of nanomechanical experiments and simulations. In particular, instrumented nanoindentation and micropillar compression tests were carried out in different orientations as a function of strain rate and temperature (25ºC to 400ºC) and compared with numerical simulations in which the nanolayered structure was explicitly taken into account. As a result, the role played by the plastic deformation of the matrix, the constraint imposed by the ceramic layers and the metal-ceramic interfaces on the deformation and fracture of the nanolaminates was elucidated as a function of the volume fraction and layer thickness of each constituent for different strain rates and temperatures. This information is critical for the design of novel metal-ceramic nanolaminates with enhanced mechanical properties under different regimes [5].

References

[1] S. Lotfian, J. M. Molina-Aldareguía, K. E. Yazzie, J. LLorca, N. Chawla. Phil. Mag. Lett., 92 (2012) 362-367.
[2] S. Lotfian, M. Rodríguez, K.E. Yazzie, N. Chawla, J. LLorca, J. M. Molina-Aldareguía. Acta Mater., 61 (2013) 4439-4451.
[3] S. Lotfian, C. Mayer, N. Chawla, J. LLorca, A. Misra, J. M. Molina-Aldareguía. Thin Solid Films. In press.
[4] W. M. Mook, R. Raghavan, J. K. Baldwin, D. Frey, J. Michler, N. A. Mara, A. Misra. Mater. Res. Lett. 1 (2013) 102-108.
[5] M. Monclús, S. J. Zheng, J. R. Mayeur, I. J. Beyerlein, N. A. Mara, T. Polcar, J. LLorca, J. M. Molina-Aldareguía, APL Materials, 1 (2013) 052103.

The use of higher gradient theories during analysis of sub-micro-structures

W.H. Mueller, C. Liebold

Technische Universität Berlin, Institut für Mechanik, LKM, Einsteinufer 5, 13591 Berlin, Germany
wolfgang.h.mueller@tu-berlin.de

Experiments on micro-specimens have shown that the deformation behavior of materials can be size dependent. The size dependence for some materials is, for example, reflected in a stiffer elastic response on the sub-microscale. A quantitative understanding of the size effect is important during the design phase of micro- and nanosize systems which, for example, is accompanied by finite element (FE) simulations. In our research project higher-order theories of elasticity will be presented and used for the description of the bending behavior of micro-beams and micro-plates. These theories include additional material parameters in order to describe the size effect. Thus they go beyond the limits of the classical Boltzmann continuum. Special attention is paid to such non-local theories as the strain gradient- and the couple stress theory of linear elasticity. The latter is based on the ideas of E. and F. Cosserat (1909) by introducing an independent degree of freedom intrinsic to the material, named rotation.

We interpret the material points of a body as rigid particles. As a consequence we require only one material length scale parameter for connecting the rotation vector to the mathematical rotation of the displacement gradients. The objectives of the research project are to determine the material length scale parameter by analyzing experimental data obtained from force-displacement measurements on extremely small cantilever beams or plates with analytical as well as numerical analysis tools based on higher gradient theory. In particular, deflection measurements were performed and force data was recorded for submicron beams made of silicon and silicon nitride and for micro plates made of the polymer BCB. Simple beam bending and plate bending experiments were performed with decreasing thicknesses of the beams and plates. This is in line with the corresponding "method of size effect" from Lakes (1995). Bending rigidities and effective strains will be measureable in our labs with the help of atomic force microscopy and Raman spectroscopy, respectively.

The analytical solutions of Euler-Bernoulli beam theory or Kirchhoff plate theory incorporating the terms of higher gradient theory are presented. In contrast to existing work on the implementation of the superior strain gradient theory in terms of a finite element solution the crucial differential equation used here is consistently based on the balance of linear momentum and on the uncoupled balance of angular momentum. The resulting analytical formulae, the obtained data from the numerical modeling and the obtained data from the experiments could be used for evaluation of higher gradient coefficients. The developed variational formulation of the couple stress theory is implemented into an open-source finite element code, FEniCS©, using equidistantly distributed tetrahedral and continuous Lagrange elements with a polynomial degree of two in observance to the rank of the resulting elliptical partial differential equation. This novel open-source FE-software provides a collection of open-source packages for automated, efficient solutions of various differential equations. The experiments were performed by using a highly sensitive atomic force microscope (MV-1000 from Nanonics Imaging Ltd.). In addition, Raman spectroscopy was used for recording strains (Renishaw© RS). Raman spectroscopy takes advantage of the morphic effect in opaque materials: The spectroscopic detection of a modification in the characteristic phonon frequencies can be attributed to mechanical strains. These strain data could be used to fit the solutions of strain gradient theories.

Keynotes

Keynote 1

On the macroscopic Elasto-plastic response of metal-matrix composites

M. Agoras, R. Avazmohammadi, P. Ponte Castañeda

Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104-6315, USA
ponte@seas.upenn.edu

Keywords: Micromechanics, metal-ceramic composites, particle-shape effects, homogenization.

In this paper, we develop constitutive models for the macroscopic response of particle-reinforced composites consisting of an elastoplastic, metallic matrix and a random distribution of linear-elastic, ceramic particles. The proposed model makes use of the variational homogenization technique [1] to approximate the effective behavior of the nonlinear composite by means of that of a linear comparison composite (LCC) consisting of a linear viscoelastic matrix with a suitably chosen viscosity constant and the same particle phase as in the actual nonlinear composite. By making the approximation that the elastic strains in the LCC are uniform-per-phase, the homogenization problem for finding the effective behavior of the LCC becomes mathematically equivalent to the corresponding problem for "thermoelastic" composites with constant-per-phase thermal strains. This problem is solved by means of appropriate estimates [2] for the LCC, and an explicit time-discretization scheme is used to integrate the evolution equations describing the macroscopic constitutive response of the composite. For simplicity, we restrict our attention to the special case of incompressible composites consisting of an elastic-ideally plastic matrix and random distribution of aligned, ellipsoidal elastic particles. We propose an empirical modification of the model to improve its accuracy in the purely elastic regime, and we compare the results with recent results [3] for cyclic loading of particle-reinforced composites with spherical reinforcement. We then use of the model to investigate the effect of the particle shape, volume fraction and elastic modulus on the macroscopic response of the fiber-reinforced composites with spheroidal fibers subjected to general loading conditions.

References

[1] P. Ponte Castañeda, The effective mechanical properties of nonlinear isotropic composites, J. Mech. Phys. Solids 39 (1991) 45-71.

[2] P. Ponte Castañeda and J. R. Willis, The effect of spatial distribution on the effective behavior of composite materials and cracked media, J. Mech. Phys. Solids 43 (1995) 1919-1951.

[3] N. Lahellec and P. Suquet, Effective response and field statistics in elasto-plastic and elasto-viscoplastic composites under radial and non-radial loadings. Int. J. Plasticity 42 (2013) 1–30.

Keynote 2

On void growth in metal ceramic systems

Viggo Tvergaard

Department of Mechanical Engineering, Solid Mechanics
Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
mailto:viggo@mek.dtu.dk

The lecture will review a number of micromechanical studies for metal ceramic systems. Special focus will be given to cases where void growth in the metals is affected by the presence of a ceramic phase. This will include metals reinforced by short ceramic fibres, ceramics bonded by a thin metal layer, and ceramics reinforced by metal particles.

When aluminium alloys are reinforced by short SiC fibres, final failure often occurs by the growth of voids to coalescence. Voids can develop from porosity present in the metal initially, from debonding at the matrix-fibre interface, or from fibre fracture. A great deal of insight can be obtained from numerical studies considering a characteristic volume element, containing only one or a few fibres.

Brittle ceramics can be given increased toughness by adding ductile reinforcements. The effect of the reinforcements is that when bridging a crack in the brittle matrix, they will provide some of the properties of a ductile material. However, during the deformation of the ductile particles the surrounding ceramic will give a high constraint on plastic flow, which will result in a high stress triaxiality that has a strong effect on void growth. Studies of this type of behavior will be discussed, both for a modelled ductile particle and for a laboratory model of this type of material. Similar constraint on plastic flow will occur in thin metal layers used to bond two ceramic blocks. Also for such configurations the effect of the high stress triaxiality on void growth will be discussed.

Keynote 3

Crystal plasticity in fatigue

Georges Cailletaud[1], Stéphanie Basseville[2], Yoann Guilhem[3]

[1]CDM, MINES ParisTech, PSL Res. Univ.,CNRS UMR 7633, BP 87, 91003 Evry, France
[2]LISV, University of Versailles Saint-Quentin, 45 av. des Etats-Unis, 78000 Versailles, France
[3]LMT, ENS de Cachan, CNRS UMR 8535, 61 av. du Pdt Wilson, 94235 CACHAN Cedex, France
Georges.Cailletaud@mines-paristech.fr

Keywords: Fatigue crack initiation, surface effect, crystal plasticity, grain cluster effect, roughness effect.

Fatigue crack initiation in metallic alloys generally occurs at the surface of the material. The process is then linked with intrusion-extrusion phenomena produced by slip planes, this is why the purpose of most of the numerical studies at a microscale deal with crystallographic aspects. The question is to know in what extent stress and strain fields differ at the surface and in the bulk, how they are affected by grain size, or grain shape. The effect of grain clusters is also critical, since the local stress state can be influenced by the neighboring grains. Nevertheless, free surface effect depends also on the local geometry, and roughness comes into play, by introducing local stress concentrations that can be more critical than crystallographic effects. This presentation will provide a synthetic view on several studies that have characterized the local stress and strain fields in metallic polycrystals.

The main results are the following:
- It has been shown that the primary crystallographic orientation of a grain remains the most critical parameter for the evaluation of local fields, but there is a non negligible influence of the relative grain size and the shape of the surface grain: a “full”, or “closed” grain in a polycrystal behaves like an isolated grain, meanwhile a “open” grain, cut by the surface, will take its state from the surrounding grains [1].
- A new indicator characterizing intrusion/extrusion steps gives information on the initiation sites, and is compared with in-situ test results [2].
- The hydrostatic pressure is an interesting indicator in polycrystal aggregate computations.
- A full characterization of the local 3D fields allows us to exhibit the local patterns inside a material element, and to characterize the heterogeneity. The analysis involves surface maps and transparent volumetric views.
- The roughness effect is predominant in the first layer of surface grains even if the asperities are small with respect to grain size. A study of the competition between crystallographic influence and roughness effect is quantified by means of a new parameter. The way this parameter decreases gradually under the surface is shown [3].

References

[1] Y. Guilhem, S. Basseville, F. Curtit, J.-M. Stephan, G. Cailletaud, G., Investigation of the effect of grain clusters on fatigue crack initiation in polycrystals, Int. J. Of Fatigue, **32**, 2010, pp.1748-1763.
[2] Y. Guilhem, S. Basseville, F. Curtit, J.-M. Stephan, G. Cailletaud, Numerical investigations of the free surface effect in three-dimensional polycrystalline aggregates, Computational Materials Science, **70**, 2013, pp.150-162.
[3] Y. Guilhem, S. Basseville, H. Proudhon, G. Cailletaud, Influence of surface roughness on local mechanical fields in polycrystalline aggregates, Congrès Français de mécanique, CFM 2013, Bordeaux, France, 26-30 août 2013

Keynote 4

Implementation of a Cohesive Zone Model in History-Dependent Materials

L. Hakim[1], S.E. Mikhailov[2]

[1] Dept. of Computing, Imperial College London, London, SW7 2AZ, UK
[2] Dept. of Mathematical Sciences, Brunel University London, Uxbridge, UB8 3PH, UK
sergey.mikhailov@brunel.ac.uk

Keywords: Cohesive zone, Time dependent fracture, Abel integral equation, Viscoelasticity

A non-linear history-dependent cohesive zone model of crack propagation in linear elastic and visco-elastic materials is presented. The viscoelasticity is described by a linear Volterra integral operator in time. The normal stress on the cohesive zone satisfies the history dependent yield condition, given by a non-linear Abel-type integral operator presented in [1]. The crack starts propagating, breaking the cohesive zone, when the crack tip opening reaches a prescribed critical value. A numerical algorithm for computing the evolution of the crack and cohesive zone in time is discussed along with some numerical results obtained in [2].

References

[1] Mikhailov S. E., Namestnikova I. V. History-sensitive accumulation rules for life- time prediction under variable loading, *Archive of Applied Mechanics*, 81 (2011) 1679-1696.

