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Strength properties of nanoporous materials: A 3-layered based non-linear homogenization approach with interface effects

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ABSTRACT

In this paper, the strength properties of a ductile nanoporous material are investigated by means of a non-linear homogenization approach based on the modified secant method. The material is described as a rigid-ideal-plastic solid matrix, obeying to a von Mises strength criterion, and containing isotropically-distributed spherical nanovoids. Aiming to properly account for local strain-rate heterogeneities, a 3-layered model is adopted. A novel closed-form macroscopic strength criterion is established, and successfully compared with available numerical data. Proposed approach results in an effective enhancement of the non-linear homogenization-based model recently provided by Dormieux and Kondo (2013).

1. Introduction

The development of materials characterised by a nanosized microstructure has recently given rise to a growing research interest, involving experimental tests, numerical simulations and theoretical models, aiming to investigate the influence of nano-inclusions or nanopores on the overall material response (Arico, Bruce, Scrosati, Tarascon, & Van Schalkwijk, 2005; Jenkins, 2010; Lu, Zhao, & Wei, 2004).

An important class of nanostructured materials consists in nanoporous media, characterised by reduced mass density, high surface-to-volume ratio, good levels of both stiffness and strength, and generally exhibiting a ductile behaviour. Furthermore, due to the nanosize of cavities, these challenging materials are chemically active, exhibiting a high capability to interact with ions and molecules. Through these attractive properties, nanoporous materials are of the most interest in several technical fields, including civil and environmental engineering, geophysics, petroleum industry, biomechanics and chemistry, opening towards groundbreaking multifunctional applications (Jenkins, 2010).

From a mechanical point of view, one of the most important aspect concerns the influence, for a fixed porosity value, of the size of voids on the macroscopic material properties. As a matter of fact, with reference to strength features, recent

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nano-indentation tests (Biener, Hodge, Hamza, Hsiung, & Satcher, 2005; Biener et al., 2006; Hakamada & Mabuchi, 2007) have proven a significant increase of the yield stress when the void size decreases. The same dependency has been shown in numerical studies based on Molecular Dynamics approaches (Brach, Dormieux, Kondo, & Vairo, 2016a; Mi, Buttry, Sharma, & Kouris, 2011; Traiviratana, Bringa, Benson, & Meyers, 2008; Zhao, Chen, Shen, & Lu, 2009), where strength predictions decrease towards asymptotic values when the void size increases.

The physical origin of such a phenomenon has been addressed in literature by analysing the solid-void interphase regions at the atomic length-scale (Cammarata, 1994; Gibbs, 1906; Murr, 1975; Orowan, 1970; Shuttleworth, 1950). Indeed, it has been well recognized that, due to the nanovoid presence, a local perturbation in the atomic arrangement occurs close to the void surface, leading to self-equilibrated interactions which can be interpreted as surface stresses (Needs, Godfrey, & Mansfield, 1991). Surface-induced effects, usually negligible for classical porous materials, become relevant for nanoporous ones (Duan, Wang, Huang, & Karihaloo, 2005), resulting in the experimentally- or numerically-observed void-size dependency of effective mechanical properties.

In the framework of a continuum approach, surface-induced stress fields have been generally addressed by introducing interface models (e.g., Duan, Wang, Huang, & Luo, 2005; Gurtin & Murdoch, 1975, 1978; Wang et al., 2011), defined in the zero-thickness limit of the transition zone affected by the perturbation of the atomic arrangement. Reference is usually made to coherent and imperfect interface laws, resulting in the continuity (resp., discontinuity) of the displacement field (resp., stress vector) across the interface (Duan, Wang, Huang, & Karihaloo, 2005; Gurtin & Murdoch, 1975, 1978; Povstenko & Z., 1993).

Early works involving surface-stress effects have been focused on the effective elastic properties of nanoporous or nanocomposite materials (Brisard, Dormieux, & Kondo, 2010a, 2010b; Duan, Wang, Huang, & Karihaloo, 2005; Duan, Wang, Huang, & Luo, 2005; Le Quang & He, 2007; Sharma & Ganti, 2004; Sharma, Ganti, & Bhate, 2003). In contrast, few attention has been paid so far to the influence of surface stresses (and thereby of void-size effects) on the material plastic behaviour.

Referring to limit-analysis approaches (Salençon, 1983), the well-established yield function proposed by Gurson (1977) for ductile classical porous media has been extended to nanoporous ones by Dormieux and Kondo (2010), taking advantage of a plastic generalization of a two-dimensional stress-interface model (Monchiet & Bonnet, 2010). The same interface description has been used by Monchiet and Kondo (2013) for deriving a nanoporous strength criterion in the case of spheroidal cavities, incorporating then both void-shape and void-size effects.

An alternative to limit-analysis models consists in non-linear homogenization (NLH) methods based on the so-called modified secant-moduli approach (Suquet, 1995, 1997), which have been proven to be equivalent to the variational procedure proposed by Ponte Castañeda (1991). Referring to the linear formulation by Herve and Zaoui (1993) and addressing a n-layered spherical composite assembly, semi-analytical strength criteria for classical porous materials have been derived by Bilger, Auslender, Bornert, and Masson (2002) and by Vincent, Monerie, and Suquet (2009), numerically-experiencing more accurate strength estimates higher the number n of layers. As regards nanoporous materials and by adopting imperfect-coherent interfaces approaches, some void-size dependent strength criteria have been recently proposed by Goudarzi, Avazmohammadi, and Naghdabadi (2010), Moshtaghin, Naghdabadi, and Asghari (2008), Zhang and Wang (2007), Zhang, Wang, and Chen (2008), and Zhang, Wang, and Chen (2010). Nevertheless, in these cases, the corresponding macroscopic yield functions are questionably expressed in terms of surface elastic properties, in contrast with the proper definition of limit-stress states. A consistent generalization to nanoporous materials of the porous strength criterion by Ponte Castañeda (1991) has been proposed by Dormieux and Kondo (2013), including surface-induced effects via an interface stress model. However, as it will be shown in the following, such a strength model (denoted as DK) strongly overrates available numerical evidence (Morin, Kondo, & Leblond, 2015; Trillat & Pastor, 2005), especially for high stress-traxiality levels. Such an occurrence is mainly due to a rough description of local strain-rate heterogeneity in the limit state, and it clearly highlights the need of a further research effort to enhance non-linear homogenization-based strength estimates for nanoporous materials.

In this light, present paper aims to establish a consistent and accurate strength model for nanoporous media, properly accounting for void-size effects and able to recover available benchmarking evidence. In detail, strength properties of ductile nanoporous materials are investigated via a non-linear homogenization procedure based on a 3-layered description and including surface-stress effects by means of an imperfect-coherent interface model. The paper is organized as follows. In Section 2 basic elements of the adopted theoretical framework are presented. Section 3 is devoted to the derivation of a novel analytical strength criterion for nanoporous materials, whose effectiveness and accuracy is discussed in Section 4. Finally, some conclusions are traced in Section 5.

2. Preliminary background

2.1. Problem statement

Aiming to investigate strength properties of a nanoporous material via a non-linear homogenization (NLH) approach, let Ω be a material representative volume element (RVE), whose exterior boundary is $\partial\Omega$. Let the RVE be comprised of internal isotropically-distributed spherical cavities of radius a and of a rigid-ideal-plastic solid matrix Ω^s (Fig. 1). Therefore, material strength properties are straight identified by referring to the yield limit state.

It is observed that the rigid-ideal-plastic assumption on the local mechanical response is a fundamental requirement of the limit analysis theory. Such an hypothesis has been widely adopted in both classical and more recent literature focus-