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Computational homogenization of cellular materials

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ABSTRACT

In this work we propose to study the behavior of cellular materials using a second-order multi-scale computational homogenization approach. During the macroscopic loading, micro-buckling of thin components, such as cell walls or cell struts, can occur. Even if the behavior of the materials of which the micro-structure is made remains elliptic, the homogenized behavior can lose its ellipticity. In that case, a localization band is formed and propagates at the macro-scale. When the localization occurs, the assumption of local action in the standard approach, for which the stress state on a material point depends only on the strain state at that point, is no-longer suitable, which motivates the use of the second-order multi-scale computational homogenization scheme. At the macro-scale of this scheme, the discontinuous Galerkin method is chosen to solve the Mindlin strain gradient continuum. At the microscopic scale, the classical finite element resolutions of representative volume elements are considered. Since the meshes generated from cellular materials exhibit voids on the boundaries and are not conforming in general, the periodic boundary conditions are reformulated and are enforced by a polynomial interpolation method. With the presence of instability phenomena at both scales, the arc-length path following technique is adopted to solve both macroscopic and microscopic problems.

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1. Introduction

Nowadays, cellular materials are used in many engineering applications because of their attractive properties, e.g. light weight, high specific stiffness, good damping, high shock absorbability, etc. (Lorna and Gibson, 1997). Their mechanical properties depend not only on the intrinsic properties of the materials of which the cell walls and cell struts are made but also on the micro-morphology, i.e. the spatial distribution of cells (e.g. size, shape, etc). Because of the increase of material requirements for specific applications, for which the required mechanical properties can be achieved by manipulating the micro-structure, the relation between the structural behavior and the microscopic properties must be evaluated.

In experimental studies the cellular materials exhibit a complex mechanical behavior because of the presence of the size effects, as shown for example by Andrews et al. (2001), and of the localization phenomena due to micro-buckling of thin components (cell walls, cell struts), as discussed for example by Papka and Kyriakides (1998), Zhu and Mills (2000), Bart-Smith et al. (1998), or Jang and Kyriakides (2009), which may be enhanced by plastic deformation and reduces strongly the structural stiffness. In finite element analyzes, there are basically three different approaches used to study the behavior of cellular materials: (i) the microscopic approach, (ii) the macroscopic approach, and (iii) the multi-scale computational approach. In the first approach, the detailed structure is considered by using the standard finite element formulation such as beam elements as proposed by Tekoglu et al. (2011), Mangipudi and Onck (in press), Lorna and Gibson (1997) and Chen and Fleck (2002). However, the use of direct simulations to model large problems by finite element analyzes can lead to an enormous number of unknowns. The solution of the resulting equations is still a challenge for actual modern computers. Therefore, this method is suitable for the problems with limited sizes. In the second one, the cellular structure is considered as a continuum medium and the phenomenological material model is applied, see for example the works by Forest et al. (2005) and Hanssen et al. (2002). Although the efficiency is higher than for the first approach, this method is still limited by the fact that the material model and its parameters are difficult to be identified. Moreover the micro-structure evolution during the macroscopic loading cannot be observed. The last method, also-called FE^2, is a combination of the two first approaches in which two separate boundary value problems (BVPs) are defined at two separate scales, see Fig. 1. At the macroscopic scale, the macroscopic BVP is considered as a continuum medium and, at the microscopic scale, a microscopic BVP is associated to each macroscopic material point and contains all heterogeneities. Each microscopic BVP is defined on a representative

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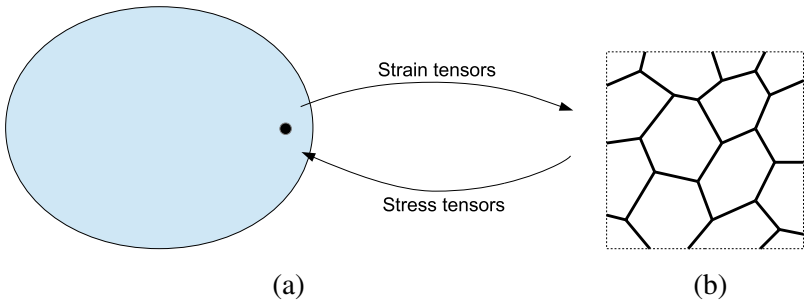

Fig. 1. Multi-scale computational modeling of cellular materials: (a) macroscopic homogenized continuum medium and (b) micro-structure with cell walls and void parts. In the scale transition, the microscopic problem defines its boundary condition depending on the macroscopic strains and computes the macroscopic stresses and macroscopic tangents.

volume element (RVE) and is associated with an appropriate microscopic boundary condition related to the macroscopic quantities, e.g macroscopic strains. The geometrical and material non-linearities at work on the micro-structure are explicitly modeled by using an arbitrary geometrically non-linear framework and arbitrary non-linear constitutive models. From the resolution of the microscopic BVPs, the macroscopic stress–strain relation is always available under the form of a homogenized constitutive law to be used in a macro-scale problem, see for example the developments by Yvonnet et al. (2007), Laroussi et al. (2002), Ohno et al. (2002) and Okumura et al. (2004, 2002), or under the form of a scale transition problem, see for example the developments by Sehlhorst et al. (2009), Kouznetsova (2002, 2004), Ebinger et al. (2005) and Onck (2002).

