Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 67 (2014) 252–265

Acta MATERIALIA

www.elsevier.com/locate/actamat

Scaling laws of nanoporous metals under uniaxial compression ☆

N. Huber [a,*], R.N. Viswanath [a,b], N. Mameka [a], J. Markmann [a,c], J. Weißmüller [a,c]

[a] Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, Max-Planck-Strasse 1, 21502 Geesthacht, Germany
[b] Surface and Nanoscience Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, India
[c] Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

Received 30 August 2013; received in revised form 5 December 2013; accepted 5 December 2013
Available online 1 February 2014

Abstract

This study is motivated by discrepancies between recent experimental compression test data of nanoporus gold and the scaling laws for strength and elasticity by Gibson and Ashby. We present a systematic theoretical investigation of the relationship between microstructure and macroscopic behaviour of nanoporous metals. The microstructure is modelled by four-coordinated spherical nodes interconnected by cylindrical struts. The node positions are randomly displaced from the lattice points of a diamond lattice. We report scaling laws for Young's modulus and yield strength, which depend on the extension of nodal connections between the ligaments and the solid fraction. A comparison with the scaling laws of Gibson and Ashby revealed a significant deviation for the yield stress. The model was applied for identifying a continuum constitutive law for the solid fraction. Matching the model's predicted macroscopic stress–strain behaviour to experimental data for the flow stress at large compression strain requires the incorporation of work hardening in the constitutive law. Furthermore, the amount of disorder of the node positions is decisive in matching the model results to the experimental observations of an anomalously low stiffness and an almost complete lack of transverse plastic strain.

Keywords: Nanoporous; Structure–property relationship; Plastic deformation; Compression test; Finite-element simulation

1. Introduction

Nanoporous metal made by dealloying takes the form of macroscopic (millimetre- or centimetre-sized) porous bodies with a solid fraction around 30% [1–3]. The material exhibits a network structure of 'ligaments' with a uniform characteristic ligament diameter that can be adjusted between 5 and 500 nm. Current research explores the use of nanoporous metal, and specifically nanoporous gold, made by dealloying as functional material with regard to catalysis [4–7], actuation [8–10] and sensing [11]. Mechanical performance is of relevance for each of these fields. It is therefore noteworthy that the strength of nanoscale objects – such as the ligaments in nanoporous gold – increases systematically with decreasing size. Nanoporous network structures made by dealloying offer themselves as suitable model systems for (i) exploring this phenomenon in experiment and (ii) implementing the high strength of individual nano-objects into a materials design strategy that yields macroscopic functional and/or structural materials which exploit the strength of nanoscale objects.

The first experimental studies of the mechanical behaviour of nanoporous gold used nanoindentation or micropillar compression. Their results, as summarized in Refs. [3,12,13], were found to agree with the Gibson–Ashby foam scaling equations [14] for the variation of strength with solid fraction and with the power-law relation between strength and structure size [15–17]. More recently, two studies using atomistic simulation have confirmed the general trends of the early experiments while suggesting corrections to the scaling law [18] and pointing towards

* Corresponding author.
E-mail address: norbert.huber@hzg.de (N. Huber).

1359-6454/$36.00
http://dx.doi.org/10.1016/j.actamat.2013.12.003

deviations [19] between the plastic behaviour in compression and in tension. Yet, while experiments with macroscopic samples of nanoporous gold that can be deformed to large strain in compression [20,21] document the constitutive behaviour in the form of stress–strain curves that can be compared to theory and simulation, the opportunity for comparison remains yet to be exploited. This would be all the more interesting as the compression experiments expose a number of nontrivial features, most importantly a significant work hardening and, hence, uniform deformation in compression, the absence of transverse plastic strain, an apparent yield stress that is considerably below that inferred from the nano- or microscale experiments, and the accumulation of lattice defects in the form of a dislocation cell structure at large strain [20]. The most recent experiments have also shown that the flow stress of macroscopic nanoporous gold samples can be reversibly varied by up to a factor of two by simply transferring electric charge to the surfaces through electrochemical double-layer charging or reversible electrosorption, highlighting the role of the surface for the deformation behaviour [21]. Furthermore, the compression–tension anisotropy of the work hardening – which leads to instable plastic flow and brittleness in tension – can be suppressed by impregnating the pore space with a polymer [22]. This opens the way to ductilizing nanoporous gold in tension. Here, we investigate the elastic and plastic deformation behaviour of nanoporous gold in a micromechanical approach, emphasizing the comparison between the modelling and the recent experimental data for the transverse plastic behaviour, as well as the work hardening during large-strain plastic deformation under compression.