[2] Hakim L., Mikhailov S.E.Numerical Implementation of a Cohesive Zone Model in History-Dependent Materials, arXiv:1403.3708, (2014) 1-26.

Keynote 5

Discrete to scale-dependent continua for complex materials. A generalized Voigt approach using the principle of virtual powers

Patrizia Trovalusci

Department of Structural and Geotechnical Engineering, *Sapienza*-University of Rome,
via Gramsci, 53, 00197 Rome, Italy
patrizia.trovalusci@uniroma1.it

Keywords: Composites, coarse-graining/homogenization, non-classical continua.

The mechanical behaviour of complex materials, characterised at finer scales by the presence of heterogeneities of significant size and texture, strongly depends on their microstructural features. By lacking in material internal scale parameters, the classical continuum does not always seem appropriate for describing the macroscopic behaviour of such materials, taking into account the size, the orientation and the disposition of the heterogeneities. This often calls for the need of non–classical continuum descriptions obtained through multiscale approaches aimed at deducing properties and relations by bridging information at proper underlying micro–level via energy equivalence criteria.

Firstly, focus will be on physically–based corpuscular–continuous models as originated by the molecular models developed in the 19th century to give explanations ‘per causas’ of elasticity [1]. Current researches in solid state physics as well as in mechanics of materials show that energy–equivalent continua obtained by defining direct links with lattice systems are still among the most promising approaches in material science [2]. The aim is then to point out the suitability of adopting discrete–continuous Voigt–like models, based on a generalization of the so-called Cauchy–Born rule used in crystal elasticity and in classical molecular theory of elasticity, in order to identify continua with additional degrees of freedom (micromorphic, multifield, etc.) which are essentially non–local models with internal length and dispersive properties and which, according to the definition in [3], are called ‘non–simple’ continua. It will be shown as microstructured continuous formulations can be derived within the general framework of the principle of virtual powers that, on the basis of a correspondence map relating the finite number of degrees of freedom of discrete models to the continuum kinematical fields, provides a guidance on the choice of the most appropriate continuum approximation for heterogeneous media, allowing us to point out in particular when the micropolar description is advantageous [4]. Some applications of the mentioned approach to fibre reinforced composite materials, ceramic matrix composites and masonry–like material will be reported and discussed.

References

[1] P. Trovalusci, Molecular approaches for multifield continua: origins and current developments, in T. Sadowski, P. Trovalusci (Eds.), *Multiscale Modeling of Complex Materials: Phenomenological, Theoretical and Computational Aspects,* CISM Series, 556, Springer, Berlin, 2014, pp. 211-278.

[2] P. Trovalusci, D. Capecchi and G. Ruta. Genesis of the multiscale approach for materials with microstructure. Arch. Appl. Mech. 79 (2009), pp. 981–997.

[3] G. Capriz, P. Podio-Guidugli. Whence the boundary conditions in modern continuum physics. In Atti dei Convegni Lincei, Vol. 210, 19–42, 2004.

[4] P. Trovalusci, A. Pau, Derivation of microstructured continua from lattice systems via principle of virtual works. The case of masonry-like materials as micropolar, second gradient and classical continua. *Acta Mech.*, 225 (2014), pp. 157-177.

Keynote 6

Multiscale approach to study deformation behaviour and designs of thermal barrier (protective) coatings

Panin S.V[1,2], Moiseenko D.D.[1], Lyukshin B.A.[1], Lyukshin P.A.[1], Sergeev V.P.[1,2] and Panin V.E.[1,2]

[1] Institute of Strength Physics and Materials Science SB RAS, Academicheskii Ave. 2/4, 634021, Tomsk, Russia,
[2] National Research Tomsk Polytechnic University, Lenin Ave, 30, 634050, Tomsk, Russia
svp@ispms.tsc.ru

Structure-heterogeneous materials and their reaction onto external loadings (being applied nonuniformly or in localized manner) are traditionally the objects of investigations within the concept of physical mesomechanics of materials. It is defined by hierarchy of stress concentrators to originate at their numerous interfaces under loading. "Coating-substrate" compositions are by definition objects of the inquiry of the physical mesomechanics that is related not only to wide practical interest of their design but also to possibility of physical modeling of the processes to occur in heterogeneous materials under loading.

From the materials science point of view there are two main directions of design coatings intended for operating under severe loadings: 1) protection against intensive mechanical affects which can consist of wear, impact loading, etc. (this problem can be successfully solved at the expense of formation of composite materials with a ductile matrix reinforced by (ultra)fine-dispersed phases (inclusions)); 2) protection against the thermal flows causing thermally induced degradation of the structure and properties of a coating as well as origination of discontinuities due to difference of the thermal expansion coefficients of coating and substrate materials (this problem can be solved by the development of new thermally stable materials of thermal-barrier coatings, as well by formation (deposition) of additional damping sublayers).

In the present work a representing set of results of theoretical and experimental investigations are described in order to illustrate the possibility of using the approach of the physical mesomechanics for design of the coating of these types. As the main statements used in the paper, it is necessary to note the following:

1) formation of nonflat "coating-substrate" interfaces is an effective way of redistribution of stress concentrators and allows to eliminate origination of adhesive and thermal fatigue cracks;

2) multiple cracking of coatings is the undesirable phenomenon, but in some cases allows to avoid the formation of the main through macrocracks and catastrophic fracture of composites;

3) formation of multilevel (hierarchical) structure in a coating under mechanical or thermal loading allows to involve in plastic deformation the significant amount of scale (structural)

levels, that, in the certain extent is related to the concept of adhesive-cohesive strength balance discussed in the literature;

4) formation of multilevel (hierarchical) structure in the "coating-substrate" compositions can be realized due to the high-frequency modulated mechanical effect or the radiation initiating the processes of mutual penetration, mass transfer and a "chess-like" distribution of stresses and deformations at internal interfaces.

A multi-level model of energy propagation along interfaces between the various structural elements of a solid with taking into account mutual energy transformations of various kinds was developed. An algorithm for calculating the local moments of forces is offeed for the case of material rotation and torsion. The relationship for the accumulated elastic energy is supplemented with a dissipation term. Numerical experiments were carried out on high-energy impact on polycrystalline copper specimens with different grain sizes. It is shown that during the nanostructuring of material surface layer, the dissipation of elastic energy gives rise to the rotation of structural elements. This makes it possible to prevent the occurrence of stress concentrators with peak values typical of coarse-grained specimens and reducing their mechanical properties.

The deformation behavior of thermal barrier coatings was investigated. The mechanism of occurring instabilities in such coatings based on their representation in the form of a plate located on an elastic foundation was studied. Loss of stability manifests itself in the form of a doubly periodic system of intrusion and extrusion zones that is qualitatively consistent with the well-known experimental results. Typical features of stability loss and its dependence on the properties of conjugated materials have been investigated by the example of the thermal loading simulation of the copper specimen with a protective ceramic coating. The influence of the thermo-mechanical properties anisotropy of the coating material on the character of the emerging instability has been estimated.

Section 1: Processing & Experiments

Monday 2nd of March, 2015

(S1-1 to S1-7)

Micromechanics determination of effective properties of voided magnetoelectroelastic materials

Jan Sladek[1], Vladimir Sladek[1], Slavomir Krahulec[1], Peter Solek[2]
[1] Institute of Construction and Architecture, Slovak Academy of Sciences, 84503 Bratislava, Slovakia
[2] Faculty of Mechanical Engineering, Slovak Technical University, Bratislava, Slovakia
jan.sladek@savba.sk

Keywords: Scaled boundary finite element method, 2-d problem, smart material.

Defects, cracks or voids are occurring very frequently in magnetoelectroelastic ceramics. The presence of voids affects material properties and functionality of these elements in smart structures. Modern smart structures made of piezoelectric and piezomagnetic materials offer certain potential performance advantages over conventional ones due to their capability of converting the energy from one type to other. For determination of influence of voids on material properties in a simplified case with uniform distribution of voids, it is efficient to analyze the representative volume element (RVE). This technique is frequently utilized in fiber reinforced composites. The same technique has been applied for determination of effective material properties in voided piezoelectric materials by Wang et al. [1].

The scaled boundary finite element method (SBFEM) developed by Song and Wolf [2] has emerged as a promising technique for analyzing general boundary value problems. It combines the main advantages of the finite element method and the boundary element method (BEM). In this method, only the boundary is discretized with elements leading to a reduction of spatial dimension by one and sparing the human and computational efforts in mesh generation. In contrast to the boundary element method, no fundamental solution is required, which permits to analyze general boundary value problems, where the conventional BEM cannot be applied due to missing fundamental solution. In this method, a scaling center O is selected at a point from which the whole boundary is directly visible. By scaling the boundary S in the radial direction with respect to the scaling center O with a scaling factor x which is smaller than 1 for bounded domain and larger than 1 for unbounded domain, the whole analyzed domain is covered. Applying either the weighted residual technique or virtual work principle for finite-element approximation along the boundary, the governing partial differential equations can be transformed into ordinary differential equations for displacements in elasticity with the radial coordinate x as an independent variable. Recently, Li et al. [3] have applied the SBFEM to crack analyses in piezoelectric composites. In the present paper the SBFEM is extended to problems of voided magnetoelectroelastic solids.

References

[1] H. Wang, G. Tan, S. Cen, Z. Yao, Numerical determination of effective properties of voided piezoelectric materials using BNM, Eng. Anal Bound. Elem. 29 (2005) 636–646.
[2] C. Song, J. Wolf, The scaled boundary finite-element method alias consistent infinitesimal finite-element cell method for elastodynamics, Computer Meth. Appl. Mech. Engn. 147 (1997) 329-355.
[3] C. Li, C. Song, H. Man, E.T. Ooi, W. Gao, 2D dynamic analysis of cracks and interface cracks in piezoelectric composites using the SBFEM, Int. J. Solids Struct. 51 (2014) 2096–2108.

Functional Role of Grain Boundaries in Hall-Petch Equation

V.E. Panin, D.D. Moiseenko, S.V. Panin

Institute of Strength Physics and Materials Science SB RAS, Akademicheskii av. 2/4, 634021, Tomsk, Russia
paninve@ispms.tsc.ru

Keywords: polycrystals, multiscale model, engineering of grain boundaries, Hall–Petch equation.

The behavior of a polycrystal is much commonly described using the empirical Hall–Petch equation $s = s_0 + kd^{-1/2}$ [1]. Classic interpretation of the Hall–Petch equation fits the single-scale approach in which the grain boundary in a 3D crystal is treated as a planar defect being a barrier to intragranular plastic dislocation motion [2].
The authors propose a multiscale model of deformed polycrystals according to which the basis for self-consistent deformation of grains is rotational wave flows of planar structural transformations at their boundaries. This approach to the description of a deformable solid treats grain boundaries in a polycrystal as an autonomous planar functional subsystem. At the grain boundaries, planar structural transformation flows develop generating strain-induced defect sources into the 3D crystal subsystem [3]. Such nonlinear planar structural transformation flows give rise to rotational moments and associated rotational deformation modes in the deformed polycrystal. Proposed multiscale excitable cellular automata method [4] allows simulating relay-race transfer of perturbations from one scale to another through explicitly accounting for local moments of forces and angular velocities of flows.
Computer-aided engineering of grain boundaries reveals two types of rotational wave flows defined by the misorientation angle of adjacent grains. Grain boundary flows of the first type develop at low-angle boundaries and feature low curvature. These flows generate dislocations in the grain bulk and the Hall–Petch equation for them has the form $s = s_0 + kd^{-1/2}$. Grain boundary flows of the second type develop at high-angle boundaries and feature high curvature. These flows generate curvature bands in the grain boundary and inject them into the grain bulk, resulting in fragmentation of grains and breakdown of translation invariance. For such self-consistency of grains in a polycrystal, the Hall–Petch equation has the form $s = s_0 + kd^{-1}$. Experimental data in support of the proposed multiscale model are presented.

The work was supported by projects of the Russian Foundation for Basic Research (Nos. 14-01-00789, 13-01-00403 and 13-08-90402) and Grant of the President of the Russian Federation for Support of Leading Scientific Schools (No. NSh 2817.2014.1).

