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Research paper

A computational insight into void-size effects on strength properties of nanoporous materials

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ABSTRACT

In this paper, strength properties of nanoporous materials are addressed aiming to establish novel insights into the influence of void-size effects. To this end, a virtual spherically-nanovoided sample of an aluminium single crystal is investigated by adopting a Molecular-Dynamics computational approach. Elasto-plastic mechanical response, under triaxial strain-based conditions and including axisymmetric and shear states, are numerically experienced, identifying the corresponding limit stresses. Computed strength measures are used to furnish estimates of strength domains, described in terms of meridian and deviatoric profiles. The influence of void-size effects on the computed strength properties is clearly quantified for different porosity levels, numerical results confirming a strengthening of the sample when the void radius reduces. Moreover, it is shown that the occurrence and the amount of void-size effects are strongly dependent on the Lode angle, resulting in a shape transition of both meridian and deviatoric strength profiles when the void radius is varied. Finally, present results suggest porosity-dependent threshold values for the void radius above which void-size effects tend to disappear. With respect to the actual state-of-the-art, useful benchmarks for assessing the effectiveness of available theoretical models are provided, resulting in a novel incremental contribution towards the definition of advanced modelling strategies for describing strength properties of nanoporous materials.

1. Introduction

In the last decades, since the development of novel and challenging nano-technologies, nanostructured materials have yielded a growing research interest, involving experimental tests, theoretical formulations and numerical models (Arico et al., 2005; Lu et al., 2004; Jenkins, 2010). An important class of nanostructured materials consists in nanoporous media, characterized by very fascinating properties or combination of properties in terms of mechanical, chemical and electromagnetic features. In particular, due to the presence of nanoscale cavities, these materials exhibit a high capability to interact, absorb and cooperate with atoms, ions and molecules. Moreover, they are characterised by reduced mass density, high surface-to-volume ratio, good levels of both stiffness and strength, and they generally exhibit a ductile behaviour. Accordingly, nanoporous materials open towards groundbreaking functional applications in several technical fields, including civil and environmental engineering, geophysics, petroleum industry, biomechanics, chemistry. For instance, they are used to conceive multifunctional devices for aerospace/automotive applications, energy storage, ion-exchange, molecular biosensing and bioseparation, drug delivery, catalysis, filtration, sensoring (Jenkins, 2010).

From a mechanical point of view, one of the most fundamental aspect consists in identifying and describing the constitutive response and the strength properties of these materials, as dependent on the size of voids (which is in the order of some nanometres), as well as on their shape and arrangement (Dormieux and Kondo, 2010; 2013; Huang et al., 2005; Li and Huang, 2005; Monchiet et al., 2008; Monchiet and Kondo, 2013). As regards void-size effects, well-established experiments (usually based on nano-indentation tests) have shown that a reduction in the length-scale of nanovoids induces an improvement of the material strength (Biener et al., 2005; 2006; Hakamada and Mabuchi, 2007). Such an effect cannot be theoretically described by classical approaches for porous materials (e.g., Gurson, 1977; Ponte Castaneda, 1991),

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that are generally conceived to predict porosity effects only, and thereby resulting in void-size-independent strength criteria.

The influence of void size on the mechanical behaviour of nanoporous materials are related to the presence, at the cavity boundaries, of self-equilibrated surface stresses (Needs et al., 1991). These latter can be modelled via interface laws (Gurtin and Murdoch, 1975) and they reveal fundamental in describing the mechanical response of nanoscale structures (Amelang and Kochmann, 2015) and nano-structured materials (e.g., Duan et al., 2005b,a), as well as for modelling strength properties of nanoporous media (e.g., Dormieux and Kondo, 2010; 2013; Goudarzi et al., 2010; Monchiet and Kondo, 2013; Moshtaghin et al., 2012). As an example, by applying a limit-analysis approach on a hollow spherical domain, Dormieux and Kondo (2010) extended the well-known strength criterion proposed by Gurson (1977) for ductile porous media to the case of nanoporous materials, aiming to predict void-size effects. The void-size-dependent strength criterion by Dormieux and Kondo (2010), as well as the porous model by Gologanu et al. (1993; 1994), have been successively extended by Monchiet and Kondo (2013) to the case of nanoscale spheroidal cavities, thereby incorporating both void-shape and void-size effects. Other analytical formulations have been proposed by Dormieux and Kondo (2013), Goudarzi et al. (2010), Zhang and Wang (2007) and Zhang et al. (2010), by combining non-linear homogenization techniques and variational arguments, and resulting in a generalization of the Ponte–Castaneda's strength criterion (Ponte Castaneda, 1991) to nanoporous materials.

