GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK e.V.
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS

86th Annual Meeting

of the International Association
of Applied Mathematics and Mechanics

March 23-27, 2015
Lecce, Italy

Book of Abstracts - Extract

2015

UNIVERSITÀ DEL SALENTO

jahrestagung.gamm-ev.de

Scientific Program - Timetable

Sunday 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	9:30					
	9:45					
	10:15	Registration		von Mises prize lecture		
	10:30					
	10:45					
	11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	11:30					
	11:45					
	12:15		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	12:30					
	12:45					
	13:15	Opening	Lunch	Lunch	Lunch	
	13:30					
	13:45	Univ. Chorus Performance				Closing
	14:15	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	14:30					
	14:45					
	15:15	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
	15:30					
	15:45					
Registration pre-opening	16:15	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	16:30	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	16:45					
	17:15					
	17:30					
	17:45					
	18:15		Public lecture Francesco D'Andria			
	18:30					
	18:45					
	19:15	Opening reception at Castle of Charles V				
	19:30					
	19:45					
	20:15			Conference dinner at Hotel Tiziano		
	20:30					
	20:45					
	21:15					
	21:30					
	21:45					

GAMM 2015

Università del Salento

Table of contents

S08: Multiscales and homogenization

This section is dedicated to discuss recent advances in multiscale and homogenization techniques. Topics of particular interest are nonlinear homogenization techniques, multiscale modelling of failure processes and localization phenomena, FE2 methods, multiphysics phenomena, atomistic to continuum coupling, contact homogenization, numerical techniques for bridging the gap between scales, coarse graining methods, model reduction techniques and multiscale techniques for dynamic problems.

A two scale phase field model for elastic shape optimization

Sascha Tölkes
Institute for Numerical Simulation
University of Bonn

In a two scale model for elastic deformations on perforated domains the macroscopic material properties are determined by a microscopic geometry. This talk discusses the optimization of a cost functional with respect to the microscopic geometry, which is described by phase field functions (compare [1]). The cost functional decomposes into a compliance type cost, a material cost, and a rescaled perimeter of the microscopic perforation selecting a particular microscopic cell size. The approach is discretized using piecewise affine finite elements both on the micro and the macro scale. For the optimization scheme Newton's method is applied to the associated Lagrangian. The relation to microstructures described by sequential laminates [2] is exploited. Further numerical experiments allow material optimization in more complex scenarios with macroscopically non-homogeneous two-scale materials.
This is joint work with M. Rumpf.

References

[1] P. Penzler, M. Rumpf, and B. Wirth. A phase-field model for compliance shape optimization in nonlinear elasticity. ESAIM: Control, Optimisation and Calculus of Variations, 18(1):229-258, 2012.

[2] Allaire, G. Shape optimization by the homogenization method Springer-Verlag, 2002, 146

Study on Statistically Similar RVEs for real microstructures based on different statistical descriptors

Lisa Scheunemann[1], Daniel Balzani[2], Dominik Brands[1], Jörg Schröder[1]

[1]Institut für Mechanik, Abteilung Bauwissenschaften, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany
[2]Institut für Mechanik und Flächentragwerke, Fakultät Bauingenieurwesen, Technische Universität Dresden, 01062 Dresden, Germany

lisa.scheunemann@uni-due.de, daniel.balzani@tu-dresden.de, dominik.brands@uni-due.de, j.schroeder@uni-due.de

In the field of microheterogeneous materials, the internal microstructure is important for the simulation of the macroscopic behavior of the material. For example, in a dual-phase (DP) steel, the interaction of its two phases, martensite and ferrite, are important contributors to the advantageous properties of the material, such as high strength and good formability. The consideration of the microstructure in the form of a representative volume element (RVE) can be incorporated into the modeling using computational homogenization approaches, such as the FE^2 method, see e. g. [1]. Therein, a microscopic boundary value problem considering an RVE is evaluated at every macroscopic gauss-point and the macroscopic quantities are computed using suitable averages of the microscopic counterparts. The incorporation of an RVE based on a real microstructure raises the issue of high computational costs, since an expensive discretization is necessary to account for the complex microstructure morphology. This drawback can be circumvented using statistically similar RVEs (SSRVEs), as proposed in [2], which are governed by a similarity with respect to specific statistical measures and the mechanical behavior, but which are much smaller in size and contain a lower level of complexity in their morphology. SSRVEs are constructed by minimizing a least-square functional which takes into account the differences of statistical measures computed for an underlying real microstructure and the SSRVE. In [3], a staggered optimization approach was proposed, which consists of an inner optimization problem comparing the statistical measures and an outer optimization problem evaluating the similarities in the overall mechanical response to obtain a suitable SSRVE. The statistical measures used in the construction of SSRVEs plays a crucial role. Different measures capture different aspects of the morphology of a microstructure; it was shown in [3] that hybrid approaches comparing a set of multiple statistical measures are beneficial, as well as the consideration of statistical descriptors of higher order. The spectral density and lineal-path function have proven to be suitable measures for the construction of SSRVEs. In this contribution measures based on certain Minkowski functionals, cf. [5], are proposed and applied in the construction process of SSRVEs. The SSRVEs obtained using different sets of statistical descriptors are evaluated regarding their mechanical response compared with the real microstructure and further considering the efficiency of the optimization process.

References

[1] C. Miehe, J. Schröder, J. Schotte. Computational homogenization analysis in finite plasticity. Simulation of texture development in polycrystalline materials. Computer Methods in Applied Mechanics and Engineering, 171 (1999), 69-94.

[2] J. Schröder, D. Balzani, D. Brands. Approximation of random microstructures microstructures by periodic statistically similar representative volume elements based on lineal-path functions. Archive of Applied Mechanics, 81 (2011), 975-997.

[3] D. Balzani, L. Scheunemann, D. Brands, J. Schröder. Construction of Two- and Three-Dimensional Statistically Similar RVEs for Coupled Micro-Macro Simulations. Computational Mechanics (2014), doi: 10.1007/s00466-014.1057-6.

[4] C.L.Y Yeong and S. Torquato. Reconstructing random media. Physical Review E. 57 (1998), 495-506.

[5] G.E. Schröder-Turk, W. Mickel, S. Kapfer, M. Klatt, F. Schaller, M. Hoffmann, N. Kleppmann, P. Armstrong, A. Inayat, D. Hug, M. Reichelsdorfer, W. Peukert, W. Schwieger, K. Mecke. Minkowski Tensor Shape Analysis of Cellular, Granular and Porous Structures. Advanced Materials, 23 (2011), 2535-2553.