References

[1] E.O. Hall, Deformation and Ageing of Mild Steel, *Proc. Phys. B*, **64** (1), 747–753, 1951.
[2] M. Meyers and K.K. Chawla, *Mechanical Behaviour of Materials*, Upper Saddle River, N-J: Prentice Hall Inc., 1999.
[3] V.E. Panin, V.E. Egorushkin and A.V. Panin, Nonlinear Wave Processes in a Deformable Solids as a Multiscale Hierarchically Organized System, *Physics-Uspekhi*, **55** (12), 1260–1267, 2012.
[4] D.D. Moiseenko, V.E. Panin and T.F. Elsukova. Role of Local Curvature in Grain Boundary Sliding in a Deformed Polycrystal, *Phys. Mesomech.*, **16** (4), 335–347, 2013.

Simulation of ablation for laser-matter-interaction on ceramic coatings with metal substrate

Peter Weidmann, Ulrich Weber, Siegfried Schmauder

Institute for Materials Testing, Materials Science and Strength of Materials (IMWF)
University of Stuttgart. Pfaffenwaldring 32, 70569 Stuttgart, Germany
peter.weidmann@imwf.uni-stuttgart.de

Key words: ablation, ceramic coating, laser-matter-interaction

Ceramic coatings are commonly used to improve the wear or heat resistance of many technical components. But due to their application process, i.e. plasma or high velocity oxygen fuel spraying, rather high residual stresses can build up within the coating and underneath. In order to determine these stresses it is possible to drill a hole into the component and measure the occurring deformations, which can be recalculated to get the governing residual stress. [1]

Normally these holes are drilled stepwise by a mechanical drill. But this procedure leads to a slow overall determination process and a direct contact between the drill and the specimen is unavoidable. To overcome these disadvantages, the mechanical drill shall be exchanged by a laser driven process. To investigate quality determining features, like the resulting surface topologies, a numerical solution of this specific laser-matter-interaction is required. Furthermore, aspects like heat expansion due to laser impact are, if at all, only measurable at great efforts.

The hereby presented numerical model allows the calculation of the laser induced surface heating, resulting ablation speed and temperature distribution. Therefore, a finite difference approach for an adaptive mesh is used while the model also considers temperature dependent material properties, the intensity absorbance which is related to the changing surface angle and the different material properties of coating and substrate. [2]

With the imposed model it will be possible to investigate influencing factors, i.e. the laser intensity distributions or material properties, and their effects on the evolving cutting hole geometry and temperature distribution during the cutting process. Hence, the cutting process can be optimized and possible sources of errors during the measurement of surface displacements can be excluded.

References

[1] Y.Y. Santana et. al., Measurement of residual stress in thermal spray coatings by the incremental hole drilling method, *Surface & Coatings Technology* **201**, 2092-2098, 2006.
[2] Michael F. Modest, Three-dimensional, transient model for laser machining of ablating/decomposing materials, *Int. J. Heat Mass Transfer* **39** (2), 221-234, 1996.

S1-4

In Situ Deformation of Metallic Interlayers

R. Hao, E. Saiz, B. Britton, F. Giuliani

Department of Materials, Imperial College London, UK
f.giuliani@imperial.ac.uk

Keywords: *In situ* testing, interlayers, SEM, laue

There are many interesting mechanical properties that can be achieved with metal/ceramic multilayers especially if they are defined more broadly to include structures such as MAX phases. However, the deformation mechanisms, such as hysteresis, can be complex. To simplify the problem, in this work we have concentrated on the effect of a single metal interlayer within a ceramic bi-crystal. The samples were produced by sputtering Niobium on to sapphire substrates and then diffusion bonding the two coated crystals together. This allowed the production of sapphire micropillars with containing a ~50-200 nm niobium layer. These were then loaded *in situ* within a microbeam laue set up. By varying the layer thickness the measured strength of the pillar could be varied along with the magnitude of the hysteresis. This hysteresis was tracked by the load-displacement trace along with the movement and elongation of diffraction spots associated with the interlayer.

Smoothed Particle Hydrodynamicssimulation of friction stir Welding

Dominik Hamann [1], Fabian Spreng [1], Peter Eberhard [1], Martin Werz [2], Siegfried Schmauder[2]

[1] Institute of Engineering and Computational Mechanics,University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany
[2] Institute for Materials Testing, Materials Science and Strength of Materials (IMWF),University of Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany
dominik.hamann@itm.uni-stuttgart.de

Keywords: Smoothed Particle Hydrodynamics, Friction Stir Welding

Friction Stir Welding (FSW) is increasingly used in industry. A tool stiring the workpiece by generating heat and transferring mechanical forces is shown in Fig. 1. This solid-state welding process works also for pairs of dissimilar materials like copper and aluminum. Due to large deformations and complex interdependencies of different physical effects, FSW is a challenging process to be modeled and, thus, gains more and more attention in engineering science. The program package Pasimodo is developed, which provides the particle-based simulation method Smoothed Particle Hydrodynamics (SPH). The SPH method is not limited by a mesh. However, for the simulation-based analysis of the FSW process, there is a need for modifications. For example, friction and plasticity as well as heat generation caused by dissipation have been enhanced and validated. Furthermore, adaptive discretization schemes, as shown in Fig. 2, were developed, used for the improvement of applications with high local stresses or discontinuities, typical characteristics of multi-phase composite materials and components influenced by material failure [1].

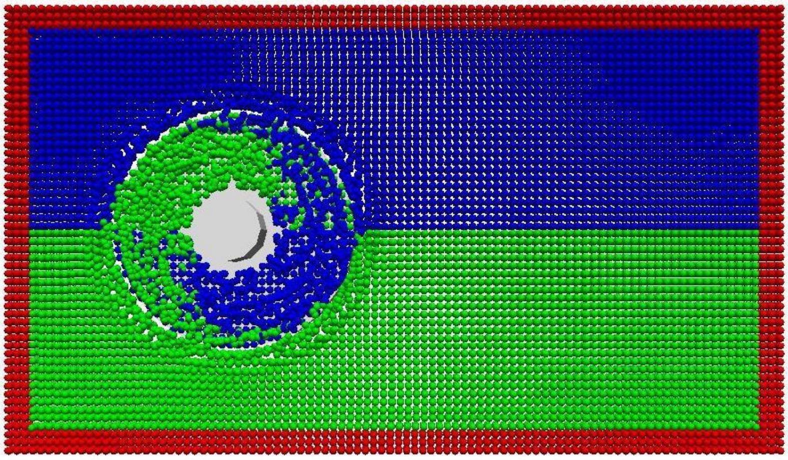


Figure 1: SPH simulation of a Friction Stir Welding process

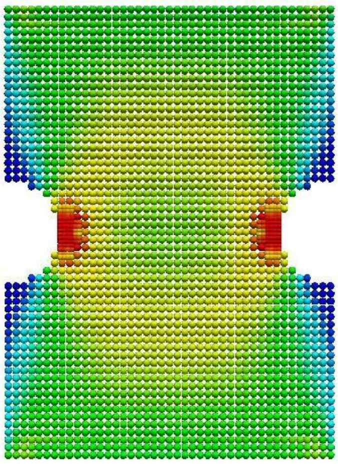


Figure 2: Notched tensile specimen with adaptive discretization [2]

References

[1] Schmauder, S.: Crack Growth in Multiphase Materials, Encyclopedia of Materials Science and Technology, Elsevier Science Ltd., pp. 1735-1741, 2001

[2] Spreng, F.; Schnabel, D.; Mueller, A.; Eberhard, P.: A local adaptive discretization algorithm for Smoothed Particle Hydrodynamics. Computational Particle Mechanics, Vol. 1, No. 2, pp. 131-145, 2014

S1-6

Prediction of fracture toughness of ceramic composites as function of microstructure

Min Zhou

The George W. Woodruff School of Mechanical Engineering, School of Materials Science and Engineering Georgia Institute of Technology, Atlanta, GA 30332-040, USA

min.zhou@gatech.edu

Keywords: ceramic composites, fracture toughness, prediction, microstructure.

Lower-scale structures determine the macro-scale fracture toughness of materials through the activation of different fracture and dissipation mechanisms. To tailor the fracture toughness through microstructure design, it is important to establish relations between microstructure and fracture toughness. To this end, systematic characterization of microstructures, explicit tracking of crack propagation process and realistic representation of deformation and fracture at different length scales are required. We present a cohesive finite element methods (CFEM) based multi-scale framework for predicting the fracture toughness of brittle materials such as ceramic composites and ductile materials such as alloys as a function of microstructure and basic material attributes. The framework does not involve curve fitting and accounts for the effects of microstructural heterogeneity, phase morphology, constituent behavior and interfacial bonding between constituents in materials. The approach uses the J-integral to calculate the initiation/propagation fracture toughness, allowing explicit representation of realistic microstructures and fundamental fracture mechanisms. Based on the CFEM results, a semi-empirical model is developed to provide a quantitative relation between the propagation toughness and statistical measures of microstructure, fracture mechanisms, and constituent and interfacial properties. The model provides deeper insights into the fracture process as it quantitatively predicts the proportion of each fracture mechanism in the heterogeneous microstructures. For example, to enhance the fracture toughness of two-phase ceramic composites, fine microstructure size scale, rounded reinforcement morphology and appropriately weak bonding strength should be introduced to promote interface debonding and discourage particle cracking. Another insight is that there are optimal levels of interfacial stiffness/toughness that maximize the fracture toughness. The relations and conclusions can be used in the selection of materials and the design of new materials with tailored properties.

References

[1]. Y. Li and M. Zhou, Prediction of Fracture Toughness of Ceramic Composites as a Function of Microstructure: I. Numerical Simulations, *Journal of the Mechanics and Physics of Solids*, **61**, 472–488, 2013.

[2]. Y. Li and M. Zhou, Prediction of Fracture Toughness of Ceramic Composites as a Function of Microstructure: II. Analytical Model, *Journal of the Mechanics and Physics of Solids*, **61**, 489–503, 2013.

Simulation of crack propagation on Al6061 laser welded joints

H. Y. Tu, S. Schmauder, U. Weber

Institute for Materials Testing, Materials Science and Strength of Materials (IMWF)
University of Stuttgart, D-70569 Stuttgart, Germany
haoyun.tu@imwf.uni-stuttgart.de

Keywords: Aluminum laser welded joints, Rousselier model, crack propagation, FE simulation

In this paper, the Rousselier damage model is used to investigate the fracture behavior of an Al6061 laser welded butt joint. Hardness test across the welded joints are performed at four different positions. The dimensions of different weld regions are fixed according to the hardness profile across the welded joint. Tensile tests of flat specimens extracted from the base material (BM), from the fusion zone (FZ) and from the heat affected zone (HAZ) are made. The mechanical properties of the different weld regions will be used as finite element model input in the simulation work. Metallographic investigations on the BM, the FZ and the HAZ are performed respectively and the initial void volume fraction (f_0) and the average void distance (l_c) are determined. Fracture toughness tests are performed on compact tension specimens (C(T)25 with reduced thickness B=6 mm) with the initial crack located in the BM (C(T)-BM), in the center of the FZ (C(T)-FZ) and at the interface between the FZ and the HAZ (C(T)-HAZ), respectively. The tensile test results of C(T) specimens are shown in the form of Force vs. Crack Opening Displacement (COD) and fracture resistance (J_R) curves.

Based on the metallographic information from the BM, the FZ and the HAZ, the Rousselier parameters (l_c, f_0, σ_k) are calibrated on the notched round specimens extracted from the BM, the FZ and the HAZ respectively. The same Rousselier parameter set is used to predict the crack propagation of C(T) specimens from the welded joints. Simulation results are compared to the experimental F-COD and J_R curves and very good agreement is found. The Rousselier model is also adopted to describe the strain variation and to predict the damage of the flat specimen under tensile test. In order to monitor the strain variation on the surface of the flat specimen extracted from Al6061 laser welded joints, the ARAMIS system is used during the tensile test process.

References

[1] G. Rousselier. Ductile fracture models and their potential in local approach of fracture. Nucl Eng Design 105 (1987), pp. 97-111

[2] P. Nègre, D. Steglich, W. Brocks. Crack extension in aluminium welds: a numerical approach using the Gurson-Tvergaard-Needleman model. Eng Fract Mech 71 (2003), pp. 2365-2383.

[3] P. Nègre, D. Steglich, W. Brocks. Crack extension at an interface: prediction of fracture toughness and simulation of crack path deviation Int J Fract 134 (2005), pp. 209-229.

