### **SPECIAL ISSUE**

## MULTISCALE MECHANICAL MODELLING OF COMPLEX MATERIALS AND ENGINEERING APPLICATIONS 3

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#### **FOREWORD**

The present volume is a special issue of articles by authors who participated in the third edition of a special symposium session on *Multiscale and Multiphysics Computational Methodologies for Complex Materials (M2-CM2)* organized within the framework of the fourth European Conference on Computational Mechanics (ECCM2010), which took place in Paris, France, on May 16–21, 2010. The primary focus of the symposium was to bridge the gap between mechanical engineering and material science providing a forum for the presentation of the fundamental, theoretical, experimental, and practical aspects of mechanical modeling of materials with complex microstructures and complex behaviour. This volume follows the issues already edited in the occasion of the first and second editions of two symposium sessions on the same topics (Vancouver, July 2006; and Berlin, August 2009, within the framework of the International Conference on Processing and Manufacturing of Advanced Materials) (Trovalusci, 2007; Trovalusci and Ostoja-Starzewski, 2011). Each contribution has undergone a standard review process, and only papers that received positive recommendations from at least two international referees, have been included.

The purpose of this special issue is to give an overview of the interdisciplinary research oriented to the mechanical modeling of complex materials. The papers provide a survey of the multiscale approaches proposed to describe materials with complex internal structure. Attention is focused on the description of material complex behaviours dominated by microstructure sizes, such as damage, plasticity, viscosity, etc. Advanced numerical tools and computational strategies developed for the solution of related boundary problems are also presented and addressed to engineering applications. The main guideline connecting papers can be recognized in the formulation of constitutive models for materials with internal length in such a way to account for any kind of nonlocality, implicit (as in the case of continua with additional degrees of freedom) or explicit (through the introduction of integral descriptions). A synthesis of all the contributions are given below.

The paper by Trinh, Janicke, Auffray, Diebels, and Forest deals with present-day issues related to the homogenization methods for micromorphic continua, which widely prove their suitability in describing the constitutive behaviour of various kinds of composite materials. In particular, these approaches are effective when the characteristic length associated with the variation of the applied loading conditions becomes of the same order of magnitude of the size of the material inhomogeneities. This work focuses on the choice of polynomial boundary conditions that have to be imposed to the unit cell of microcontinua in order to enhance classical affine conditions for displacements. Differences in the evaluation of standard and nonstandard overall elastic moduli, related to additional fluctuation fields, are studied in the general micromorphic case, as well as in the second gradient and micropolar subcases. The numerical results obtained for two-phase periodic composites as microcontinua of the three cases considered are then compared. The problem of identification of the representative size of the volume element for such microcontinua is also undertaken and a new method to derive size-independent elastic moduli is proposed.

Within the framework of configurational/material thermomechanics, the work by Bargmann and Svendsen proposes an incremental variational formulation for a crystal plasticity model of the strain-gradient type. Generalized plasticity theories are involved in order to predict energetic hardening, taking into account scale-dependent behaviour; here described by the variation of plastic strain gradients. This size-dependent plasticity model includes geometrically necessary dislocations as integrant parts of the evolution process. Besides the strain-gradient contribution generally accounted for in the specific literature, the evolution equations for the dislocation density contain contributions from self-hardening and interaction-hardening mechanisms as well as a term arising due to large deformations. The algorithmic formulation of the model is obtained using the explicit discrete variational approach extended to the inelastic nonlocal/phase field context. Some numerical simulations for a two-dimensional polycrystal in simple tension show the capability of the model in predicting length-scale-dependent hardening.

The aim of the paper by Grégoire, Rojas-Solano, and Pijaudier-Cabot is to achieve a consistent description of the continuous—discontinuous transition involved in the failure process of materials, accounting for the variation of the internal length with the state of the damage. In particular, the authors numerically investigate the performances of different integral-type nonlocal formulations that act in competition in terms of internal length evolution as a function of damage. Attention is then focused on the combined effect of the transfer of information through a damaged area, which leads to a decrease in the internal length and of the interactions between growing voids; which conversely leads to an increase of the internal length itself. Results obtained for two one-dimensional problems show that the combination of two specific models provides better results in terms of convergence with respect to mesh refinements, continuum—discontinuum transitions, and mesh-independent damage distributions.