Polynomial shape functions on the logarithmic space: the LogFE method

Christian Schröppel, Jens Wackerfuß
Emmy Noether Research Group MISMO,
Institute of Structural Analysis, University of Kassel

In order to obtain robust and rapid convergence in multi-grid methods, it is desirable that the approximation algorithms operating on the meshes of different coarseness, including the prolongation and restriction steps, work primarily on their respective length scales, thus achieving a separation of the shape functions in the (spatial) frequency domain. At the same time, the space of deformations in the low-frequency domain must be rich enough so as to avoid locking phenomena.

To realize these objectives, we propose the "Logarithmic finite element" (LogFE) method, a finite element approach that focuses on the approximation of the low-frequency part of a deformation, using a small number of degrees of freedom. In contrast to the standard Ritz-Galerkin approach, the (internal and external) degrees of freedom are given as coefficients of shape functions on a Lie algebra, allowing to reduce the number of degrees of freedom without incurring the locking phenomena associated with linear shape functions.

Equation (1) shows the transformation of a point at position $\mathbf{x}(\xi)$ by the deformation function $g(\mathbf{u})$, resulting from a set of shape functions associated with a given node at the initial position $\mathbf{v}$. $N_i(\xi)$ and $\bar{N}_j(\xi)$ denote scalar-valued shape functions, u_i and $\bar{u}_j$ are the respective degrees of freedom. The bases $\mathbf{e}_i$ and $\mathbf{B}_j$ generate linear subspaces of the larger vector space $\mathbf{V} := \langle \mathbf{e}_i \rangle \oplus \langle \mathbf{B}_j \rangle$ of the Lie algebra. For $\bar{N}_j(\xi) \equiv 0$, the proposed LogFE method collapses to the special case of the commonly used displacement-based finite element method.

$$\mathbf{x}(\xi) \hookrightarrow (\mathbf{x}(\xi), \mathbf{v}) \overset{g(\mathbf{u})}{\longmapsto} \left(\mathrm{e}^{\sum_j \bar{u}_j \bar{N}_j(\xi) \mathbf{B}_j} (\mathbf{x}(\xi) - \mathbf{v}) + \mathbf{v} + \sum\nolimits_i u_i N_i(\xi) \mathbf{e}_i, \mathbf{v} + \sum\nolimits_i u_i N_i(\xi) \mathbf{e}_i \right) \tag{1}$$

The shape functions induce a tight coupling of translations, rotations and dilatations within a single finite element. Choosing appropriate basis vectors on the Lie algebra and suitable shape functions is of crucial importance for the performance of the model.

We will present models based on the LogFE method for 2D beams as well as for 3D beams, and provide comparisons of the results with reference solutions obtained from displacement-based FE models, including commercially available finite element programs.

Convergence Properties of GMRES for FFT-based Galerkin Homogenization of Periodic Media

Nachiketa Mishra[1], Jaroslav Vondřejc[2,1], Jan Zeman[1,3]

[1]Faculty of Civil Engineering,
Czech Technical University in Prague,
Thakurova 7, 166 29 Prague, Czech Republic
e-mail: nachiketa.mishra@fsv.cvut.cz

[2]Faculty of Applied Sciences,
University of West Bohemia in Pilsen,
Univerzitni 22, 306 14 Pilsen, Czech Republic
e-mail: vondrejc@kme.zcu.cz

[3]Centre of Excellence IT4Innovations,
Technical University in Ostrava,
17. listopadu 15/2172, 708 33 Ostrava-Poruba, Czech Republic
e-mail: zemanj@cml.fsv.cvut.cz

The central result of the homogenization theory for linear elliptic partial differential equations (PDEs) with periodic oscillating coefficients states that the limit problem attains the form of the homogenized elliptic PDE with constant coefficients determined from the periodic corrector (or cell) problem. In the present contribution, we are concerned with FFT-based methods for the solution of the cell problem, originally based on an iterative solution to an integral equation of the Lippman-Schwinger type [1]. Recently, it has been demonstrated by Vondřejc et al. [2, 3] that this approach is equivalent to a Fourier-Galerkin discretization of the cell problem, resulting in a linear system of the form:

$$F^{-1}\widehat{G}FAx = F^{-1}\widehat{G}FAb \text{ with } x \in \mathbb{E}. \tag{1}$$

Here, $\mathbb{E}$ is a subspace of $\mathbb{R}^n$, F^{-1} and $F \in \mathbb{C}^{n\times n}$ are the inverse and forward Fourier transform operators, $\widehat{G} \in \mathbb{R}^{n\times n}$ is a sparse projection matrix from $\mathbb{R}^n$ to $\mathbb{E}$ in the Fourier domain, sparse $A \in \mathbb{R}^{n\times n}$ collects the coefficients at the cell level, and $b \notin \mathbb{E}$ is a given vector. Our goal is to solve the system using GMRES, but its standard application leads to the failure of the Arnoldi orthogonalization step because of the singularity of the system matrix. In the talk, we will outline possibilities how to overcome these difficulties in GMRES and compare its convergence properties with other Krylov subspace-based solvers of (1).

AMS Subject Classification: 74Q99, 65M12, 65F10

References

[1] H. Moulinec, P. Suquet, A fast numerical method for computing the linear and nonlinear mechanical properties of composites, Comptes rendus de l'Académie des sciences. Série II, Mécanique, physique, chimie, astronomie, 1994, 318(11):1417–1423.
[2] J. Vondřejc, J. Zeman, I. Marek, An FFT-based Galerkin Method for Homogenization of Periodic Media, Computers & Mathematics with Applications, 2014; 68(3):156-173
[3] J. Vondřejc, J. Zeman & I. Marek (2014), arXiv:1404.3614

Acknowledgments.
This work was supported by the European Union under the project No. CZ.1.07/2.3.00/30.0034.

A two-scale homogenisation approach for fluid saturated porous media

B.Sc. Florian Bartel[1], Prof. Dr.-Ing. Tim Ricken[1], Prof. Dr.-Ing. Jörg Schröder[2]
[1]TU Dortmund University, Germany
[2]Duisburg-Essen University, Germany

Thinking about the description of biomaterials, e.g. human tissue, plants or sponges, we always have to take into account a global design composed of various substructures with different characteristics on a lower level. Examples of such substructures are pores which can be saturated with fluids or gases, fibres with different orientations or cells which can be influenced by chemical reactions. For the theoretical description of the behaviour, enhanced continuum mechanical models give promising approaches. Up to now, due to the high complexity, it has not been possible to simulate a biological system with only one design model. Hence, it is necessary to think about techniques which simplify the model but still consider the essential characteristics.
This contribution will present a two-scale homogenisation approach for fluid saturated porous media with a reduced two-phase material model, which covers the behaviour of large poro-elastic deformation. The main aspects of theoretical derivation for the weak form, the lower level boundary conditions and the averaged macroscopic tangent moduli will be pointed out and a numerical example will be shown.