[4] U. Mühlich, D. Steglich, J. Besson, W. Brocks. A User-Material Subroutine of the Rousselier-Model of Porous Metal Plasticity, GKSS Research Center, 2001.

[5] H. Y. Tu, S. Schmauder, U. Weber. Numerical simulation and experimental investigation of damage behaviour on Al6061 laser welded joints. Key Eng Mater 627 (2015), 105-108.

Section 2: Micromechanics of deformation and fracture

Tuesday 3rd of March, 2015

(S2-1 to S2-5)

A Comparison of Constitutive Models for Short Fibre Reinforced Brittle Materials

Heiko Herrmann[1,2]

[1]Institute of Cybernetics at Tallinn University of Technology,
Akadeemia tee 21, 12618 Tallinn, Estonia.
[2]Institute of Physics, Technische Universität Chemnitz,
Reichenhainer Str. 70, 09126 Chemnitz, Germany.
hh@cens.ioc.ee

Keywords: composite, constitutive modeling, fibres.

Many modern materials are composites with engineered properties, because theproperties of a single component are not sufficient for the given task. Quite often composites consist of a matrix material to which other phases are added. When improving the properties of a matrix material, the addition of short fibers has become very popular, there are many examples from glassfiber plastics over ceramics to building materials. The addition of short fibers often leads to anisotropic and sometimes inhomogeneous material properties, when the fiber orientation distribution is anisotropic and nonhomogeneous.

The fiber orientation distribution can influence mechanical properties like the Young's modulus or fracture toughness, and also thermal properties. In most cases, in the theoretical modeling, the fibers are considered to be straight (rodlike), if the actually used fibers have a different shape, like hooked ends or undulating, this is still approximated by a straight fiber. However, the influence of the, e.g., hooked ends can be noticeable, as will be demonstrated. This leads to the conclusion, that a different theoretical model is needed. Possible approaches will be discussed in the presentation.

Thermo-Elasticity in FGM Beams with Constrained Cross-Sections

Stephan Kugler[1], Justin Murin[2], Peter Fotiu[1], Dominik Haselbacher[1], Juraj Hrabovsky[2]

[1] Dep. of Applied an Numerical Mechanics, University of Applied Sciences in Wiener Neustadt, Wiener Neustadt, Austria
[2] Slovak University in Bratislava, Faculty of Electrical Engineering, Bratislava, Slovakia
kugler@fhwn.ac.at

Keywords: Thermo-Elasticity, FGM-Beams, Two-stage Algorithm, Homogenization.

Important classes of structural components within mechatronic devices made of **F**unctionally **G**raded **M**aterials (FGM) are beams and rods. A functionally graded material shows an arbitrary continuous or discontinuous variation of material properties in order to achieve specific functions and applications. Frequently, numerical analyses are carried out in a multi-physical regime such as thermo-elasticity or electro-thermo-elasticity, and many procedures and solution strategies are proposed by Murin and co-workers (see e.g. [1]). Superior algorithms can be found in literature (see [1] and references therein) to evaluate global solution variables such as deformations within beam structures made of FGMs. However, the analysis of a three-dimensional thermal stress state in constrained cross-sections like axisymmetric (see Fig. 1a)) or box-shaped cross-sections (see Fig. 1b)) is still an issue, if constitutive parameters like Young's modulus E and thermal expansion α show continuous or discontinuous (layer-wise) variations.

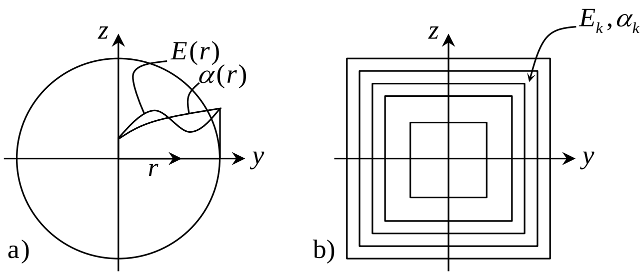


Fig. 1: Constrained cross-sections with continuous or discontinuous varying properties

In order to resolve that open question, here, a two stage algorithm is proposed. Within the first step global solution variables (displacements $u_z(x)$, bending angles $\varphi_y(x)$ and axial strain fields $\varepsilon_{xx}(x,z)$) are evaluated using beam elements. This rather classical step [1] incorporates suitable homogenization procedures to deal with specially varying constitutive parameters. The resulting axial strain field $\varepsilon_{xx}(x,z)=\varepsilon_0+\kappa z$ in connection with temperature elevations ΔT is the applied onto a finite element model of the cross-section causing internal loads. There, axial or planar symmetry conditions can be used in order to establish an effective analysis strategy. The solution of this second model delivers a three dimensional stress state which is in good agreement compared to three dimensional continuum approaches.

References

[1] V. Kutiš, J. Murín, R. Belák, J. Paulech, Beam element with spatial variation of material properties for multiphysics analysis of functionally graded materials, Computers & Structures, Volume 89, Issues 11–12, June 2011, Pages 1192-1205.

Scale effects in homogenization of metal matrix composites

S. Schindler[1], M. Zimmermann[2], J.C. Aurich[2], P. Steinmann[1]

[1]Chair of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
[2]Institute for Manufacturing Technology and Production Systems, University of Kaiserslautern, Germany
Stefan.Schindler@ltm.uni-erlangen.de

Keywords: multi-scale, scale effects, homogenization

In this contribution a multi-scale finite element model of mechanical and thermal properties of silicon particle reinforced aluminium is presented.

In a first step macroscopic thermal and elastic properties of a metal matrix composite (MMC) are determined from a micro-scale model by homogenization. Therefore a representative volume element (RVE) is designed for a homogeneous distribution of silicon particles inside an aluminium matrix. For both phases of the composite temperature dependent material properties are available from the literature. For the composite material properties are only available at room temperature. After a verification of the numerically determined elastic and thermal properties at room temperature, these can also be numerically determined for a large temperature range. The elastic and thermal behaviour is only dependent on the volume fraction of both components and not on the size of a single particle.

In a second step also the plasticity of the MMC is investigated. In contrast to the elastic and thermal behaviour, the plasticity depends not only on the volume fraction of the particles but also on their size. The conventional homogenization approach cannot consider those size effects. One approach to account for size effects on the microscopic scale has been presented in [1] for nonlinear elasticity. This approach is transferred to plasticity. The surfaces of the microscopic features, in this case the silicon particles, are endowed with their own (energetic) structure. The thereby defined surface energy causes a scale effect when homogenizing the microscopic stress response in order to determine the macroscopic stress response with a Hill-type averaging condition. The surface energy provides the possibility to adjust the numerically calculated yield stress to experimentally determined yield stresses of MMCs with various particle sizes.

In a third step the plasticity properties could be numerically extrapolated to high temperatures and high strain rates. At high strain rates almost adiabatic heating through dissipation takes place and consequently temperature dependent thermal properties are required.

References

[1] Javili et. al., Micro-to-macro transition for continua with surface structure at microscale, IJSS 50 (2013) 2561-2572.

Micro-scale modelling of metal ceramic composites behavior using statistical approach

Mikhail Tashkinov

Perm National Research Polytechnic University, Komsomolsky Ave. 29, Perm, Russia
m.tashkinov@pstu.ru

Keywords: boundary value problem, moment functions, microstructural characteristics, deformation and fracture, 3D modelling

One of the features of the metal ceramic composites is randomness of the geometrical and physical parameters of their internal microstructure. In general, this random distribution as well as such parameters as volume fraction of particles, orientation, shape, size and spatial distribution of inclusions can affect the indentation response of composites [1, 2].

One of the analytical methodology for investigation of the non-periodic randomly reinforced composites is based on statistical methods and the theory of random functions [3]. It implies that mechanical properties of microstructural components are defined with conventional phenomenological equations and criteria while the effective properties of composite and characteristics of its microscopic deformation fields are computed using the solutions of boundary value problems with piecewise constant coefficients equations. As the characteristics of the deformation processes for the components of the material, the multipoint statistical moments of the stochastic stress and strain fields are being used.

This work is devoted to development and implementation of such approach regarding to multicomponent metal ceramic composites. The 3D models of materials' representative volume elements (RVE) were built. Their microstructure was characterized with multipoint correlation functions. The approximated solutions of the boundary value problems in elastic and elastoplastic cases were obtained with the Green's functions method. These solutions along with the moment functions were used for deriving the analytical expressions for such statistical characteristics as mean values and dispersions (or first and second order moments) of stress fields in different components of composites. These moments were used for calculation of failure probability of the composites' phases under specified load.

The numerical results for the statistical characteristics were calculated for several specific types of composites' microstructure.

References

[1] S. Torquato Random heterogenous materials, microstructure and macroscopic properties. Springer, 2001.
[2] R. Ekici, M.K. Apalak, M. Yıldırım, F.Nair Effects of random particle dispersion and size on the indentation behavior of SiC particle reinforced metal matrix composites, Materials and Design 31 (2010) 2818–2833.
[3] M. Tashkinov Statistical characteristics of structural stochastic stress and strain fields in polydisperse heterogeneous solid media, Computational Materials Science 94 (2014) 44–50. DOI: 10.1016/j.commatsci.2014.01.050.

Mechanical aspects of deformation-induced roughening in surface-modified materials

Varvara Romanova[1,2], Ruslan Balokhonov[1,2], Olga Zinovieva[1,3],
[1]Institute of Strength Physics and Materials Science, Tomsk, Russia
[2]National Research Tomsk Polytechnic University, Tomsk, Russia
[3]National Research Tomsk State University, Tomsk, Russia
varvara@ispms.tsc.ru

Plastic deformation of metals is known to be accompanied by free surface roughening developing through all length scales. Comprehensive classification of the multiscale roughness patterns and pertinent mechanisms involved is given by Raabe et al. [1]. A specific surface pattern develops on a meso scale where whole grain groups are involved in cooperative motion to form surface valleys and ridges.

In the majority of engineering applications, surface roughening accompanied by multiscale plastic strain localization has an adverse effect on the material fatigue strength, wear resistance, adhesion, weldability, reflectability and other mechanical properties. It is a challenge, therefore, to develop efficient methods of roughening suppression, at least within certain scale range.

Experimental studies have shown that surface roughening may be somewhat affected by preliminary surface treatment by means of coating deposition or severe surface hardening. Yet, the conclusions drawn from the experiments for different materals and surface treatment techniques are contradictory. In comparison to the unhardened materials, surface under deformation is smoother in some cases and more roughened in others. What is more, surface modification leading to roughness suppression on a certain length scale may intensify its growth on the other scales [2].

While extensive experimental and theoretical studies along these lines have been done, the factors responsible for the resulting roughening patterns in surface-modified materials and pertinent mechanisms involved require to be explored yet. In this paper, we have numerically studied the surface hardening effect on the mesoscale surface roughening in uniaxial tension. Basing on the experimental findings, we have constructed three-dimensional microstructure-based constitutive models of the unhardened and surface-hardened polycrystalline specimens which mechanical behavior is analyzed numerically by a finite-difference method.

The results obtained suggest the following conclusions:

(1) Grain boundaries are the sources of stresses directed perpendicular to the axis of tension. Acting from the inside across the free surface, these stresses give rise to the surface out-of-plane displacements in the form of ridges and valleys.

(2) In the unhardened specimen, the surface roughness exhibits a well-defined pattern of two sets of folds. The finer surface folds are associated with the displacements of individual grains relative to each other and the larger ones referred to as mesoscale roughness are formed by grain ensembles involved in a cooperative motion.

(3) The surface-hardened layer moves the grain structure away from the free surface, thus suppressing the low-scale surface displacements and smoothing out the mesoscale ones. The thicker is the hardened layer, the lower are the normal stresses near the surface and the smoother is the surface relief.

(4) The presence of a hardened layer postpones roughness appearance and decreases its growth rate.

This work is partially supported by the Russian Science Foundation (14-19-00766), the Russian Foundation for Basic Research (14-08-00277-A) and a program to increase the competence of Tomsk Polytechnic University.

References

[1] D. Raabe et al., Acta Mater. 51 (2003) 1539-1560.
[2] A.V. Panin et al., Phys. Mesomech. 15 (2012). 94-106.

