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MULTI-SCALE MODELLING OF FAILURE THROUGH DELAMINATION AND DECOHESION

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Summary. *This paper shortly addresses the computational homogenization of plastically deforming microstructures in which delamination and decohesion events occur. Particle-reinforced materials and structured thin sheets are thereby the main applications of interest. The use of special boundary conditions applied to a small scale volume allows to construct a two-scale homogenization framework that applies to both cases examined.*

1 INTRODUCTION

In the past decades, considerable progress had been made in bridging the mechanical engineering aspects of materials to the field of materials science. This is mainly due to a fruitful combination of micromechanics and multi-scale approaches, with a steadily increasing multi-disciplinary character. Several improved micromechanical theories and associated numerical models have been proposed and implemented, where a lot of interaction with materials science is involved. The developed understanding of single phases and complex interfaces in materials is optimally used in multi-scale homogenization techniques, where it is aimed to predict the collective multi-phase response of materials. Large deformations, damage and cracking, phase transformations, etc. can thereby be taken into account.

This paper focuses on the upscaling of decohesion or delamination in plastically deforming microstructures or multi-layered structured thin sheets. Two types of applications are thereby envisaged: (1) particle-reinforced materials with a decohering phase and (2) thin multi-layered sheets like e.g. flexible displays. A second-order computational homogenization is then elaborated to solve a 2D continuum upscaling procedure for both solids and beam like structures. The homogenization of thin structured sheets towards rollable macroscopic shells is thereby the main goal. Previous work has shown the necessity of a second-order scheme to handle softening as the result of the gradual degradation of the microstructure or sheet[1,2,3,4,5].

Theoretical concepts of the applied second-order approach needed will be addressed and some details on the numerical implementation will be given. Two examples will be given, highlighting the intrinsic properties of decohering elastic particles in a plastic matrix and the upscaling of multi-layered thin structures as needed for the analysis of irreversible deformations and failure in flexible displays.

2 REPRESENTATIVE VOLUME ELEMENTS AND BOUNDARY CONDITIONS

A higher-order RVE has been introduced recently in the context of a gradient-enhanced computational homogenization scheme[2]. One of the key ingredients are the enriched boundary conditions applied to the RVE.

The second-order case departs from a Taylor series expansion of the classical nonlinear deformation map, applied to a finite material vector in the deformed state. Using such a Taylor series expansion, the macroscopic (coarse scale) kinematics is determined through the deformation gradient tensor $\boldsymbol{F}_M$ and its Lagrangian gradient ${}^3\boldsymbol{G}_M = \vec{\nabla}_{0,M}\boldsymbol{F}_M$. Imposing kinematical scale transition relations on the volume, results in two constraints formulated as boundary integrals. The first constraint is typically satisfied by requiring periodicity of the micro-fluctuation field $\vec{w}$ at the boundaries. The second constraint, see[2,3], typically imposes the boundary to accommodate the macroscopic shape in the average sense. The constraint equation in its general form reads

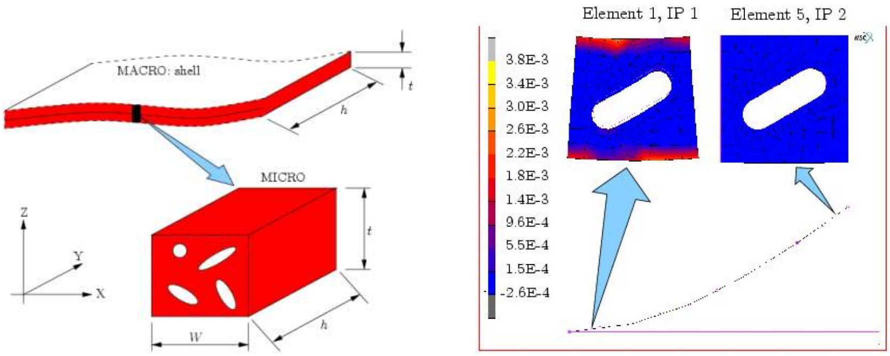
$$\int_{\Gamma_0} \left(\vec{X}(\vec{w} - \vec{w}_1)\vec{N} + \vec{N}(\vec{w} - \vec{w}_1)\vec{X} \right) d\Gamma_0 = {}^3\mathbf{0} \tag{1}$$

where $\vec{X}$ represents the undeformed position vector, $\vec{N}$ the boundary normal, $\vec{w}_1$ the micro-fluctuation in one of the corner nodes.