An Extended Cascade Micromechanics Model for the Effective Diffusivity of Porous Materials accounting for Pore-Size Distribution

J. J. Timothy, G. Meschke
Ruhr University Bochum, Germany

The effective molecular diffusivity D_{eff} of porous materials such as cementitious or geological materials is strongly affected by the complexity of the pore-space which may span across multiple scales from the nanometer to the sub-millimeter range. Recently, a semi-analytical Cascade Continuum Micromechanics (CCM) Model [1, 2] was presented, which allows to compute estimates of D_{eff} given the porosity ϕ, the intrinsic diffusivity of molecules in the pore-fluid D and a complexity parameter n. In contrast to existing micromechanics models, the CCM model is able to predict a physically consistent percolation threshold.

The CCM model recursively solves for the effective diffusivity based on the Eshelby Matrix-Inclusion morphology characterized by the complexity parameter n that is also the recursion index. However, in order to incorporate a realistic pore-size distribution it is necessary to have explicit access to the volume fraction of pores that are homogenized at a particular cascade level. To this end, an extension of the CCM model is proposed to account for a particular volume fraction of porosity characteristic of a particular size at a particular recursion index n. The recursion index n now characterizes the scale of a particular REV. At a specified scale n, a particular volume fraction $\psi^{(n)}$ of the homogeneous REV (representative of a porous material with smaller pores $r^{(n-1)} << r^{(n)}$) material is de-homogenized into impermeable solid spherical particles and spherical pores. The de-homogenization process transforms the original homogeneous REV into a heterogeneous REV which is now re-homogenized using the Eshelby Matrix-Inclusion technique.

The unknown $\psi^{(n)}$ at each level can be specified given a particular pore-size distribution by using an inverse transformation. For porous materials with the same porosity, but different pore size distributions, the model predicts a higher effective diffusivity for materials with dominating volume fraction of large pores in comparison to a porous material with a larger volume fraction of smaller pores. The predictions from the semi-analytical extended CCM model are compared to numerical pore-network simulations.

References

[1] J. J. Timothy, G. Meschke. Micromechanics model for tortuosity and homogenized diffusion properties of porous materials with distributed micro-cracks. Proc. Apl. Math. Mec. 11 (2011), 555–556.

[2] J. J. Timothy, G. Meschke. Diffusion in Fracturing Porous Materials: Characterizing Topological Effects using Cascade Micromechanics and Phase-Field Models. Poromechanics V (2013), 2250–2259.

Grain-scale-based simulation of granular material

Sami Bidier, Wolfgang Ehlers
Institute of Applied Mechanics (CE), Chair of Continuum Mechanics, University of Stuttgart

In recent years, new developments in experimental mechanics, e. g., particle-tracking methods using X-ray micro-tomography, have provided a new insight into the material behaviour of granular media. The possibility to capture the individual grain displacement and rotation of all particles within a sample provides a new fundament for a reliable numerical simulation of granulates. This is, in particular, the case for deformation localisation in shear zones as they are observed in bi- and triaxial compression tests, where the exact thickness of the localised zone as well as the amount of accompanying grain displacements and rotations are measurable in a precise and direct way.

In this context, the Discrete-Element (DE) Method has become a promising and frequently used modelling technique for granular materials. In contrast to macroscopically based continuum-mechanical approaches, the DE approach treats each particle as a rigid and uncrushably body and is, therefore, defined on a microscopic level of description. This consequently allows a direct comparison with experimental data from grain-scale tracking methods. In the present contribution, the DE method is applied in order to solve problems of localisation in granular media. Therefore, constitutive inter-particle contact laws are formulated for forces and torques which are transferred between interacting particles. The formulations are based on the assumption of an inter-particle contact area and a subsequent idealisation towards a point contact, which can be effectively implemented within a DE approach. This again allows the application of a simplified model based on spherical particles but still incorporating the characteristic effects due to particle shape and distribution. The corresponding set of material parameters needs to be calibrated with respect to experimental data in order to overcome the gap between a qualitative and a quantitative description of the material behaviour.

With a given solution of initial-boundary-value problems on the microscale, a computational homogenisation procedure leads to macroscopic quantities purely stemming from microscopic information. Herein, a particle-centre-based volume averaging technique leads to macroscopic quantities which correspond to quantities known from micropolar continuum theories. The contribution presents a framework for the homogenisation in all time steps in a fully 3-dimensional context and discusses the activation of micropolar effects in the localised zone. Furthermore, the admissible size of the chosen representative elementary volume is addressed.

Materials design of elastic properties of multiphase polycrystalline composites using model functions

M. Lobos, T. Yuzbasioglu, T. Böhlke
Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT)
Karlsruhe 76131, Germany

The present work presents a method for the materials design of elastic properties of multiphase polycrystalline composites. The method follows inverse design methodologies, as presented, e.g., in [1] for general materials and in [2] and [3] specialized for cubic materials. The method takes into consideration the material constants and the orientation distribution of each arbitrarily anisotropic phase. Based on the material constants of each phase, zeroth-order bounds are used in order to decide which combination of materials are physically suitable for prescribed effective properties. This is an approach which can be easily used also within large local or online data bases in order to reflect design possibilities of anisotropic materials and composites based on energetic principles. For the chosen combination of materials, a crystallite orientation distribution function for each phase is formulated as a superposition of analytic central model functions, as the ones presented, e.g., in [4]. It is shown that the chosen central model functions allow the analytic integration of orientation averages of arbitrarily anisotropic fourth-order tensors. Based on this result, the first-order bounds and the geometric average of the stiffness can be expressed explicitly in closed forms for arbitrarily anisotropic polycrystalline materials and number of phases depending on the volume fractions and the influence of the crystallographic texture of each constituent. These expressions are then used in design examples for the determination of volume fractions and orientation distribution of selected materials for prescribed properties.

References

[1] B.L. Adams, S.R. Kalidindi, D.T. Fullwood. Microstructure Sensitive Design for Performance Optimization. Butterworth-Heinemann, Waltham, MA. (2013).

[2] T. Böhlke, M. Lobos. Representation of Hashin-Shtrikman bounds of cubic crystal aggregates in terms of texture coefficients with application in materials design. Acta. Mater. 67 (2014), 324–334.