Section 3:

Functionally graded materials

Tuesday 3rd of March, 2015

(S3-1 to S3-4)

On vibrations of functionally graded metal-ceramic thin plates

Holm Altenbach[1], Victor A. Eremeyev[1,2]

[1] Otto von Guericke University Magdeburg, Universitätplatz 2, 39106 Magdeburg, Germany
[2] South Federal University and South Sci Center of RASci, Milchakova str, 8a,
Rostov on Don, Russia
holm.altenbach@ovgu.de

Keywords: Functionally graded plate, effective properties, vibrations

The paper addresses analysis of free and forced vibrations of functionally graded plates made of metal-ceramic composites. Such composites are popular in engineering and used, for example, as a thermal coating. Within the framework of the linear first order shear deformable plate theory with rotatory inertia [1, 2] we discuss the effective properties of the plates that is effective tangential and bending stiffness parameters. Since the distribution of material properties across the cross-section of the plate is non-homogeneous, in general, the stiffness parameters include also the stiffness tensor describing the coupling between in-plane and out-of-plane deformations. Here we restricted ourselves by isotropic material behaviour. The theory is supplemented by few examples of oscillations for rectangular and circular plates. The dispersion curves are obtained and analyzed for various boundary conditions and ceramic distribution law across the thickness of the plate.

In addition, using technique of [3] we discuss bounds for the spectrum of eigenfrequencies for plates of general shape in plane. In particular, considering the Rayleigh quotient we estimate the least eigenfrequency using the eigenfrequancies obtained for homogeneous plates and plates with various distributions of metal-ceramic across the plate thickness. This bounds are useful for rapid estimation of eigenfrequencies and vibrations of plates with complex law of ceramic distribution across the cross-section.

References

[1] H. Altenbach, V.A. Eremeyev, Direct approach based analysis of plates composed of functionally graded materials, *Arch. Appl. Mech*. 78 (2008) 775–794.
[2] H. Altenbach, V.A. Eremeyev, Eigen-vibrations of plates made of functionally graded material. *CMC: Computers, Materials, & Continua*, 9 (2009) 153–178.
[3] H. Altenbach, V.A. Eremeyev, Vibration analysis of non-linear 6-parameter prestressed shells, *Meccanica*, 49 (2014) 1751–1761.

Predictions in strength and fracture of sandwich composites under time varying loads

Vyacheslav N. Burlayenko[1], Tomasz Sadowski[2], Svetlana Dimitrova[1]

[1] National Technical University Kharkiv Polytechnic Institute, Kharkiv, Ukraine
[2] Lublin University of Technology, Lublin, Poland
burlayenko@yahoo.com

Keywords: Dynamic fracture, skin-to-core debond, sandwich plates, finite element analysis.

Skin-to-core debonding that implies the partial separation between the constitutive layers of composite three-layered sandwich material can threaten the structural integrity of a whole composite structure [1]. Time varying loads may promote the onset and evolution of the debond growth along the skin/core interface [2]. Consequently, a clear motivation exists for examining the skin-to-core interface strength and dynamic fracture process in sandwich materials to ensure their reliability and endurance in engineering applications.

Capacities available in commercial finite element analysis codes, such as ABAQUS® [3], enable simulations of skin/core debonding. The accuracy, however, of such simulations depends significantly on the adequacy between the finite model developed and the real fracture process being studied. The goal of this research is to evaluate the strength and to analyze in details the dynamic fracture of the skin-to-core interface of three-layered sandwich plates by using the finite element analysis within the ABAQUS code. The damage mechanics approach, implemented in ABAQUS through cohesive elements is applied to predict debonding fracture. The bilinear traction separation law is used to evaluate the damage initiation and to describe the damage growth which degrades the stiffness of the cohesive element according to the linear softening assumption. Due to mixed-mode loading in the skin-to-core interface, the criteria of debonding initiation and defending evolution are defined based on equivalent displacements. Herewith, the stress-based quadratic stress failure criterion specifies the onset and the energy-based Benzeggagh-Kenane fracture criterion governs the progression. Instead of time- and cost-consuming experimental tests to define interfacial strength and debond toughness used in fracture models of ABAQUS, virtual testing of standard fracture specimens for studied sandwich materials are carried out by using the finite element models of DCB, ENF and MMB standard fracture specimens. Two types of dynamic loading such as transient and harmonic forces were applied to sandwich plates with a pre-existing skin/core debond. The researches showed that debonding propagates in a stick-slip manner. It jumps from one arrest position to another one depending on the existing dynamic stress state at the current instant of time. Herewith, the dynamic stress state combines incident and reflecting stress waves that are generated by both the external loads and due to intermittent contact between the detached skin and core.

References

[1] L.A. Carlsson, G.A. Kardomateas, Structural and Failure Mechanics of Sandwich Composites, Springer Science+Business Media B.V., 2011.
[2] J. Lambros, A.J. Rosakis, An experimental study of dynamic delamination of thick fiber reinforced polymeric matrix composites, *J. Experimental Mechanics* **37 (1997)** 360-366.
[3] ABAQUS User Manual, ABAQUS Inc., Pawtucket, Rhode Island, USA, 2006.

BIEM modeling of elastic waves in a graded half-plane with position-dependent velocity containing cavities

Ioanna-Kleoniki Fontara[1], Petia Dineva[2], George Manolis[3] and Frank Wuttke[1]

[1] Institute of Applied Geoscience, Christian-Albrechts University of Kiel, Germany
[2] Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria.
[3] Department of Civil Engineering, Aristotle University, Thessaloniki, Greece
fontara@gpi.uni-kiel.de

Keywords: graded media, boundary elements method, wave propagation

Functionally graded media comprise a class of advanced materials because of 'smart' improvements over the more traditional ones such as those with layered structure. In general, wave motion in continuously inhomogeneous media with heterogeneities has multiple applications in fields such as seismic wave propagation in soils, sound waves in the ocean and ultrasonic non-destructive techniques for composite materials.
The aim of the present work is to develop, validate and to conduct intensive numerical simulations using an efficient boundary integral equation method (BIEM) for the anti-plane strain dynamic problem involving a graded half-plane with multiple cavities. This heterogeneous continuum is subjected to either incident, time-harmonic SH waves or to body waves radiating from a point source. Two different types of material gradient are considered: (a) type A, where the material is pure elastic, but the density $\rho(x_2)$ and shear modulus $\mu(x_2)$ vary proportionally in quadratic way in respect to the depth, and in this case the phase velocity is constant, see Ref. [1]; (b) type B, where the material is viscoelastic of Kelvin-Voigt type with the shear modulus and density varying with respect to the spatial coordinates in arbitrary fashion, so that the phase velocity is both frequency and position–dependent, see Ref. [2]. For the above mentioned types of material gradient, two different frequency dependent BIEM schemes are developed based on (a) the Green's function for quadratically graded half-plane in the case of material profile of type A; (b) fundamental solution for the full plane in the case of material profile of type B. The system of BIEs is solved in respect to displacements along all boundaries by using standard discretization and collocation techniques.
In terms of results, we consider a number of anti-plane strain elastodynamic problems for a graded half-plane containing an arbitrary number of cavities with different shapes and location. These are solved via the frequency dependent BIEM. The results reveal the sensitivity of the elastic wave field to the following key factors: type and characteristics of the material gradient, type and characteristics of the applied load, shape, position and number of cavities, interaction between cavities and cavity-free surface interaction.

References

[1] Wuttke F, Fontara I-K, Dineva P, Rangelov T. SH-wave propagation in a continuously inhomogeneous half-plane with free-surface relief by BIEM. ZAMM (2014) 1 – 16 / DOI 10.1002/zamm.201300198.
[2] Karakostas CZ, Manolis GD. Transient signal simulation due to explosion in heterogeneous soil media. The International Journal of BEM Communications (1997) 8:160-167.

Modeling of brittle fracture of functionally graded coatings subject to thermo-mechanical loading

Vera Petrova [1,2], Siegfried Schmauder [1]

[1]Institute for Materials Testing, Materials Science and Strength of Materials (IMWF)
University of Stuttgart, D-70569 Stuttgart, Germany
[2] Voronezh State University, University Sq.1, Voronezh, 394006, Russia
veraep@gmail.com

Keywords: Thermal Fracture, Functionally Graded Material, Singular Integral Equations, Stress Intensity Factors

The work is devoted to the problem of thermal fracture of functionally graded coatings (FGCs) on a homogeneous substrate (semi-infinite medium). The specimen is under the influence of thermal loading (residual thermal stresses due to sudden cooling) and mechanical loading (tension). It is supposed that arbitrarily located cracks are placed in the FGC. In the present formulation we assume that the thermal and mechanical properties are continuous functions of the thickness coordinate and different models for FGMs are used, e.g., exponential function, power-law function and the rule of mixture based on the volume fraction of materials.

The problem is formulated by means of singular integral equations. The solution of the equations is obtained numerically. Similar methods of singular integral equations were used for the study of thermal fracture of FGC/homogeneous structures due to residual stresses arising during the cooling process and caused by non-uniform coefficients of thermal expansion of the constituent materials (see, for example, [1]). These stresses were accounted as additional stresses on the crack surfaces. Some results for an FGC were obtained also in [2]. This method is applicable when the material gradation of the FGM is not steep.

After the solution of the thermo-elastic problem the stress intensity factors at the crack tips are obtained as well as fracture angles (the direction of initial crack propagation). Then, the influence of geometry of the problem and material non-homogeneity on the stress intensity factors is analyzed. These models for functionally graded materials in combination with a detailed parametric analysis can help to optimize gradation of the FGC (material parameters) and structure (geometrical parameters) in order to improve the fracture resistance of FGC/homogeneous systems. Some examples of real material combinations for FGCs (ceramic/ceramic and ceramic/metal) are discussed.

References

[1] A.M. Afsar, H. Sekine, Crack spacing effect on the brittle fracture characteristics of semi-infinite functionally graded materials with periodic edge cracks. Int. J. Fract. 102 (2000) L61–L66.
[2] V. Petrova, T. Sadowski, Theoretical modeling and analysis of thermal fracture of semi-infinite functionally graded materials with edge cracks, Meccanica 49 (2014) 2603–2615.

Section 4:

Fracture and failure I

Wednesday 4th of March, 2015

(S4-1 to S4-8)

Modified cohesive zone models for high speed dynamic fracture of ductile materials

Chong-Qing Ru

Department of Mechanical Engineering
University of Alberta, Edmonton, Canada T6G 2G8
cru@ualberta.ca

In this presentation, a new cohesive zone model is proposed to study the inertia effect of cohesive zone which has not been considered in existing cohesive zone models. This new model predicts a terminal limiting crack speed comparable to the observed terminal crack speed of some ductile materials. On the other hand, a strain rate-dependent cohesive zone model and related finite element model (FEM) are developed to analyze speed-dependent dynamic fracture of pipeline steels observed in recent tests. The FEM results showed that the strain rate-effects could be largely responsible for the observed speed-dependent dynamic fracture phenomena of pipeline steels. The presented theoretical and numerical models can be used to simulate high speed fracture of pipeline steels especially when the related experiments are difficult or too expensive.

The effect of composite polycrystalline microstructure on the deformation and fracture of aluminum alloys with friction stir welds. Numerical simulation

R.R. Balokhonov [1,2], V.A. Romanova [1,2], A.V. Zinoviev [1], S.A. Martynov [1], O.S. Zinovieva [1]

[1] Institute of Strength Physics and Materials Science, SB, RAS, 634021, Tomsk, Russia
[2] National Research Tomsk Polytechnic University, 634050, Tomsk, Russia
rusy@ispms.tsc.ru

Keywords: computational mesomechanics, microstructure, fracture, polycrystals

Mesomechanical numerical analysis [1] of the microstructure effect in deformation and fracture of a high-strength aluminum alloy with the friction stir weld is presented. The simulated polycrystalline microstructures (Fig.1) correspond to the microstructures found experimentally in different weld zones: weld nugget, thermo-mechanically affected zones (TMAZ) both at retreating and advancing sides (Fig.2).

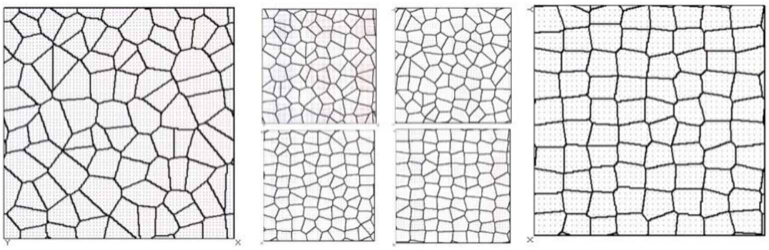


Fig.1 Model microstructures with different orientations observed in the nugget and TMAZ.