When considering FE^2 methods, the scale transition can be formulated as a first-order scheme by using the standard continuum theory at both macro- and micro-scales (Sehlhorst et al., 2009; Kouznetsova, 2002) or as a second-order scheme with a generalized continuum theory applied at the macro-scale, e.g. a Cosserat continuum (Ebinger et al., 2005; Onck, 2002) or a Mindlin strain gradient continuum (Kouznetsova et al., 2004). Compared to the first-order schemes, the second-order ones can deal with size effects and some localization phenomena because of the accounting of the higher-order terms related to the higher-order strains (e.g. gradient of deformation gradient, etc). However, the second-order schemes cannot resolve the strong localization bands exhibiting deformations beyond a quadratic nature in the displacement field (Geers et al., 2010). In case of a strong localization band, other approaches should be used, e.g. multi-scale enhanced schemes with a discontinuity enrichment at the macro-scale, see the work of Nguyen et al. (2011), Massart et al. (2007) and Coenen et al. (2012). In spite of their limitations, the second-order schemes are applicable for moderate localization phenomena in cellular materials. This work is thus restricted to the study of localization onsets and of moderate loadings for which the self-contact phenomena of cell walls have not yet happened.

In this work the presence of localization phenomena in cellular structures motivates the use of the second-order multi-scale computational homogenization scheme using a macroscopic Mindlin strain gradient continuum (Kouznetsova et al., 2004; Kaczmarczyk et al., 2008; Nguyen et al., 2013). In this second-order scheme, both the deformation gradient and its gradient are used to define the microscopic boundary condition. The macroscopic stresses (first Piola–Kirchhoff and higher order ones) are calculated by using the generalized version of the Hill-Mandel homogenization principle. For cellular materials, the thickness of the localization band is comparable to or slightly larger than the characteristic size of the micro-structure. As it will be shown in this paper, although we are clearly at the edge of the separation of scales, the second-order homogenization method remains accurate when the localization band present at the macroscopic scale is of a size larger than the RVE size. For periodic cellular materials it is the case as the microscopic BVP can be limited to a single cell study. In that case, the usual microscopic boundary conditions can still be used. Note however that to capture instability phenomena we introduce some different randomness in each micro-problem studied at each macroscopic Gauss point. As the instabilities are considered at both scales, the path following method (Wempner, 1971; Riks, 1979, 1992; Bellini and Chulya, 1987; Fafard and Massicotte, 1993; Zhou and Murray, 1995; Kouhia and Mikkola, 1999; Grognec and Le van, 2008; Grognec et al., 2009) is used to solve both the macroscopic and the microscopic BVPs.

In order to solve the Mindlin strain gradient continuum in this second-order scheme, instead of using a specific finite element formulation as the mixed formulation (Kouznetsova et al., 2004; Kaczmarczyk et al., 2008), an implementation based on a discontinuous Galerkin method is shown to be particularly efficient to constrain weakly the continuities of the displacement field and of its gradient (Nguyen et al., 2013). This method can be easily integrated into conventional finite element codes and parallelized at the macroscopic scale by using face-based ghost elements (Becker et al., 2011; Wu et al., 2013). In that context the homogenization is viewed as a usual constitutive law from the macro-finite element, and this constitutive law solves another finite-element problem: the microscopic problem. In order to consider large problems, the multi-scale problem is not only parallelized at the macro-scale by face-based ghost elements but also by distributing the microscopic problems of a macro-partition between several processors.

At the microscopic scale, classical finite element resolutions of RVEs are considered. In a general problem, three classical boundary conditions, which are linear displacement boundary condition (Dirichlet condition), minimal kinematic boundary condition (Neumann condition) and periodic boundary condition can be used. Many numerical studies show that the periodic boundary condition provides a better estimation than other boundary condition types (Kanit et al., 2003; Terada et al., 2000; Larsson et al., 2011; Nguyen et al., 2012). For problems involving localization at the micro-scale, the boundary condition should be reformulated to account for this localization direction (Coenen et al., 2012). However, in this work, the localization bands at the macro-scale have a size larger than the size of the micro-scale problem and the classical microscopic boundary conditions can be used. The periodic boundary condition is chosen because of its efficiency. The implementation of the periodic boundary condition in case of conformal meshes is easily implemented by constraining matching nodes. But meshes generated from the cellular materials are normally non-conformal because of their random spatial distribution. For these non-conformal meshes, some methods are available to enforce the periodic boundary condition in first-order schemes, such as the master/slave approach (Yuan and Fish, 2008), the weak peri-

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