The formulation of constitutive models for microcracked bodies is also addressed in the paper by Bongue Boma, Sudak, and Federico, developed within the framework of generalized continua theory. The macroscopic behavior of these materials has been derived from a micro/macro change of scale, based on the description of the geometry of the crack field. In particular, at the macrolevel a nonlocal (second-gradient type) constitutive law and an additional nonlinear constitutive law for a scalar configurational force are derived from a nonlocal single-crack model described at the underlined microlevel. The micro/macro transition is obtained via volume averaging accounting for the effect of interactions with neighboring cracks. Some numerical tests show the influence of the crack-to-crack interactions on the strength and stiffness of the body.

Again working in the conceptual framework of generalized continua, Stefanou and Sulem perform a homogenization procedure leading to the identification of a third-order micromorphic continuum for the analysis of masonry columns. The macroscopic model is obtained starting from a discrete description of the structure and by imposing a kinematical map (third-order differential expansion) that guarantees a one-to-one correspondence between the set of degrees of freedom of the discrete system and the continuum kinematic vector fields. It is also required that the power of the internal forces of the discrete system and its kinetic energy correspond to the continuum internal density power and kinetic energy density, respectively. Dispersion curves (phase velocities versus wavelength) evaluated for the model show good agreement between both the discrete and continuum models, in a given range of ratios between the wavelengths and size of the elementary cells.

The paper by Aigner, Lackner, and Eberhardsteiner presents a rheological model for the analysis of the time-dependent behaviour of asphalt under a high-temperature regime. The behavior of the material in such conditions is obtained extending toward plasticity a purely viscoelastic model previously formulated by the same authors. This is done by introducing a friction element. The viscoelastic and viscoplastic constitutive relationships (inclusive unloading) are obtained using a multiscale procedure that allows the dialog among five observation scales. The constitutive relations at the macroscopic level are suitable for the analysis of flexible pavements in order to capture the main failure mechanisms (rutting, low-temperature cracking, and fatigue). Some numerical analyses are performed using the material parameters identified from a bending-beam rheometer. The comparison with the results of triaxial cyclic compression tests of asphalt in-service conditions in the case of high-temperature loading show satisfactory correspondence.

In the paper by Boso and Lefik the mechanical behavior of materials with a complex geometric internal structure is investigated. Attention is focused on wire ropes made of several bundles of wires arranged according to a hierarchical structure and twisted into strands, such as cables used in magnet technology. The problem of identification of the material terms of the rope related to multilevel helix geometry and to twist pitches, which causes some coupling

effects not accounted for in the classical Euler–Bernoulli beam model, is tackled by resorting to an artificial neural network (ANN) approach. In particular, a multilevel recursive procedure is performed, aimed at substituting a bundle of wires with an equivalent single wire, taking into account the complex geometry and the contact phenomena. The numerical tests affected by using a hybrid finite-element/ANN code allow investigating the influence of twist pitches and of nonlinear contact interactions on the material response.

We hope these research issues will provide opportunities to identify and discuss future developments in the field of multiscale modeling and design of advanced materials. Finally, our special thanks are given to the editor Jacob Fish for his invitation to select and collect papers in a special issue of this journal and for assisting us in the editorial work.

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### **REFERENCES**

Trovalusci, P. (Ed.), Multiscale mechanical modelling of complex materials and engineering applications, *Int. J. Multiscale Comput. Eng.*, vol. **5**, no. 2, 2007.

Trovalusci, P. and Ostoja-Starzewski, M. (Eds.), Multiscale mechanical modelling of complex materials and engineering applications 2, *Int. J. Multiscale Comput. Eng.*, vol. 9, no. 5, 2011.