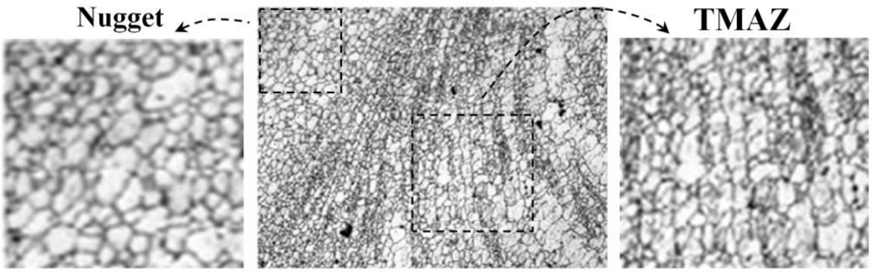


Fig.2 Microstructure in the nugget and TMAZ at the advancing side of the weld [2].

Macromechanical strength of local mesovolumes in different zones and plastic strain localization and fracture patterns are shown to depend on the microstructure parameters.

This work is supported by the Ministry of Education and Science of the Russian Federation (ID №RFMEFI57814X0045).

References

1. R.R. Balokhonov, V.A. Romanova, S. Schmauder, S.A. Martynov, Zh.G. Kovalevskaya, A mesomechanical analysis of plastic strain and fracture localization in a material with a bilayer coating, Composites: Part B. 66 (2014) 276–286.
2. M. Dumont, A. Steuwer, A. Deschamps, M. Peel, P.J. Withers Microstructure mapping in friction stir welds of 7449 aluminium alloy using SAXS. Acta Materialia, 54 (2006) 4793–4801.

Delamination of functionally graded thin films on elastic substrates

Marco Paggi[1], José Reinoso[1,2,3]

[1] IMT Institute for Advanced Studies Lucca, Piazza San Francesco 19, 55100 Lucca, Italy
[2] Institute of Structural Analysis, Leibniz Universität Hannover, Appelstr. 9A, 30167, Germany
[3] Group of Elasticity and Strength of Materials, University of Seville, Camino de los Descubrimientos, 41092, Seville, Spain
marco.paggi@imtlucca.it

Keywords: Multilayered graded structures, Delamination, Cohesive Zone Model, Nonlinear FEM, Thin films

Stiff films on substrates are used in a wide range of technological applications such as electronic devices [1,2], thermal coatings [1], shield engine blades, among many others. These substrates can be coated with different typologies of thin films. In particular, Functionally Graded Materials (FGMs) with a heterogeneous composition are generally incorporated in such applications through a combination of metallic and ceramic phases. This metallic-ceramic grading is particularly beneficial in case of heat-transfer barrier coatings that have to withstand severe thermo-elastic deformations [3]. However, delamination of thin films from the substrate to which they are attached to is one of the most prominent failure modes that remarkably affect their reliability and practicability. In this regard, to date, most of the studies on fracture mechanics of FGM coatings have almost been focusing on two-dimensional analyses under the assumptions of linear elasticity and small displacements, so that linear elastic fracture mechanics can be employed and, in some cases, semi-closed form solutions [1,4] or simple finite element schemes [1,2,5] can be proposed.

In the present study, aiming at investigating the phenomenon of delamination of thin FGM layers from elastic substrates, we propose a general nonlinear computational framework that comprises nonlinear fracture mechanics based on a novel interface element formulation undergoing large displacements [6]. Due to the nonlinear character of the problem under investigation, in the three-dimensional setting, a large-displacement continuum shell element with grading of the elastic properties over its thickness is developed as a generalization of [7]. This shell element is then coupled with the nonlinear three-dimensional interface element for large displacement analyses, assuring a perfect kinematic compatibility between both element topologies. Through the use of the developed numerical tools, a comprehensive numerical investigation of such delamination problems is carried out, paying a special attention to the investigation of the potential postbuckling and wrinkling induced failures as in [2].

References

[1] Choi, S.R., Hutchinson, J.W., Evans, A.G., Delamination of multilayer thermal barrier coatings, Mech. Mat., 31, 431–447 (1999).
[2] Mei, H., Landis, C.M., Huang, R., Concomitant wrinkling and buckle-delamination of elastic thin films on compliant substrates, Mech. Mat., 43, 627–642 (2011).
[3] Carpinteri, A., Paggi, M., Thermo-elastic mismatch in nonhomogeneous beams, J. Eng. Math., 61, 371–384 (2008).
[4] Erdogan, F., Fracture mechanics of functionally graded materials, Compos. Eng., 7, 753–770 (1995).
[5] Kim, J.-H., Paulino, G.H., Mixed-mode fracture of orthotropic functionally graded materials using finite elements and the modified crack closure method, Eng. Fract. Mech., 69, 1557–1586 (2002).
[6] Reinoso, J., Paggi, M., A consistent interface element formulation for geometrical and material nonlinearities, Comp. Mech., in press, doi:10.1007/s00466-014-1077-2.
[7] Bischoff, M., Ramm, E., Shear deformable shell elements for large strains and rotations, Int. J. Num. Meth. Eng., 40, 4427–4449 (1997).

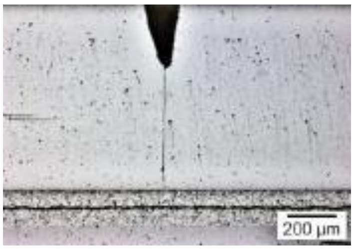
Application of a coupled stress-energy criterion to model the crack propagation in ceramic laminates with compressive embedded layers.

D. Leguillon[1], O. Sevecek[2], E. Martin[3], R. Bermejo[4]

[1] Institut Jean le Rond d'Alembert, CNRS UMR 7190, Sorbonne Universités, UPMC Université Paris 06, F-75005 Paris, France.
[2] Institute of Solid Mechanics, Mechatronics and Biomechanics, Faculty of Mechanical Engineering, Brno University of Technology, 616 69 Brno, Czech Republic.
[3] Laboratoire des Composites Thermo-Structuraux, CNRS UMR 5801,Université de Bordeaux, F-33600 Pessac, France.
[4] Institut für Struktur und Funktionskeramik, Montanuniversität Leoben, A-8700 Leoben, Austria.
dominique.leguillon@upmc.fr

Keywords: Ceramic laminates, residual stresses, fracture mechanics.

One novel approach to improve the apparent toughness of ceramics is to fabricate laminates promoting surface crack deflection in order to delay the final fracture of the whole structure. This can be achieved using weak interfaces by adding a material as a fuse (pyrocarbon, porous layer) or utilizing strong interfaces to create compressive residual stresses in embedded layers in order to trap or deflect these surface cracks.



Four-point bending tests were conducted on V-notched laminates made of alumina-based ceramics to demonstrate the effect of the compressive layers on the propagation of surface cracks [1]. Depending on the v-notch depth, a crack was observed to initiate at the root of the notch either directly after cooling when processing the notch or later under the mechanical loading. In both cases, following this nucleation, the crack penetrates the compressive layer on a short length, then stops.

The aim of this work is to show that the coupled stress-energy criterion [2,3] can predict these mechanisms in a fairly accurate way. This criterion states that crack onset occurs if two conditions are fulfilled simultaneously, the first one specifies that there is enough available energy to create a crack and the second that the tensile stress is greater than the tensile strength all along the expected crack path. A particular feature, derived from the theory and in agreement with observations, is that the crack appears abruptly and jumps a given length.

According to this criterion, the role of the v-notch depth can be analyzed. It is shown that beyond a critical depth, crack nucleation occurs spontaneously after the cooling phase when processing the notch and is unstable: the crack passes entirely through the first layer. Moreover, it is possible to predict the crack penetration length in the next compressive layer.

References

[1] Bermejo R., Torres Y., Sanchez-Herencia A.J., Baudin C., Anglada M., Llanes L., Residual stresses, strength and toughness of laminates with different layer thickness ratios, Acta Mater. 54 (2006) 4745-4757.

[2] Leguillon D., Strength or toughness? A criterion for crack onset at a notch, Eur. J. Mech. – A/Solids 21 (2002) 61-72.

[3] Martin E., Leguillon D., Energetic conditions for interfacial failure in the vicinity of a matrix crack in brittle matrix composites, Int. J. Solids Structures 41 (2004) 6937-6948.

Homogenization via unfolding in periodic elasticity with contact on closed and open cracks.

Julia Orlik, Vladimir Shiryaev

Fraunhofer ITWM, Fraunhoferplatz 1, 67663 Kaiserslautern, Germany
orlik@itwm.fhg.de

Keywords: Homogenization, periodic cracks, debonded inclusions.

We consider the elasticity problem in a heterogeneous domain with a periodic micro-structure, including multiple micro-contacts between the structural components. These components can be a simply connected matrix domain with open cracks or inclusions completely surrounded by cracks, which do not touch the outer boundary. The contacts are described by the Signorini and friction contact conditions. The Signorini condition is described mathematically by a closed convex cone, while the friction condition is a nonlinear convex functional over the interface jump of the solution on the oscillating interface. The difficulties appear when the inclusions are completely surrounded by cracks and can have rigid displacements. In this case, in order to obtain preliminary estimates for the solution in the periodic domain, the Korn inequality should be modified, first in the fixed context and then for the periodic case. Additionally, for all states of the contact (inclusions can freely move, or are locked/stuck to the interface with the matrix, or the frictional traction is achieved on the inclusion-matrix interface and the inclusions can slide in the tangential to the interface direction) we obtain estimates for the solution in the periodic domain uniform with respect to the small parameter, denoting the period of the structure. An asymptotic analysis for the nonlinear functionals over the growing interface is carried out, based on the application of the periodic unfolding method for sequences of jumps of the solution on the oscillating interface. This allows to obtain the homogenized limit elasto-plastic problem. The algorithm is illustrated by a numerical result (application to technical textiles).

References

[1] D. Cioranescu, A. Damlamian, J. Orlik, Homogenization via unfolding in periodic elasticity with contact on closed and open cracks, Asymptotic Analysis, volume 82, issue 3-4, 2013

[2] V. Shiryaev, J. Orlik, Modelling and design optimization of textiles via homogenization, Proc.Appl. Math. Mech., 14 (2014).

Multiscale Modeling of Mechanical Properties of Particle-reinforced Aluminum-Based Metal-Matrix composites

Sergey Lurie[1], Dmitrii Volkov-Bogorodskii [1], Yuri Soliaev [1], Ragudin Rizachanov [2], Leonid Agureev [2]

[1] Institute of Applied Mechanics of RAS, Leningradskii pr. 7. Moscow, Russia
[2] Keldysh Research Centre -State Research Centre of RF, Onegskaya str. 8. Moscow, Russia

salurie@mail.ru

Keywords: Metal-matrix composites, gradient elasticity, scale effects.

In the work the dependence of the young's modulus and strength of aluminum-based metal-matrix composites by volume fraction and size of carbide and oxide dispersed inclusions. we consider the metal-matrix composites reinforced by the micro/nanoscale inclusions of silicon carbide with a large volume fractions, as well as composites containing extremely low volume fraction of oxide inclusions (<0.15%) with the size of inclusions 1-100 microns. We simulated experimental non-monotonic dependences of the mechanical properties from the bulk contents and size of inclusions, which reflect the large-scale effects.

We study the effective properties and stress state of the filled aluminum-based metal-matrix composites with spherical inclusions and take into account the the porosity and clustering capabilities inclusions.

The generalized gradient theories are involved to describe the anomalous behavior of materials with rich internal structural heterogeneity [1]. It was used the accurate solution of the Christensen-Eshelby problem for gradient elasticity connected with definition of the effective characteristics of the composites reinforced with spherical inclusions. This solution was received on the basis of the Eshelby integral representation generalized for gradient models [2].

Modeling of the experimentally observed effects of scale amplification of strength characteristics of metal-matrix composites depending on the volume fractions of particles on the basis of gradient elasticity, self-consistent method of three and four spherical phases and the method of radial factors are given in the work.

