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Void-shape effects on strength properties of nanoporous materials

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Abstract

In this paper, strength properties of nanoporous materials with spheroidal nanocavities are investigated via a Molecular Dynamics approach applied to a nanovoided aluminium single crystal, in the case of a fixed porosity level, and for prolate, oblate and spherical void shapes. Estimates of the effective strength domain are provided, by considering several mechanical loadings including axisymmetric and shear strain-rate states. Void-shape effects are quantified for different values of the void aspect ratio, mainly resulting in an overall weakening of the sample as the spheroidal nanovoid assumes either an oblate or a prolate shape, in comparison to the case of a spherical void. Finally, it is observed that the computed strength profiles exhibit the following specific features: (i) a strong dependence on the hydrostatic, second-order and third-order deviatoric stress invariants, (ii) more significant void-shape effects for triaxial-expansion stress states with a small hydrostatic component, and (iii) a more pronounced influence of the spheroid shape, as the aspect ratio is varied, in the presence of an oblate nanovoid rather than of a prolate one.

Keywords: Strength properties, void-shape effects, nanoporous materials, Molecular Dynamics

1. Introduction

Plastic failure in ductile metals has been recognized to occur for the subsequent nucleation, growth and coalescence of voids in an otherwise bulk material. Specifically, experimental traction and compression tests performed on an alloy steel [1] showed that prolate ellipsoidal voids were nucleated from second-phase particles, leading to ductile fracture through internal necking. Conversely, oblate ellipsoidal voids were observed to grow from cleavage cracks in dual-phases microstructures [22].

As such, since a number of pioneering research works (e.g., [9, 18, 25]), several studies have been proposed in order to investigate void-shape effects on strength properties of ductile porous materials. Numerical computations on plastic or viscolplastic media embedding spheroidal cavities were carried out in [11], pointing out the role of both initial void shape and void orientation upon cavity growth and evolution. Later, the well-known Gurson's model [9] was extended via limit analysis approaches to the case of ductile materials containing prolate or oblate spheroidal voids [6, 7, 8]. Similar modelling strategies were adopted in [5], with reference to porous media with prolate cavities. More recently, macroscopic yield criteria for ductile materials embedding spheroidal cavities have been proposed [19, 20], also including the combined effect of void shape and matrix anisotropy on the effective strength properties [19].

Nonetheless, despite the interest of above-mentioned studies, progress in developing predictive approaches is needed in analyzing void-shape effects on ductile failure of materials containing nanosized cavities. The latter issue represents one of the most challenging research topics in nano-mechanics, since the enormous technological effort recently afforded to conceive ultra-high-performance engineering devices based on nanoporous materials.

A notable attempt to investigate the combined influence of void-shape and void-size effects in nanoporous media was proposed in [21], by providing a macroscopic yield criterion for ductile materials containing spheroidal nanosized cavities. On the contrary, there is still a lack of numerical benchmarking evidence, which might be useful for both the assessment and the calibration of theoretical models. As a matter of fact, when ductile failure of nanoporous materials is addressed in computational literature, the focus often consists in the characterization of void growth and coalescence [4, 13, 14, 15, 16, 23, 26, 28, 29]. Conversely, there is in general little concern about the investigation of void-shape effects on effective strength properties, recent computational studies only addressing the case of nanoporous materials embedding spherical cavities [2, 30].

Motivated by the above observations, the present paper aims to provide numerical estimates of the effective strength domain of nanoporous materials with spheroidal cavities. Void-shape effects on predicted strength properties are analyzed by referring to a single-crystal computational domain embedding prolate, oblate or spherical cav-

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