It is worth observing that available strength models for nanoporous materials are based on a number of a priori assumptions. In fact, they generally include a very simple limit behaviour of the bulk matrix, as well as a simplified representation of the physics underlying nanoscale effects (usually faced by introducing fictitious plastic interfaces). Nevertheless, available experimental results are not sufficient to support these assumptions, so that current theoretical models can be neither properly validated nor suitably calibrated. As a matter of fact, apart from some qualitative indications of the void-size influence on the material strength level, no further information can be deduced from the experimental literature either on the three-dimensional material strength domain or on the influence of the void size as a function of the loading state. In this context, numerical methods may be considered as an effective alternative to provide comparative benchmarks, allowing also to successfully control a number of possible coupled effects, and thereby resulting in useful indications towards advanced modelling strategies.

Computational methods usually employed for modelling macro- and/or micro-mechanical response are not able to automatically provide helpful insights on nanoscale effects, since they do not include a satisfactory description of the material structure at that length-scale. On the contrary, and as confirmed by recent investigations (e.g., Bringa et al., 2010; Borg et al., 2008; Mi et al., 2011; Tang et al., 2010; Traiviratana et al., 2008; Zhao et al., 2009), numerical methods based on Molecular Dynamics (MD) approaches allow to describe the material arrangement at the atomistic level, and thereby they can be considered as promising tools for investigating the elasto-plastic behaviour of nanoporous materials.

As a matter of fact, available studies based on MD approaches mainly address the identification and the characterization of atomistic mechanisms underlying failure processes related to void growth and coalescence (e.g., Farrissey et al., 2000; Lubarda et al., 2004; Lubarda, 2011; Marian et al., 2004; 2005; Pogorelko and Mayer, 2016; Ruestes et al., 2013; Tang et al., 2010; Traiviratana et al., 2008). On the other hand and at the best of the authors' knowledge, very few attempts have been provided in order to employ these numerical strategies to furnish indications towards the definition of engineering strength measures for nanoporous materials. For instance, an attempt to put in relationship strength properties at the macroscale with MD-based evidence has been provided by Mi et al. (2011) and Traiviratana et al. (2008), referring to the void-size-independent Gurson model. Nevertheless, current MD studies are generally limited to the analysis of particular admissible stress states only, computed under uniaxial (Farrissey et al., 2000; Tang et al., 2010), volumetric or shear conditions (Marian et al., 2004; 2005), and therefore defining only few discrete points on the a-priori unknown material strength surface, without considering more complete multiaxial scenarios. In fact, a comprehensive three-dimensional characterization of material strength properties requires a proper investigation of failure mechanisms under multiaxial loading conditions. Furthermore, no numerical evidence has been yet provided concerning the influence of void size on material strength domains. Accordingly, with respect to the previously-discussed state-of-the-art, a parametric multiaxial loading strategy is expected to pave the way for a number of original contributions, such as: (i) complete identification of failure surfaces and of the influence of stress invariants on material strength properties; (ii) analysis of void-size effects on strength domains; (iii) assessment of novel and effective comparative benchmarks for validating and calibrating available theoretical formulations, as well as for drawing advanced modelling strategies.

It must be pointed out that porous and nanoporous materials may be generally characterised by irregular patterns and randomly-distributed voids. Nevertheless, as it is customary in classical elasto-plastic theoretical approaches for micro/nano-structured materials, simple geometrical descriptions are often considered. This is the case of single-voided domains and of hollow sphere models (Gurson, 1977), widely adopted in porous metal plasticity and limit analysis approaches (Dormieux and Kondo, 2010; Monchiet and Kondo, 2013; Tvergaard and Needleman, 1984). Corresponding results are strictly valid for the particular, but realistic, considered microstructure (in the case of hollow sphere models, the microstructure is the so-called Hashin Composite Sphere Assemblage, (Hashin, 1962; Leblond et al., 1994; Michel and Suquet, 1992)), but they generally furnish also helpful indications on statistically-equivalent arrangements. In this framework, domains embedding a single spherical nanovoid have been adopted in many recent MD-based computational studies (e.g. Farrissey et al., 2000; Marian et al., 2004; 2005; Traiviratana et al., 2008), addressing plastic mechanisms in nanoporous materials.

In this paper, strength properties of an aluminium single crystal containing a spherical nanovoid are addressed via a Molecular Dynamics approach. A parametric analysis with respect to the void radius and for different porosity levels is carried out, by considering different strain paths (shear, triaxial expansion and triaxial compression) and a wide range of triaxiality scenarios (from pure deviatoric conditions to pure hydrostatic ones). The computational model is defined in Section 2, drawing also basic elements of the adopted numerical procedure. With the aim to present simulation results in the framework of a customary notation in plasticity, and by referring to average stress and strain measures, the Haigh–Westergaard (HW) coordinates are introduced. Section 3 is devoted to analyse some preliminary results, in terms of both stress-strain relationships and dominant atomistic mechanisms, in order to identify suitable strength measures for estimating limit stress conditions for the in-silico samples. Analyses of numerically-experienced strength properties are provided in Section 4, wherein meridian and deviatoric representations of computed strength domains are proposed, highlighting and discussing the influence of void-size effects. Finally, main concluding remarks are traced in Section 5.