Also employed model of multilayer inclusions and finite element method for modeling in the framework of classical theory of elasticity. We use simulation results to determine the size range of inclusions where it is possible to use the classical methods of modeling. Based on a comparison with experimental data the additional parameters non-classical models are determined that help to explain the impact of scale effects (the size of the inclusions) on the properties of composites.

References

[1] S. Lurie, D. Volkov-Bogorodsky, V. Zubov, N. Tuchkova, Advanced theoretical and numerical multiscale modeling of cohesion/adhesion interactions in continuum mechanics, Comp. Mater. Sc. 45(3) (2009) 709-714

[2] S. Lurie, D. Volkov-Bogorodsky, A. Leontiev, E.Aifantis, Eshelby's inclusion problem in the gradient theory of elasticity. Int. J. Eng. Sci. 49 (2011) 1517-1525

Initiation and Propagation of Local Curvature at Grain Boundaries during Intergranural Sliding in Deformed Polycrystal

D.D. Moiseenko, V.E. Panin, P.V. Maksimov

Institute of Strength Physics and Materials Science SB RAS, Akademicheskii av. 2/4, 634021, Tomsk, Russia
mdd@ispms.tsc.ru

Keywords: physical mesomechanics, structure curvature, open systems, grain boundaries, computer simulation, cellular automata.

According to physical mesomechanics, initial plastic flow in a deformed polycrystal is related to clustered nonlinear wave-like flows of atoms in surface layers and to grain boundary sliding [1]. The analytical theory of such flows [2] describes them as nonlinear waves of local structural transformations that strongly depend on curvature of flux. It is very important because curvature of grain boundary flow causes the generation of deformation defects at grain boundaries. Moreover, high curvature of grain boundary flow leads to a crack nucleation and material fracture. A new original method of excitable cellular automata (ECA) [3] is developed to describe the propagation of rotational-wave defect flows. The method is intended for the simulation of processes in which local moments of forces are taken into account and could not be described in the framework of classic methods. An essential feature of the proposed approach is that an active element describes not a discrete mesovolume of the material but a fixed region of space through which the material flows. This concept opens up new avenues for the numerical simulation of flows of matter and energy of different origin.

A network of active elements that make up a specimen is divided into clusters, each of which models a grain with its own lattice orientation with the Eulerian angles, and grain boundaries are explicitly taken into account according to their misorientation angles. The developed algorithm for the simulation of mechanical energy transfer was supplemented with the procedure of calculating the vectors of moments of forces acting on a local mesovolume.

Dynamics of matter and energy flows along grain boundaries is studied using ECA method. It is shown that these flows have a rotational-wave nature and depend on the loading conditions of a grain boundary. All theoretical investigations are in good agreement with experiment.

The work was supported by projects of the Presidium RAS Program No.25, the Russian Foundation for Basic Research (Nos. 14-01-00789, 13-01-00403, 13-08-00616 and 13-08-90402) and Grant of the President of the Russian Federation for Support of Leading Scientific Schools (No. NSh 2817.2014.1).

References

[1] V.E. Panin, V.E. Egorushkin and A.V. Panin, Nonlinear Wave Processes in a Deformable Solids as a Multiscale Hierarchically Organized System, *Physics-Uspekhi*, **55** (12), 1260–1267, 2012.

[2] V.E. Egorushkin, Dynamics of Plastic Deformation: Waves of Localized Plastic Deformation in Solids, *Russ. Phys. J.*, **35** (4), 316-334, 1992.

[3] D.D. Moiseenko, Yu.I. Pochivalov, P.V. Maksimov and V.E. Panin, Rotational Deformation Modes in Near-boundary Regions of Grain Structure in a Loaded Polycrystal, *Phys. Mesomech.*, **16** (3), 248–258, 2013.

Three collinear cracks interaction in pre-stressed elastic composites

E.M. Craciun, T. Sadowski, A. Rabaea, L.Marsavina

Crack initiation at a crack tip, propagation direction, cracks tip elds and cracks interaction in static orthotropic plane linear elasticity are the main themes for mathematical modeling and simulation and represent important problems of Fracture mechanics. Assume that the admissible equilibrium states of the body are plane strain states relative to Ox1x2 plane. In this case the equilibrium states of the material can be represented by two complex potentials de ned in two complex planes. We shall use Guz's representation of the elastic state, without initial deformation, in a weakly modifed form due to Soos.
Our first aim is to determine the elastic state produced in the body using complex potentials. We suppose that our material is unbounded and contains three equal and collinear cracks situated in the same plane Ox1x2. The cracks faces are acted by normal stresses, symmetrically distributed relative to the plane containing the cracks. We formulate and give the solution of the mathematical problem, assuming that the applied normal stresses have a given constant value. The elastic state produced in the body is determined using the theory of Riemann-Hilbert problem by complex potentials.
Our second aim is to find which tip of the cracks will start to propagate first. To do this we determine singular parts of the elastic states near the cracks tips using the asymptotic method. Several fracture criteria have been suggested in the literature. Our third aim is to extend one of the first from these criteria, named maximum tangential stress criterion (MTS) due to Erdogan and Sih and to find which tip will propagate first. For doing this we consider as an example two configuration of three equal and collinear cracks in a Graphite-epoxy fiber reinforced elastic composite. Using numerical computations we determine that:
In the case when the distance between the cracks is much smaller than their length, i.e There exist a strong interaction between the cracks, first start to propagate inner tips of the cracks and cracks tend to unify;
- In the case when the distance between the cracks is much greater than their length, i.e.there exist a weak interaction between the cracks and all cracks start to propagate almost in the same time.

Section 5:

Bio/Nano Materials

Wednesday 4th of March, 2015

(S5-1 to S5-6)

Nanostructuring of interfaces in composites: Computational analysis of reserves of materials optimization

Leon Mischnaevsky Jr.

Department of Wind Energy, Technical University of Denmark, Risø Campus, Roskilde, Denmark
lemi@dtu.dk

Keywords: Nanocomposites; Interfaces; Micromechanics; Computational modelling

Mechanical properties and strength of materials can be enhanced by modifying the structures of the materials at micro- and nanoscales. One of the promising directions of the materials modification for the properties enhancement is based on the control and modification of interface properties. Interfaces, phase and grain boundaries represent often relatively instable and deformable regions of materials. The introduction of geometrical structural inhomogeneities (e.g., defects or nanoparticles) into instable phases allows to control the local stress concentration and to channels the deformation energy into the lower scale level. Thus, nanomodification of weak regions and structural defects can be used to influence the damage evolution and improve the damage resistance of the material. A series of computational micromechanical studies of the effect of nanostructuring and nanoengineering of interfaces, phase and grain boundaries of materials on the mechanical properties and strength of composite materials was carried at the DTU Wind Energy. We considered several groups of materials (composites, nanocomposites, nanocrystalline metals, wood) and explored (using numerical experiments [1-4]) how the interface structures influences the properties of the materials. Figure 1 shows an example of hierarchical FE model of a composite with nanoreinforced interphase/interface layer [1-2]. In the simulations, it was demonstrated that the availability of special structures in grain boundaries/phase boundaries/interfaces represents an important and promising source of the enhancement of the materials strength.

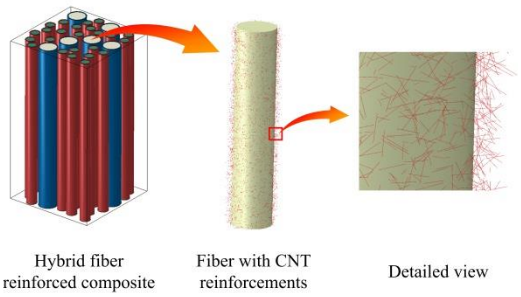


Figure 1. Schema of the multiscale modelling of CNT reinforced hybrid composites

References

[1] L. Mishnaevsky Jr., G.Dai, Hybrid and hierarchical nanoreinforced composites, Composite Structures, 117 (2014) 156–168

[2] L. Mishnaevsky Jr., Nanostructured interfaces for enhancing mechanical properties of materials, Composites Part B, 68 (2015) 75–84

[3] G. M. Dai, L. Mishnaevsky Jr., Fatigue of multiscale composites with secondary nanoplatelet reinforcement, Composites Sci. Technol.91 (2014) 71-81

[4] G.M. Dai, L. Mishnaevsky Jr., Graphene monolayer nanocomposites: 3D simulation of damage and fracture, Computational Materials Science, Vol. 95, 2014, pp. 684–692

Hydrogen enhanced slip plane fracture in alpha iron

Shinya Taketomi[1], Ryosuke Matsumoto[2], Seiya Hagihara[1]

[1] Dept. of Mechanical Engineering, Saga University, 1 Honjo-machi, Saga, 840-8502, Japan
[2] Dept. of Mechanical Engineering and Science, Kyoto University, Kyoto daigaku-katsura, Nishikyo-ku, Kyoto, 615-8530, Japan
taketomi@me.saga-u.ac.jp

Keywords: Slip plane fracture, Hydrogen embrittlement, Molecular statics, Gilman crack

Steel sometimes reveals trans-granular fracture surface in the presence of hydrogen which is known as typical feature of hydrogen embrittlement(HE). Molecular dynamics analyses for alpha iron also show that the crack propagation occurs at the slip plane[1]. However, the slip plane fracture enhancement due to hydrogen is still unclear. In this study, we investigated the effect of dislocation density and hydrogen concentration on the surface formation energy around the dislocation core using the Molecular statics method. EAM potential[2] is adopted as an interatomic potential. The results show that increasing the dislocation density, the surface formation energy decrease. This decrement mainly attribute to the increase of hydrogen concentration. Furthermore, the slip plane fracture model developed by Gilman[3] is also adopted to this study, and the critical dislocation pile-up distance for fracture is calculated.

References

[1] R.Matsumoto, S.Taketomi, S.Matsumoto, N.Miyazaki, Int. J. Hydrogen Energy, 34 (2009) 9576-9584.
[2] M.Wen, X.J.Xu, S.Fukuyama, K.Yokogawa, J.Mater.Res., 16, 12 (2001) 4396-3502.
[3] J.J.Gilman, Trans. Metall. Soc. AIME, 212, (1958) 783-791.

Computational modeling of the mechanical behavior of nanocomposites

Natalia Konchakova[1], Swantje Bargmann [1, 2]

[1]Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology, Eißendorfer Str. 42, 21073 Hamburg, Germany
[2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht, Germany
natalia.konchakova@tuhh.de

Keywords: nanocomposite, gradient crystal plasticity, ligament size, sub-micron gold, size effect.

Due to a very high local strength and a relatively regular interconnection of the nano-constituents as well as a low mass density, nanocomposite with sub-micron metals are very good candidates for fest and light-weight structural materials.

The modeling of a modern nanocomposite material is in the focus of the contribution. A gradient extended crystal plasticity theory is applied to the computation of the mechanical response of the metal part of the composite and an elastic-plastic continuum model is used for the simulation of the second material. The model of the sub-micron gold crystal with double slip system is applied for the computation. The gradient hardening contribution is included into the crystal plasticity model in order to study the influence of the ligament size.

Numerical results of the deformation of the nanocomposite under compression loading are presented. The sub-micron gold ligament diameter is varied. The simulation results are compared with the corresponding experimental data. The influences of the gold solid fraction and the gold initial yield stress on the mechanical characteristics of the nanocomposite are discussed.

References

[1] S. Bargmann, M. Ekh, Microscopic temperature field prediction during adiabatic loading in a gradient extended crystal plasticity theory, J. of Solids and Structures, 50 (2013), 899- 906.

[2] E. Husser, E. Lilleodden, S. Bargmann, Computational modeling of intrinsically induced strain gradients during compression of c-axis oriented magnesium single crystal, J. Acta Materialia, 71 (2014), 206-219.

Molecular dynamics simulations of tensile tests of Ni-, Cu-, Mg- and Ti-alloyed aluminium nanopolycrystals

Stephen Hocker[1], Martin Hummel[1], Peter Binkele[1], Hansjörg Lipp[1,2], Siegfried Schmauder[1]

[1] Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Universität Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany
[2] Institut für Theoretische und Angewandte Physik (ITAP), Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany
stephen.hocker@imwf.uni-stuttgart.de

Keywords: aluminium, polycrystal, foreign atoms, molecular dynamics, tensile test.