[3] M. Lobos, T. Böhlke. Materials design for the anisotropic linear elastic properties of textured cubic crystal aggregates using zeroth-, first- and second-order bounds. Int. J. Mech. Mater. Des. 10(3) (2014), 1–20.

[4] S. Matthies, J. Müller, G.W. Vinel. On the Normal Distribution in the Orientation Space. Texture Microstruct. 10 (1988), 77–96.

A coupled two-scale shell model for comb-like sandwich structures

D. Heller, F. Gruttmann
Technische Universität Darmstadt

In the present contribution a coupled two-scale sandwich shell model is proposed, where 4-node quadrilaterals are employed both on the global and the local scale. The coupled global-local boundary value problem is derived by means of a variational formulation and ensuing linearization. Several numerical simulations are carried out for linear elastic and elasto-plastic material behavior with small strains, as well as geometrically nonlinear large displacement calculations assuming finite rotations.

On the local scale, shell elements with 6 degrees of freedom and intersections [2] based on a Hu-Washizu functional [3] are employed to model comb-like microstructures as a representative volume element. In-plane displacements are prescribed on the lateral surfaces of the RVE, determined by the shell strains on the global scale in a specific integration point. Additionally, link conditions are applied for the out-of-plane displacements to allow for unrestricted torsional strains [1]. At the top and bottom face layers, stress boundary conditions are imposed. For simple configurations some components of the matrix of linearized stress resultants are validated using analytical expressions. Constant membrane and bending stiffness components are obtained for different feasible choices of RVEs describing the same microstructure.

The resulting coupled nonlinear boundary value problems are solved simultaneously in a Newton iteration with incremental load steps. Various types of sandwich models are investigated in the form of uni- and bidirectionally stiffened structures as well as a hexagonal honeycomb structure. For the unidirectionally stiffened beam, an analytical reference solution is present by means of classical beam theory. In addition, the numerical results of all coupled calculations are compared to full scale shell models, showing very good agreement while significantly reducing the size of occurring system matrices.

References

[1] F. Gruttmann, W. Wagner. A coupled two-scale shell model with applications to layered structures. Int. J. Numer. Meth. Engng. 94 (2013), 1233–1254.

[2] J.C. Simo. On a stress resultant geometrically exact shell model. Part VII: shell intersections with 5/6-DOF finite element formulations. Comput. Methods Appl. Mech. Engrg. 108 (1993), 319–339.

[3] W. Wagner, F. Gruttmann. A robust non-linear mixed hybrid quadrilateral shell element. Int. J. Numer. Meth. Engng. 64 (2005), 635–666.

Dual-Phase Steel Simulations Based on Representative Three-Dimensional Microstructures

D. Brands[1], D. Balzani[2], L. Scheunemann[1], J. Schröder[1]

[1] Institut für Mechanik, Abteilung Bauwissenschaften, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Germany

[2] Institut für Mechanik und Flächentragwerke, Fakultät für Bauingenieurwesen, TU Dresden, Germany

In many fields of steel applications, e.g. automotive engineering or manufacturing, the optimization of the material properties has become one of the main challenges. The reduction of weight as well as an increasing stability and crash safety are main driving forces. The properties of dual-phase (DP) steels are in good accordance with these aspects and, consequently, they are often applied in the aforementioned fields of applications. It has been shown that these properties mainly depend on microstructural factors such as volume fraction, shape, size and spatial distribution of inclusions. Consequently, for a reliable computational modeling a consideration of the microstructure should be included and for that reason we present a strategy to obtain a representative volume element (RVE) for multiscale simulations like the FE^2-method, see e.g. [1, 2]. These RVEs will be constructed by a set of tomographic measurements and mechanical tests. In order to arrive at more efficient numerical schemes we also construct statistically similar RVEs (SSRVEs), which are characterized by a lower complexity compared to the real microstructure but which represent the overall material behavior accurately, see e.g. [3].

In addition to the morphology of the microstructure, the austenite-martensite transformation during the steel production has a relevant influence on the mechanical properties and is considered in this contribution. This transformation induces a volume expansion of the martensite phase. A further effect is determined in nano indentation tests, where it turns out that the hardness in the ferrite phase increases exponentially when approaching the martensitic inclusion. To capture these gradient properties in the computational model, the volumetric expansion is applied to the martensite phase and the arising equivalent plastic strain distribution in the ferrite phase serves as a basis for a locally graded modification of the ferritic yield curve, cf. [4]. Good accordance of the model considering the gradient yield behavior in the ferrite phase is observed in the numerical simulations with corresponding data.

References

[1] C., Miehe, J. Schröder and J. Schotte. Computational homogenization analysis in finite plasticity. Simulation of texture development in polycrystalline materials. Comp. Meth. Appl. Mech. Eng. 171 (1999), 387–418.

[2] J. Schröder. A numerical two-scale homogenization scheme: the FE^2-method. Plasticity and Beyond - Microstructures, Crystal-Plasticity and Phase Transitions. CISM Lecture Notes 550, Eds. J. Schröder, K. Hackl. Springer, 2014.

[3] D. Balzani, L. Scheunemann, D. Brands, and J. Schröder. Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations. Comp. Mech. 54(5) (2014), 1269–1284.

[4] J. Schröder, D. Balzani, H. Richter, P. H. Schmitz, and L. Kessler. Simulation of microheterogeneous steels based on a discrete multiscale approach. Numisheet 2008: Proceedings of the 7th international conference and workshop on numerical simulation of 3d sheet metal forming processes, 2008.

Computational characterization of magneto-electric composites: the role of ferroelectric pre-polarization

M. Labusch[1], J. Schröder[1], M.-A. Keip[3], D.C. Lupascu[2]

[1]Institute of Mechanics, University of Duisburg-Essen,
Universitätsstraße 15, 45141 Essen, Germany
[2]Institute for Materials Science, University of Duisburg-Essen,
Universitätsstraße 15, 45141 Essen, Germany
[3]Institute of Applied Mechanics (CE), Chair I, University of Stuttgart
Pfaffenring 7, 70569 Stuttgart, Germany

The interaction between electric and magnetic fields enables smart devices, like the measurement of magnetic brain activities and their conversion into electric signals, and may find applications in sensor technology and data storage [1]. Materials showing magneto-electric (ME) coupling combine two or more ferroic characteristics and are known as multiferroics. Since natural single-phase materials show an interaction between polarization and magnetization mostly at very low temperature and at the best a too small ME coefficient at room temperature for technical applications, composite materials becomes important. These ME composites consist of ferromagnetic and ferroelectric phases and generate the ME coupling as a strain-induced *product property*, where we distinguish between the direct and converse ME effect. The direct effect characterizes magnetically induced polarization, where an applied magnetic field yields a deformation of the magneto-active phase which is transferred to the electric phase. As a result, a strain-induced polarization is observed. On the other hand, the converse effect characterizes electrically activated magnetization. Several experiments on composite multiferroics showed remarkable ME coefficients at room temperature that are orders of magnitudes higher than those of single-phase materials. Due to the large influence of the microstructure on the ME effect, we have derived a two-scale homogenization framework, which allows for the consideration of microscopic morphologies [2,3]. A further major influence on the overall ME properties is the polarization state of the ferroelectric phase. In order to account for different polarization states, a material model is implemented that considers the switching behavior of the spontaneous polarization [4] and enables a more exact comparison to experimental measurements [5].

