Journal of the Mechanics and Physics of Solids 92 (2016) 55–71

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Scaling laws of nanoporous gold under uniaxial compression: Effects of structural disorder on the solid fraction, elastic Poisson's ratio, Young's modulus and yield strength

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ARTICLE INFO

Article history:
Received 28 August 2015
Received in revised form
30 November 2015
Accepted 16 February 2016
Available online 27 February 2016

Keywords:
Nanoporous gold
Scaling laws
Finite element method
Yield strength
Young's modulus
Poisson's ratio
Mechanical behavior

ABSTRACT

In this work the relationship between the structural disorder and the macroscopic mechanical behavior of nanoporous gold under uniaxial compression was investigated, using the finite element method. A recently proposed model based on a microstructure consisting of four-coordinated spherical nodes interconnected by cylindrical struts, whose node positions are randomly displaced from the lattice points of a diamond cubic lattice, was extended. This was done by including the increased density as result of the introduced structural disorder. Scaling equations for the elastic Poisson's ratio, the Young's modulus and the yield strength were determined as functions of the structural disorder and the solid fraction. The extended model was applied to identify the elastic–plastic behavior of the solid phase of nanoporous gold. It was found, that the elastic Poisson's ratio provides a robust basis for the calibration of the structural disorder. Based on this approach, a systematic study of the size effect on the yield strength was performed and the results were compared to experimental data provided in literature. An excellent agreement with recently published results for polymer infiltrated samples of nanoporous gold with varying ligament size was found.

1. Introduction

Samples of nanoporous gold, made by dealloying, take the form of a monolithic homogenous network structure consisting of nanoscale ligaments with a uniform ligament size between 5 and 500 nm (Erlebacher et al., 2001; Hakamada and Mabuchi, 2007; Li and Sieradzki, 1992; Parida et al., 2006; Weissmüller et al., 2009). The macroscopic samples can be described as porous bodies with a solid fraction around 30% (Erlebacher et al., 2001; Li and Sieradzki, 1992). Current research focuses on the prospective use as functional material for catalysis (Ding and Chen, 2009; Snyder et al., 2010; Wang et al., 2012), actuation (Biener et al., 2009; Kramer et al., 2004) and sensing (Chen et al., 2012) applications. For each of these fields the mechanical properties are of importance. It is noteworthy that the strength of nanoscale objects–such as the ligaments in nanoporous gold–increases systematically with decreasing size (Biener et al., 2006; Volkert and Lilleodden, 2006). Resulting from the well-described manufacturing process, nanoporous gold has been established as a model system

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http://dx.doi.org/10.1016/j.jmps.2016.02.018

for the study of the mechanical properties at the nanoscale. So produced macroscopic samples of several millimeters in size provide access by micro- or macromechanical testing while exploiting the strength of nanoscale objects (Huber et al., 2014; Li and Sieradzki, 1992; Ngô et al., 2015). The crystal lattice of the initially undealloyed lattice survives the dealloying process, leading to a much larger grain than ligament size (Weissmüller et al., 2009). Nanoporous structures with a ligament size in the order of nanometers have an average grain size in the order of microns, meaning a single grain consists of billions of ligaments (Jin et al., 2009).

Porous materials can be characterized by their porosity, thus by the solid fraction $\varphi = \rho/\rho_s$, where ρ denotes the density of the porous material and ρ_s the density of the solid phase. The Gibson-Ashby scaling laws for open cell foams (Gibson and Ashby, 1997), which are well established for cell sizes in the micrometer range, are commonly applied to nanoporous metals, providing a relationship between the solid fraction and the mechanical behavior. These scaling laws do not consider specific geometric features and it is assumed, that the geometry of nanoporous gold does not fundamentally differ from the one for macroporous materials (Weissmüller et al., 2009). Therefore, the Gibson-Ashby scaling laws have been adapted to nanoporous gold and are giving a good starting point for the evaluation of the mechanical behavior in terms of the macroscopic Young's modulus E and the macroscopic yield strength σ_y by

$$\frac{E}{E_s} = C_E\,\varphi^2 \tag{1}$$

and

$$\frac{\sigma_y}{\sigma_{ys}} = C_\sigma\,\varphi^{3/2}. \tag{2}$$

In the previous equations the subscript s denotes the material properties of the solid phase and C_E and C_σ are constants determined by experiments.

The first experimental studies of the mechanical behavior of nanoporous gold used nanoindentation or micropillar compression. Their results, as summarized in (Hodge et al., 2007; Weissmüller et al., 2009; Yang and Li, 2008), were consistent with the Gibson-Ashby equations for the variation of strength with solid fraction and with a power-law relation between strength and structure size (Greer et al., 2005; Uchic et al., 2004; Volkert et al., 2006). Further work combining the analysis based on the Gibson-Ashby model with experimental investigations on nanoporous metals suggested incorporation of a Hall–Petch-type relationship between the average yield strength and the average ligament diameter (Hodge et al., 2007).

Recently, studies using atomistic simulations have confirmed the general trends of the previous experiments, while suggesting corrections to the scaling law (Sun et al., 2013) and pointing towards deviations (Farkas et al., 2013) between the plastic behavior in compressive and tensile direction. Yet being able to deform macroscopic samples of nanoporous gold to large compressive strains, further investigations led to inconsistencies to previous results (Huber et al., 2014; Jin et al., 2009; Wang et al., 2015), indicating that the material's coupling behavior between the solid phase and the macroscopic mechanical response is still not fully clarified.

2. Scaling laws for a unit cell

Huber et al. concluded in (Huber et al., 2014) that the scaling of nanoporous gold depends on the complexity of the unit cell, which also includes the degree of randomization. The scaling laws derived from a simple ball-and-stick model and the major results of a subsequent finite element study for a randomized structure, presented in (Huber et al., 2014), will be briefly summarized in the following sections.

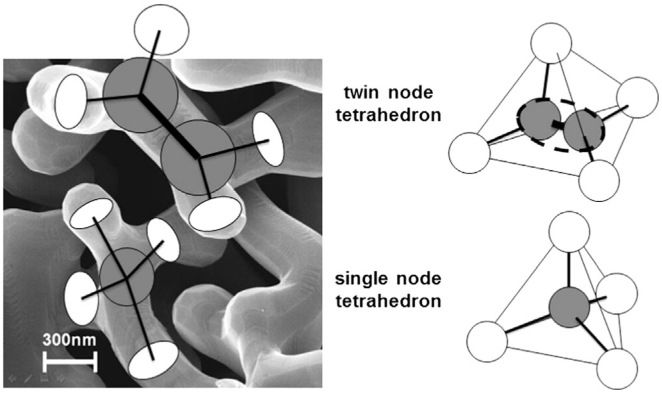

Fig. 1. Scanning electron micrograph and simplification of a three dimensional interconnected nanoporous gold structure to tetrahedral building blocks (from Huber et al., 2014).