Molecular dynamics simulations are used to investigate the tensile strengths and failure mechanisms of aluminium nanopolycrystals of in average 8 nm grain diameter with dissolved Ni, Cu, Mg or Ti atoms. It is shown that tensile strengths are influenced by several factors such as stacking fault energies as well as types, concentrations and positions of the dissolved atoms. A strong strengthening was found in case of Cu whereas Ni or Ti lead to a moderate increase of strength, while Mg even lowers the tensile strength.

It was found that both, dislocation processes as well as grain boundary dominated effects contribute to plastic failure mechanisms. Type and concentration of dissolved atoms possess a significant influence on these failure mechanisms. Whereas alloying with Ni, Cu or Mg supports grain boundary dominated failure processes, dissolved Ti atoms lead to an significant increase of stacking faults and dislocations.

Multiscale simulations on the mechanical properties of a Peptide - Zinc oxide composite

Immanuel Schäfer[1], Tuan Anh Do[2], Galina Lasko[1], Jürgen Pleiss[2], Ulrich Weber[1], Siegfried Schmauder[1]

[1]Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), University of Stuttgart, Stuttgart, Germany,
[2]Institute of Technical Biochemistry (ITB), University of Stuttgart, Stuttgart, Germany
Immanuel.Schaefer@imwf.uni-stuttgart.de

Keywords: Nacre, Simulation, Cohesive elements, Zinc oxide/peptide composite, Multiscale Modeling.

Inspired by Nacre, the shiny layer in seashells, the authors reproduced this material artificially, by using a ceramic component and a connection component for the binding of the composite. A multiscale simulation approach of coupling molecular dynamics (MD) and finite element method (FEM) simulations was established to find a protein that shows the highest binding capabilities to a Zincoxide (ZnO) surface. MD simulations of a single 6-mer peptide (Fig. 1A) adsorbed on the polar ZnO(0001)-O surface were accomplished to define the adsorbed peptide conformations and their adsorption force parameters. The results were used in FE simulations with cohesive elements to define special properties of an artificial ZnO-peptide composite material. A parameter study was performed to analyze the influence of the Young's modulus of the Peptide on the mechanical properties of the material in a three point bending test. One important finding in analyzing the Crack Opening Displacement (COD) (Fig. 1B) was that not only the binding capabilities of the protein should be considered as important for the fracture behavior of the nanocomposite, but also its Young's modulus.

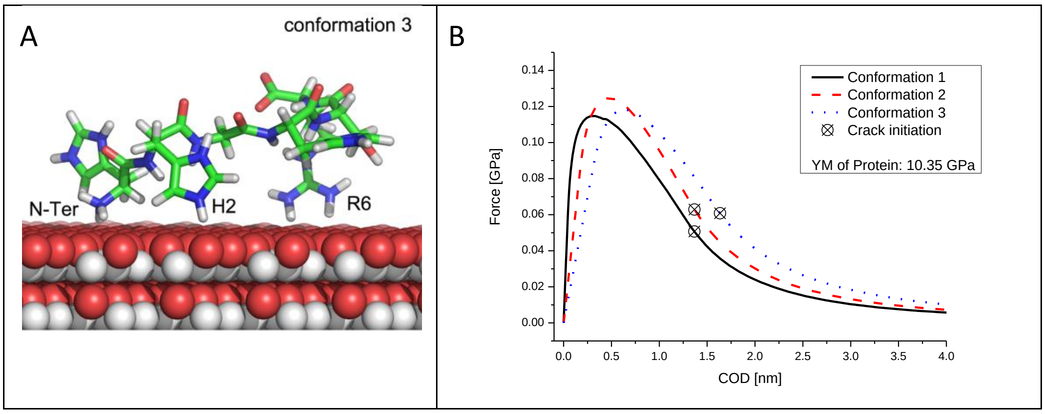


Fig. 1: A: Example conformation of the peptide on a ZnO surface. B: Comparison between different conformations of the protein [1].

Reference: I. Schäfer, T.A. Do, J. Pleiss, G. Lasko, U. Weber, S. Schmauder, Peptide - Zinc oxide interaction: Finite Element Simulation using cohesive zone models based on molecular dynamics simulation, Computational Materials Science, 2014, accepted.

[*] The authors acknowledge funding by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) project number Schm 746/88-1.

Understanding the failure behavior of bio-composites as a prototype for composites with brittle fibers

Swantje Bargmann [1, 2], Ingo Scheider [1], Songyun Ma [1]

[1] Institute of Materials Research, Materials Mechanics/ACE-Centre, Helmholtz-Zentru Geesthacht Germany
[2] Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology,Germany
swantje.bargmann@tu-harburg.de

Keywords: dental enamel, cohesive zone model, size effect, fracture behavior.

Dental enamel exhibits high fracture toughness and stiffness due to the hierarchical and graded structure. Up to 85 vol.% of enamel consist of the hydroxyapatite mineral, the rest being protein and water. Understanding the relationship between the hierarchical structure and the mechanical behavior can be helpful for developing a new high-performance fiber reinforced composite with the desired mechanical properties. In this work, a representative volume element (RVE) is adopted to study the deformation and fracture mechanism of the microstructure. Neo–Hooke and Arruda–Boyce material models are used to simulate the non- linear elastic behavior for the hard and the soft phase, respectively. In addition, the large- deformation kinematics and softening at the first hierarchy level are taken into account in the computation. Breaking of the fiber and debonding of the interface between the fiber and the matrix are captured in this work by employing the cohesive zone model with different material parameters. The strategy of identifying material parameters is developed in consideration of physical interpretation.

The computational results are verified by comparing with experimental data from bending and compression tests. A good agreement between computational and experimental results is achieved with respect to the stress-strain curve and stiffness. The dependence of the failure mechanism on the aspect ratio can be predicted reasonably well by the proposed micromechanical model. Furthermore, it is shown that twist angle reduces the strength of the column significantly. The present work provides an extensible computational approach including scale separation and bridging for modeling the fracture behavior of hierarchical materials, which can help optimizing the design of bio-inspired artificial fiber reinforced composite materials.

References

[1] S. Bargmann, I. Scheider, T. Xiao, E. Yilmaz, G.A. Schneider, and N. Huber. Towards bio-inspired engineering materials: Modeling and simulation of the mechanical behavior of hierarchical bovine dental structure. Computational Materials Science, 79:390-401, 2013.

Section 6:

Fracture and failure II

Thursday 5th of March, 2015

(S6-1 to S6-3)

Fracture Behavior of Highly Heterogeneous Composites: Damage Tolerant Mechanism in Short Carbon Fiber/Si/SiC Composite

Yutaka Kagawa
4-6-1 Komaba, Meguro-ku, Tokyo 183-0023, Japan
kagawa@rcast.u-tokyo.ac.jp

Keywords: Fracture, Toughness, Heterogeneous structure, Carbon/Si/SiC composite

Fracture stress of brittle solids is predicted by fracture toughness: *e.g.* $\sigma_F \approx K_c/\sqrt{\pi a}$. Critical stress intensity factor of ceramics is usually lower than ~10 $MPa\sqrt{m}$, and therefore achievement of higher fracture toughness has been important research fields of structural ceramics. Recently, carbon fiber/Si/SiC composites have been developed and used for severe environmental wear components, such as car brake disks. Fracture toughness of the carbon fiber/Si/SiC composite is in the range ~5 $MPa\sqrt{m}$ with a typical tensile fracture stress ~50 MPa. Although fracture toughness and tensile strength are quite low, this composite behaves tough and damage tolerant material and possible to use without failure. Under tensile/compressive loading, formed micro-cracks in the composite are stably stored within the composite by some crack arrest mechanism. In this case network of "local" crack arrest mechanism due to heterogeneous structure and dimension of the network play important role on tough and damage tolerant behaviors. The presentation focuses micro-scale damage evolution behavior of short carbon/Si/SiC composite and evolution of micro-damage behavior under tensile and compressive loading modes. Fracture strength prediction based on strain energy approach is compare with that of critical stress intensity factor approach.

Experimental study of synergy in hybrid fiber reinforced concrete

Janis Krumins, Aigars Zesers

Institute of Polymer Mechanics, University of Latvia, Aizkraukles Str 23, Latvia, LV-1006

janis.krumins1990@gmail.com

Keywords: Brittle matrix, FRC, hybrid reinforcement.

Metal ceramics composites are formed by adding metallic reinforcement to the brittle ceramic matrix. Therefore they can be classified as brittle matrix - ductile fiber composites. Another example of this class of composites is fiber reinforced concrete (FRC). In this case the main advantage of the presence of ductile fibers is the increased ductility of the composite material.

Most of commercially used FRC usually contains a small volume fraction (1-3%) of steel fibers (length ~ 50mm, diameter~1mm). It is shown, that this type of reinforcement is effective only at relatively large crack opening displacements (COD) [1]. Alternatively, microscale fibers could be used for concrete reinforcement [2]. With this type of reinforcement, the fiber bridging would take place only during micrkocracking phase. For example, the addition of polypropylene microfibers to concrete matrix can increase composite ductility without significant improvement in the load bearing capacity [3]. By using both micro and macro scale reinforcement (hybrid fiber reinforcement), crack bridging effectiveness could be increased at all stages of cracking. The mechanical properties of hybrid fiber reinforced concrete cannot be explained by superposition of individual fiber contributions, therefore it can be concluded, that some synergetic interaction between fiber types is present [3-5]. In this work, steel fiber and hybrid fiber (steel and polypropylene fibers) reinforced composites were studied by performing four point bending, single fiber pullout and compressive tests. Additionally, analysis of porosity was conducted.

References

[1] Buzzini, Davide, Dazio, Alessandro and Trüb, Martin. Quasi-static cyclic tests on three hybrid fibre concrete structural walls. vdf Hochschulverlag an der ETH Zürich (2006).

[2] Yao Wu, "Flexural Strength and Behavior of Polypropylene Fiber Reinforced Concrete Beams," *Journal of Wuhan University of Technology*, vol. 57, no. 2, p. 54, June 2002.

[3] A. Zesers, J. Krūmiņš, Experimental investigation of hybrid fiber reinforced concrete fracture, *Mechanics of composite materials*, 2014. (submitted for publishing)

[4] K. Komloš, B. Babal, T. Nurnbergerova, "Hybrid fibre-reinforced concrete under repeated loading," *Nuclear Engineering and Design*, no. 156, pp. 195-200, 1995.

[5] Nemkumar Banthia, Vivek Bindiganavile, "Performance Synergy in Hybrid Fiber Reinforced Concrete Under Impact," *Journal of Frontiers in Construction Engineering*, vol. 2, no. 4, pp. 75-82, Dec. 2013

Failure limit surface of ceramic foams based on Kelvin cell models under complex global loading

D. Zhang, M. Abendroth, M. Kuna

Institute for Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Lampadiusstrasse 4, 09596, Freiberg, Germany
dongshuan.zhang@student.tu-freiberg.de

Key words: failure limit surface, ceramic foam, Kelvin cell

Due to the favorable properties of foam structures like lightness, high relative stiffness and strength, foam structure have wide utilization. For foams made of brittle material like ceramic, the structure will fail when the material reaches the local strength limit. The Kelvin cell is suitable model to simulate regular foam structures. Under multi-axial loading the struts of the Kelvin cell experience a complex stress state. Tension, compression, shear and bending may happen at the same time. It is investigated, how the variation of the cross section of struts influences the most stressed locations. Struts with constant cross section (CCS) and variable cross section (VCS) are used to describe the failure surface and discuss the weak position under multi-axial loading. The maximum principal stress criterion is used to evaluate local and global structural failure. It is assumed that the material has the same compression and tension strength. As results multi-axial failure limit surfaces are presented.

References:

[1] J. Storm, D. Zhang, M. Abendroth, M. Kuna. Geometry dependent effective elastic properties of open-cell foams based on Kelvin cell models. Advanced Engineering Materials,15,1292-1298(2013)

[2] Kraynik, A.M., Reinelt, D.A.. Foam microrheology: from honeycombs to random foams. Technical Report. Engineering Sciences Center MS 0834, Sandia National Laboratories and Department of Mathematics, Southern Methodist University. (1999)

[3] Hill. On constitutive macro-variables for heterogeneous solids at finite strain. Proc. R. Soc. Lond. A 326, 131-147. (1972)

[4] Jang, W.-Y., Kraynik, A.M., Kyriakides, S. On the micro structure of open-cell foams and its effect on elastic properties, Int. J. Solids Struct, 45, 1845–1875 (2008).