References

[1] N.A. Spalding, M. Fiebig. The renaissance of magnetoelectric multiferroics. Materials Science 309 (2005), 391-392

[2] J. Schröder, M.-A. Keip. Two-scale homogenization of electro-mechanically coupled boundary value problems. Computional Mechanics 50 (2012), 229-244

[3] M. Labusch, M. Etier, D.C. Lupascu, J. Schröder, M.-A. Keip. Product properties of a two-phase magneto-electric composite: Synthesis and numerical modeling. Computational Mechanics 54 (2014), 71-83

[4] S.C. Lynch, R.M. McMeeking. Ferroelectric/ferroelastic interactions and a polarization switching model. Acta Metallurgica et Materialia 43 (1995), 71-83

[5] M. Etier, V.V. Shvartsman, Y. Gao, J. Landers, H. Wende, D.C. Lupascu. Magnetoelectric effect in (0-3) $CoFe_2O_4$-$BaTiO_3$ (20/80) composite ceramics prepared by the organosol route. Ferroelectrics 448 (2013), 77-85

Electro- and Magneto-active Soft Composites with Periodic and Random Microstructures

Stephan Rudykh
Technion – Israel Institute of Technology

We analyze the coupled behavior of dielectric elastomer composites (DEC) and, mathematically analogous, magnetoactive elastomers (MAE) undergoing finite deformations in the presence of external electric or magnetic fields. We specifically focus on the role of microstructures in the coupled response of these active materials. To this end we analyze the composites with (i) periodically and (ii) randomly distributed active particles embedded in soft matrix [1, 2], as well as (iii) layered composites and similar anisotropically structured composites [3]. Through the theoretical analysis and through finite element simulations we identify the key parameters that govern the electro- and magneto- mechanical coupling. We find advantageous microstructures that give rise to significant enhancement of the coupling and performance of the active materials [1]. Moreover, we show that even very similar microstructures, such as periodic composites with hexagonal and rectangular representative volume elements (RVE), exhibit very different behavior both in terms of actuation, and effective properties [2].

Furthermore, we explore the coupled electro- and magneto-elastic instabilities in DEC [4, 5, 6] and MAE [3]. We study the role of the external field (electric or magnetic), microstructure parameters, and material properties on the onset of both microscopic and macroscopic instabilities. We present the multiscale instability analysis for a particular class of periodic microstructures, namely, multilayered active composites. To determine the response of the multilayered structure to an external excitation and mechanical loadings, an analytical solution is derived [4, 3, 6]. The determined from the exact solution local fields are used in the Bloch-Floquet analysis to predict the onset of microscopic instabilities [6]. The onset of macroscopic instabilities is identified by analyzing the homogenized tensor of electro- or magneto-elastic moduli [4, 3]. The results for global bifurcation modes agree with these of the limit of infinite wavelengths in the microscopic instability analysis.

The presentation is based on the joint work with Profs. Kaushik Bhattacharya, Pedro Ponte-Castañeda, Katia Bertoldi, and Gal deBotton.

References

[1] S. Rudykh, A. Lewinstein, G. Uner and G. deBotton. Analysis of Microstructural Induced Enhancement of Electromechanical Coupling in Soft Dielectrics. App. Phys. Lett. 102 (2013), 151905.

[2] E. Galipaeu, S. Rudykh, G. deBotton and P. Ponte-Castañeda. Magnetoactive elastomers with periodic and random microstructures. Int. J. Solids. Struct. 51 (2014), 3012–3024.

[3] S. Rudykh and K. Bertoldi. Stability of Anisotropic Magnetorheological Elastomers in Finite Deformations: A Micromechanical Approach. J. Mech. Phys. Solids. 61 (2014), 949–967.

[4] S. Rudykh and G. deBotton. Stability of Anisotropic Electroactive Polymers with Application to Layered Media. Z. Angew. Math. Phys.(ZAMP) 62 (2014), 1131–1142.

[5] S. Rudykh, K. Bhattacharya, and G. deBotton. Snap-through Actuation of Thick-wall Electroactive Balloons. Int. J. Nonlinear Mech. 47 (2012), 206–209.

[6] S. Rudykh, K. Bhattacharya, and G. deBotton. Multiscale Instabilities in Soft Heterogeneous Dielectric Elastomers. Proc. Royal Soc. A 470 (2014), 20130618.

Multi-scale modeling of beam-like structures: A new boundary condition concept for the RVE

S. Klarmann, F. Gruttmann
Technische Universität Darmstadt

In this work a coupled two-scale beam model using Timoshenko beam elements [1] with finite displacements on the macro scale and fully non-linear 3D brick elements on the micro scale is proposed. The calculation is carried out with the so-called FE^2 concept. To achieve the coupling between the beam and the brick elements, the algorithm from [2] is adapted.

Within the degenerated concept of the Timoshenko beam, the introduction of a pure shear deformation leads to significant problems concerning the equilibrium condition on the micro scale. Applying this deformation mode on the RVE with periodic boundary conditions results in a rigid body rotation. Using linear displacement boundary conditions instead, the wrapping deformation is suppressed on the boundary, leading to a length dependency in the torsional deformation mode. In addition, the shear forces introduce a bending moment, which depends on the length of the RVE and adds spurious normal stresses and a length dependency of the shear stiffness.

To overcome these problems, periodic boundary conditions are applied and the displacement assumptions are modified such that the shear deformation is achieved with force pairs on both ends of the RVE. The resulting model leads to length independent results in tension, bending and torsion and a domain which is able to produce a pure shear stress state. Consequently, only this domain of the model should be homogenized which can be accomplished by modifying the variations in the algorithm [2]. The concept is validated by simple linear and non-linear test problems.

References

[1] F. Gruttmann, R. Sauer and W. Wagner. Theory and numerics of three-dimensional beams with elastoplastic material behaviour. Int. J. Numer. Meth. Engng. 48 (2000) 1675–1702.