Nanoporous metals are characterized by their solid fraction $\varphi = \rho/\rho_s$, where ρ and ρ_s denote the mass densities of the porous material and of the solid skeleton phase, respectively. Although nanoporous metals typically have a solid fraction of $\varphi > 0.25$, the Gibson–Ashby model [14] for low-density cellular open foams is commonly applied to these materials [3]. In this case the scaling of the macroscopically effective values of Young's modulus, E, and yield stress, σ_y, is given in dependence of the solid fraction by

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

and

$$\frac{\sigma_y}{\sigma_{ys}} = C_\sigma \varphi^{n_\sigma} \tag{2}$$

respectively. In these equations E_s and σ_{ys} denote the modulus and the yield stress of the solid phase.

As summarized in Ref. [23], for bending-dominated behaviour we have $n_E = 2$ and $n_\sigma = 3/2$, while for tension-dominated behaviour $n_E = n_\sigma = 1$. As a generalization of the Gibson–Ashby model, the effect of the variation in the geometry of the skeleton on the reduced modulus was studied for different unit cell geometries [24]. Values of $1.3 < n_E < 3$ were found for the random microstructures, indicating a more complex dependence than typically obtained for periodic cell theories.

Further work that combined the analysis based on the Gibson–Ashby model with experimental investigations on nanoporous metals suggested incorporating a Hall–Petch-type relation between the average yield strength and the average ligament diameter [13]. The impact of the surface excess elastic parameters on the effective elastic response has also been considered [25]. Motivated by the experimental findings for nanoporous metals having higher solid fractions ($\varphi \geqslant 0.4$), Liu and Antoniou [26] proposed a modified rectangular unit cell that accounts for the geometrical dimension of the additional mass at the junctions of ligaments. The scaling law for the elastic modulus required an extension by an additional geometric parameter characterizing the extension of this mass.

It was suggested very recently that the Gibson–Ashby model [14] should be modified for nanoporous metals according to their deformation mechanisms at the nanoscale [18]. The tensile behaviour and size effects of open-cell nanoporous gold were investigated using molecular dynamics (MD) simulations. Consistent with experimental results, it was found that the ultimate tensile strength of nanoporous Au depends on the average ligament diameter. In relation to Young's modulus, the scaling law was determined by calibration with the MD results. The result took the form

$$\frac{E}{E_s} = C_{E,b}\varphi^2 + C_{E,t}\varphi \tag{3}$$

where the two terms on the right side of Eq. (3) correspond to bending and tensile deformation of the ligaments, respectively, with $C_{E,b} = 0.14$ and $C_{E,t} = 0.136$. Furthermore, it was found that the yield strength in tension is dominated by axial yielding of the ligaments, for which $n_\sigma = 1$. The corresponding scaling law reduced to

$$\frac{\sigma_y}{\sigma_{ys}} = C_\sigma \varphi \tag{4}$$

The results of these studies suggest that the mechanics of nanoporous metals follow the relationships by Gibson–Ashby, where the scaling of the reduced modulus includes both bending and tension contributions, while the macroscopically effective yield stress is mainly controlled by tension.

From the literature discussed above, we can conclude that the scaling of nanoporous metals depends on the complexity of the unit cell, which also includes the degree of randomization. The loading direction (macroscopic tension or compression loading) determines if the dominating deformation in the ligaments is bending and/or tension. Most theoretical works concentrate on the elastic properties, while the literature on the scaling laws for yield stress, particularly for nanoporous metals under compression loading, is scarce.

Because large plastic deformation of nanoporous metals can only be obtained in compression tests, the experiment