In the context of the analysis of shells and beams towards the elaboration of a multi-scale scheme on the basis of an underlying through-thickness RVE, similar boundary constraints can be applied to the left and right boundaries. In this paper, a simplified 2D analysis will be illustrated in this sense, where shell-type or beam-type RVEs have been used as schematically illustrated in figure 1(a). Starting from the macroscopic (2D, beam) curvature κ and the normal strain ε, the homogenization of the RVE response naturally results in the bending moment M and the normal force N.

3 UPSCALING OF STRUCTURED THIN SHEETS

Using the higher-order RVE for shells or the 2D-beam RVE , bending of thin structured sheets can be easily analysed, where a direct coupling with the underlying scale is established. An example is given in figure 1(b). This procedure can be readily generalized to 3D shells, where complex deformation mechanisms can be taken into account. In particular, delamination prior to macroscopic localization in multi-layered structures is thereby an interesting application.



(a) Through-thickness RVE (b) Multi-scale bending

Figure 1: (a) Two-dimensional through-thickness RVE and (b) multi-scale bending of a substructured thin beam

4 UPSCALING OF MICROSTRUCTURES WITH DECOHERING PARTICLES

All engineering materials are heterogeneous on one or another spatial scale. The size, shape, physical properties and spatial distribution of the microstructural constituents largely determine the macroscopic overall behaviour of these multi-phase materials and consequently the process window and the life performance of a product. Void nucleation by debonding of inclusions or second phase particles plays a key role in determining the ductility and toughness of a wide variety of structural metals and metal-based composites. Void nucleation is followed by void growth and coalescence, which constitute the main sources of micro-cracking in ductile damage. Ductile damage in metals is inherently a multi-scale process. However, modelling of ductile damage is traditionally done at one scale only (micro or macro).

As a first step towards the multi-scale modelling of ductile fracture, a microstructural model has been created and tested. The model consisted of (one or more) stiff (elastic) inclusions in an elasto-plastic matrix material. The degrading interface between the matrix and the inclusion was modelled by means of cohesive zones. The overall response of such a microstructural model with the degrading interface exhibits pronounced softening. A classical (first-order) computational homogenization methods may not be applied to the fully coupled multi-scale modelling of macroscopic localization, since in this case they lead to an ill-posed problem on the macroscale. A recently developed second-order computational homogenization framework[2,3,4,5] is required to overcome this shortcoming, and to enable modelling of macroscopic localization in a truly multi-scale manner.

Based on the RVE with the boundary conditions defined above, two microstructural models have been analysed: (i) the simplest unit cell model consisting of a single inclusion in a matrix and (ii) a representative volume element (RVE) consisting of several randomly distributed inclusions. Figure 2 show the response of the RVE for different interfacial

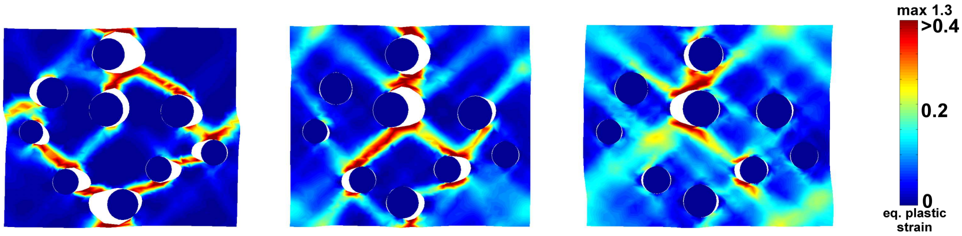


Figure 2: Decohesion at particle interfaces for different interfacial strengths

strengths. Comparison of these results with traditional unit cells, points out that the local equivalent plastic strains are significantly higher (approximately 3 times) in the random RVEs (for the same interfacial strength). Localization bands clearly develop in a different manner, which has a pronounced influence on the resulting ductility. Unit cell approaches are not adequate to pick up this effect.

5 CONCLUSIONS

The use of a higher-order RVE in bending of thin sheet and localization of softening microstructures has been briefly illustrated in the context of a second-order computational homogenization scheme.

Taking into account the fact that microstructure of structural metals and most of metal-matrix composites is random, a random microstructural model is required for the microstructural and multi-scale analysis of ductile damage initiation and development. Using simpler and computationally cheaper unit cell model may lead to erroneous conclusions with respect to both the local microstructural field distributions as well as the overall onset of softening and stress levels.

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