[2] F. Gruttmann, W. Wagner. A coupled two-scale model with applications to layered structures. Int. J. Numer. Meth. Engng. 94 (2013), 1233–1254.

Micromechanical modeling of textile materials by means of 1-D structural elements

Markus Mehnert, Sebastian Fillep, Julia Mergheim, Paul Steinmann
University of Erlangen-Nuremberg

Technical textiles show a nonlinear constitutive behavior that differs from the underlying fiber material and is significantly influenced by heterogeneities on the micro level, e. g. the structural assembly of the fibers and appearing contact zones. To reduce the time and costs for experiments for each practical application case a reliable computational method for the identification of macroscopic material properties in dependency of the micro structure in the sense of a numerical laboratory is needed.

The increased application of textiles in various technical fields is decisively influenced by the recent development of different fibre shapes and the improvement of their properties. Exemplary textiles find application in architecture as constructive structures and design materials, as geo-textiles for erosion defence of embankments or as drainage layers. Due to their adjustable porosity they are well suited as filter material. Their flexibility makes them interesting for usage as carrier material for electronic devices or flexible solar cells. Due to the variety of processable materials even bio-compatible structures for medical applications, e. g. implants, can be found.

In this contribution shell-like textiles are considered. Because of their large area-to-thickness ratio a shell specific formulation for the description of technical textiles on the macroscale is used. On the microscale the fibers that compose the representative volume element are discretized by one dimensional beam elements. Therefore the geometry on the microscale is described by a beam specific formulation. Hence a suitable multiscale method using a specific form of the Hill-Mandel condition that links the shell specific formulation on the macroscale and the beam specific formulation on the microscale is developed.

This contribution deals with the determination of the nonlinear constitutive behaviour of technical textiles. We present selected examples of the macroscopic behaviour of microscopic heterogeneous fibre structured materials.

Experimental investigation and approximation of the temperature-dependent stiffness of short-fibre reinforced polymers

L. Kehrer, V. Müller, B. Brylka, T. Böhlke
Chair for Continuum Mechanics, Institute of Engineering Mechanics,
Karlsruhe Institute of Technology (KIT)
Karlsruhe, Germany

In the last decades, polymer based composites were increasingly applied as lightweight material in various fields due to their specific material properties. Short-fibre reinforced thermoplastics exhibit advantages concerning fabrication by injection moulding and recycling. The fabrication process causes, however, inhomogeneous and anisotropic mechanical material behaviour due to introduced local fibre orientation distribution, spatial distribution, and varying geometry of the fibres. During the injection process, cooling rates lead to effects on the structure of the composite, cf. e.g. in [2] and [3]. These structures are not balanced and exhibit post-crystallisation effects. An increase of temperature restores the original amorphous structures. Particularly in case of semi-crystalline thermoplastics, the stiffness depends on the degree of crystallisation, which is linked to temperature and time. Hence, the degree of crystallisation causes changes in the mechanical properties. In addition to the anisotropic and inhomogeneous material behaviour, the effective stiffness properties depend further on temperature and strain-rate and are coupled to temperature history.

Material properties of polypropylene as well as fibre reinforced polypropylene are investigated by a tensile test under thermal loading using dynamic mechanical analysis (DMA). Both, post-crystallisation effects and viscoelastic material behaviour of matrix material are detected, while the thermal loading is varied in a range of $-50°C$ and $120°C$. These effects are discussed on the basis of experimental results.

The effective thermoelastic material behaviour of the fibre reinforced composite is modelled using the interaction direct derivative (IDD) estimate developed by [4]. Based on the three-phase model, the IDD estimate takes into account interaction between fibres and the surrounding matrix material and the fibre distribution. The mean field homogenisation with the IDD approach is performed by means of µ-CT data describing the microstructure of the composite [1]. Experimental data of polypropylene matrix obtained by the DMA are used as input parameters for the homogenisation scheme. For various time-temperature loading histories, the effective properties of the composite resulting from numerical homogenisation are compared to experimental results.

References

[1] V. Müller, B. Brylka, F. Dillenberger, R. Glöckner, S. Kolling, T. Böhlke. Homogenization of Elastic Properties of Short-Fiber reinforced Composites Based on Measured Microstructure Data. (submitted 2014).

[2] E.A. McGonigle, J.H. Daly, S. Gallagher, S.D. Jenkins, J.J. Liggat, I. Olsson, R.A. Pethrick. Physical Ageing in Poly(ethylene terephthalate) - its Influence on cold Crystallization. Polymer 40 (1999), 4977–4982.

[3] S. Meister, A. Jungmeier, D. Drummer. Long-Term Properties of Injection-Molded Micro-Parts: Influence of Part Dimensions and Cooling Conditions on Ageing Behavior. Macromolecular Materials and Engineering 297 (2012), 994–1004.

[4] Q.-S- Zheng, D.-X. Du. An explicit and universally applicable estimate for the effective properties of multiphase composites which accounts for inclusion distribution. Journal of the Mechanics and Physics of Solids 49 (2001), 2765–2788.

Coupling atomistic and continuum models with nodes having translational and rotational degrees of freedom

Florian Niederhöfer, Jens Wackerfuß
Emmy Noether Research Group MISMO,
Institute of Structural Analysis, University of Kassel

The coupling between atomistic (discrete) and continuum models is still an active field of research. It is required for multiscale simulations with atomic structures. The presence of ghost forces is one of the main problems by the definition of interfaces. This effect is the result of the coupling of a local (continuum) and a non-local (atomistic) region. The present work deals with this problem on the level of forces (force-based a/c scheme). The presented class of coupling schemes is not restricted to merge an atomistic model with a special kind of continuum element. The atomistic model can consist of bonded, multi-body interactions. In contrast to the most approaches found in literature, the nodes of the continuum models are not restricted to representative atoms with three translational degrees of freedom. The described schemes are able to deal with nodes with rotational degrees of freedom as well. In the Finite Element code mismo [1] the implementation can be done on the element level.

The coupling between an end of a carbon nano tube and a node of a 3D beam (six degrees of freedom) is presented as an application. The *dreiding* potential [2] is used considering 2-, 3- and 4-body interactions. A defined benchmark without a continuum element enables the analysis of the error resulting from the coupling under different deformations. This example can be used as a part of a multiscale simulation with beam elements and as a key to special kind of boundary conditions related to 3D beams (e.g. bending or torsion).

References

[1] J. Wackerfuß. Molecular mechanics in the context of the finite element method. International Journal for Numerical Methods in Engineering 77.7 (2009): 969-997.

[2] S. L. Mayo, B. D. Olafson, and W. A. Goddard. DREIDING: a generic force field for molecular simulations. Journal of Physical Chemistry 94.26 (1990): 8897-8909.

Representative Volume Element Size Convergence for a Parallel Fiber Bundle Micro-Model

Scott E. Stapleton,Lars Appel, Stefanie Reese
Institute for Applied Mechanics, RWTH Aachen University, Germany
Institute of Textile Technology, RWTH Aachen University, Germany

With the increasing popularity of multi-scale modelling in the field of composites, predicting the microstructure is becoming increasingly important. The local, in-situ microstructure of textile-reinforced composite parts is a result of the earlier manufacturing steps, specifically the infiltration and curing process for the matrix properties and the tow-to-textile and textile-to-preform steps for the fibers. The local fiber orientation is absolutely necessary information for parts which have significant curvatures, since angle changes due to fabric shearing occurring during the draping process can result in large differences in the stiffness and strength properties. To this end, computational models for textiles are being developed to model the draping of fabrics.

Where once only macroscopic models of textiles characterized through extensive experimental programs existed, there is now the possibility of capturing more detailed behaviors at the fiber bundle (tow / roving / yarn) scale. These textile-scale models either create a material model from a Representative Volume Element (RVE), communicate between the textile and macro scales one way or both using homogenization and localization, or only model the textile-scale. These models typically consider a tow as a homogenized continuum, and set the transverse properties of the tow to be a value much smaller than the axial properties. The transverse properties are not explicitly determined, but are estimated.

The present research introduces a fiber-scale model, where the homogenized fiber bundle properties are obtained by an RVE for cases where the fiber radius is magnitudes smaller than the cross-sectional dimensions of the fiber bundle. This RVE is generated using the discrete element method, where each fiber is modelled as a line mass, and elasticity of the fiber is only imitated through the appropriate contact law. The analysis is carried out with an explicit integration scheme where equilibrium is reached at the end of each load step. RVE size convergence is conducted for several different loading scenarios, including shear and compression perpendicular to the fibers and shear in the plane of the fibers. Additionally, the effect of packing pattern and initial pressure on the size convergence is shown. The convergence of stress response and degree of anisotropy will be used to judge convergence. These characteristics are vital to have confidence in the micro-scale response, which is then passed to the next larger scale in the simulation.

Comparison of the Interface Orientation Distribution Average to RVE simulations

Rainer Glüge, Jan Kalisch
University of Magdeburg

Analytical estimates of the effective elastic properties of a microstructured material are mostly designed for specific, idealized microstructures. To incorporate the microstructure arrangement, usually higher n-point correlation functions are needed, which can be rather complicated. Another possibility to consider arbitrary arrangements is to combine a laminate solution [1, 2] with an interface orientation distribution (IOD) average. Since any symmetry of the IOD is transferred to the effective stiffness, the IOD approach captures basic features of the morphology-induced anisotropy. From a mathematical point of view, the approach is similar to second order estimates like the sequential/iterated homogenization approaches [3, 4].

For linear elasticity, one obtains analytical expressions for the effective stiffness of mixtures of two isotropic phases with isotropic, transversely isotropic, and hexahedral IOD. The estimates are in accordance with well-established analytic results such as the Hashin-Shtrikman bounds and Hill's findings for phases with equal shear moduli. Further, at extremal volume fractions, the behavior of the IOD approach is converse to that of the self-consistent approach: both approaches coincide up to first order with complementary and mixed Hashin-Shtrikman-bounds.

For hexahedral IOD, the approach is compared to RVE simulations, where different microstructures with equal IOD are considered. We have found a reasonable agreement for phases with shear moduli of similar magnitude and for microstructures in which both phases percolate the material. Within a sequence of similar microstructures, the error attains a local minimum close to the point of equal arrangement of phases, which is at a phase mixture of 50%/50%.

References

[1] G. Francfort, F. Murat. Homogenization and optimal bounds in linear elasticity. Arch. Ration. Mech. Anal. 94 (1986), 307–334.

[2] R. Glüge, J. Kalisch. The effective stiffness and stress concentrations of a multi-layer laminate. Compos. Struct. 111 (2014), 580–586.

[3] A. Braides, D. Lukkassen. Reiterated homogenization of integral functionals. Math. Mod. Meth. Appl. S. 10 (2000), 47–71.

[4] G. deBotton, I. Hariton. High-rank nonlinear sequentially laminated composites and their possible tendency towards isotropic behavior. J. Mech. Phys. Solids 50 (2002), 2577–2595.

Continuum modeling of material interfaces and surfaces based on molecular statics computations

Christian Sievers, Jörn Mosler
Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

The effective macroscopic properties of a broad variety of different materials are defined by the properties of the involved material interfaces and surfaces. However, in contrast to classical bulk materials, the mechanical properties of material interfaces can usually only be determined indirectly. For that purpose, two different approaches are presented which allow to compute macroscopic properties of material interfaces based on molecular statics computations. While the first of those is based on the principle of energy equivalence, the second one relies on the principle of stress equivalence. The advantages and disadvantages of both frameworks are analyzed.

A multiscale contact homogenization approach for hysteresis friction of rubber on rough surfaces

Paul Wagner[1], Peter Wriggers[1], Corinna Klapproth[2], Corinna Prange[2]
[1]Institute of Continuum Mechanics, Hannover
email: wagner@ikm.uni-hannover.de, wriggers@ikm.uni-hannover.de
[2]Continental Reifen Deutschland GmbH, Hannover
email: corinna.klapproth@conti.de, corinna.prange@conti.de

Understanding the frictional behaviour of elastomers on rough surfaces is of high practical importance in many industrial applications. For example the traction of a tire is directly linked to the material properties of the considered elastomer and the surface conditions of the road track [1]. One goal of our studies is to gain a deeper understanding of the underlying contact physics at all length scales. Another aim is to determine a macroscopic coefficient of friction for varying material and surface properties and to validate the results with experimental data.

One of the main physical aspects of rubber friction on rough surfaces is the internal energy dissipation due to cyclic loading and unloading, called hysteresis. This effect is mainly influenced by the micro roughness of the surface [2]. To capture all details and information down to microscale at acceptable computational costs it becomes necessary to incorporate all physical aspects into a multiscale framework. Some multiscale approaches for sliding rubber samples are presented in [3, 4]. In this study a new FEM multiscale approach for rubber friction on rough rigid road surfaces is suggested focusing on hysteresis effects.

For modelling rubber hysteresis a finite linear viscoelastic material model containing a series of maxwell elements is used. With a spectral analysis of the considered road surface a decomposition into a micro- and macro-roughness is applied. The pressure- and velocity-dependent friction law gained from homogenized micro calculations is then incorporated at the macro scale in the FEM formulation.

We will present the main features of the multiscale framework. Furthermore a numerical validation of the method will be shown for an artificial example. The method is also applied to a measured rough surface showing the agreement of measured and calculated coefficients of friction for two different rubber materials.

References

[1] K.A. Grosch. The relation between the friction and viscoelastic properties of rubber. Proceedings of the Royal Society of London A. 274 (1963), 21–39.

[2] B.N.J. Persson. Theory of rubber friction and contact mechanics. Journal of Chemical Physics 115 (2001), 3840–3861.

[3] P. Wriggers, J. Reinelt. Multi-scale approach for frictional contact of elastomers on rough rigid surfaces. Comput. Methods Appl. Mech. Engrg. 198 (2009), 1996–2008.

[4] I. Temizer, P. Wriggers. A multiscale contact homogenization technique for the modeling of third bodies in the contact interface. Comput. Methods Appl. Mech. Engrg. 198 (2008) 377–396.

Reduced order nonlinear homogenization of composites with cohesive interfaces

Matthias Leuschner and Felix Fritzen
YIG Computer Aided Material Modeling, Karlsruhe Institute of Technology
transition to: Efficient Methods for Mechanical Analysis (EMMA) Research Group,
University of Stuttgart

The mechanical behavior of composite materials is often strongly influenced by the constitutive properties of the interface between the individual phases. For example, brittle or ductile decohesion of particle or fiber reinforcements can occur which may (i) influence the effective material response directly and (ii) trigger secondary deformation processes in the surrounding phases (fiber breakage, formation of localization bands). Therefore, the consideration of the interfaces of the materials is important for the homogenization of nonlinear materials.

In order to homogenize the mechanical behavior of solids with nonlinear interfaces we propose a reduced order model based on the pRBMOR for nonlinear solids [1, 2]. A low-dimensional basis of global ansatz functions is used to parameterize the displacement jump on the cohesive interface. Micromechanical considerations help to condense out the mechanical equilibrium equations in the bulk material. However, the cohesive tractions on the interface have to satisfy the local constitutive model which is assumed to belong to the class of SD-CZ [3]. A variational principle is used to derive a minimization problem delivering necessary conditions that can be interpreted in terms of a constitutive equilibrium in the weak sense. The resulting method is computationally efficient and has low memory requirements.

The reduced order model is applied to three-dimensional microstructures with imperfect interfaces. The accuracy of the predictions is examined and the influence of the choice of the training data for the basis identification is quantified. A comparison to kernel-based interpolation methods is carried out [4]. Future developments are briefly sketched in order to illustrate possible extensions and their significance for realistic multiscale simulations.

References

[1] F. Fritzen, M. Leuschner. Reduced basis hybrid computational homogenization based on a mixed incremental formulation. Comput. Methods in Appl. Mech. Eng. 260 (2013), 143–154.

[2] F. Fritzen, M. Hodapp, M. Leuschner. GPU accelerated computational homogenization based on a variational approach in a reduced basis framework. Computs in Method. Appl. Mech. Eng. 278 (2014),186–217.

[3] M. Leuschner, F. Fritzen, J.A.W. van Dommelen, J.P.M. Hoefnagels. Potential-based constitutive models for cohesive interfaces: Theory, implementation and examples. Composites Part B: Engineering 68 (2015), 38–50.

[4] F. Fritzen, M. Leuschner. Nonlinear reduced order homogenization of materials including cohesive interfaces. *submitted manuscript* (2015).

Use of Gurtin-Murdoch model in predicting effective properties of nano-composites with application to nanoporous gold

Lidiia Nazarenko 1, Swantje Bargmann 1,2, Henryk Stolarski 3
Institute of Continuum Mechanics and Material Mechanics, TU Hamburg, Germany 1
Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany 2
Department of Civil, Environmental and Geo- Engineering, University of Minnesota, USA 3

In this contribution a mathematical model accounting for matrix/inclusion interface effects and used in evaluation of the effective bulk modulus of random nanocomposites [1] is modified and applied to evaluation of the effective shear modulus. To this end the method of conditional moments [2] is combined with a new notion of the energy-equivalent inhomogeneity and used to predict the effective properties of a nanocomposite with randomly distributed nanoparticles. The interface effect is described via complete Gurtin-Murdoch equations [3], which requires proper identification of the energy associated with the surface gradient of displacements present in those equations. This issue constitutes the main focus in the proposed presentation.

With the help of interface energy accommodating all terms of Gurtin-Murdoch equations the real system, consisting of the inhomogeneities and their surfaces possessing different properties and residual stresses, is replaced by energy-equivalent inhomogeneities with modified bulk properties which incorporate the interface effects. Such an approach replaces the problem with interface effects by the problem without such effects, but with modified properties of the inhomogeneities. The modified properties of the energy-equivalent inhomogeneity are obtained assuming that – for the uniform state of strains within the inhomogeneity – its energy is equal to the sum of the energies of the unmodified inhomogeneity and the energy of the interface. This approach is particularly suitable in the context of the method of conditional moments used here for determination of the effective stiffness tensor of the material, as it assumes that the state of deformations within the inhomogeneities is uniform. Closed-form expressions for the effective moduli of a composite consisting of a matrix and randomly distributed spherical nanoinhomogeneities are derived for both the bulk and the shear moduli. Dependence of those moduli on the radius of nanoparticles is included in these expressions.

The presented approach is adopted to the investigation of porous open cell structures and applied for prediction of effective properties of nanoporous gold accounting for surface effects. The effective Young′s moduli of nanoporous gold are analyzed for varying volume content of the nanocavities and for two different values of the stiffness tensor of the reference medium (needed in method of conditional moments). The respectable degree of agreement between the experimental results and those obtained by the method of conditional moments in combination with energy-equivalent inhomogeneity approach illustrates versatility of the proposed method and its viability in analysis of nanomaterials of various structures, including materials with porous open cell structure.

References

[1] L. Nazarenko, S. Bargmann, H. Stolarski. Influence of interfaces on effective properties of nanomaterials with stochastically distributed spherical inclusions. Int. J. Solids Struct. 51 (2014), 985–997.

[2] L. Nazarenko, L. Khoroshun, W.H. Müller, R. Wille. Effective thermoelastic properties of discrete-fiber reinforced materials with transversally-isotropic components. Continuum Mech. Thermodyn. 20 (2009), 429–458.

[3] M.E. Gurtin, A.I. Murdoch. A continuum theory of elastic material surfaces. Arch. Rational Mech. 4 (1975), 291–323.