Acta Materialia 103 (2016) 796–808

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression

Duancheng Ma [a, *], Philip Eisenlohr [a, b], Eike Epler [c], Cynthia A. Volkert [c], Pratheek Shanthraj [a, d], Martin Diehl [a], Franz Roters [a], Dierk Raabe [a]

[a] Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
[b] Chemical Engineering and Materials Science, Michigan State University, East Lansing 48824, MI, USA
[c] Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany
[d] Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen University, Schinkelstraße 2, D-52062 Aachen, Germany

ARTICLE INFO

Article history:
Received 24 July 2015
Received in revised form
18 October 2015
Accepted 7 November 2015
Available online xxx

Keywords:
Honeycomb
Cellular material
Nanoporous gold
Crystal plasticity
Crystallographic orientation

ABSTRACT

We present a study on the plastic deformation of single crystalline stochastic honeycombs under in-plane compression using a crystal plasticity constitutive description for face-centered cubic (fcc) materials, focusing on the very early stage of plastic deformation, and identifying the interplay between the crystallographic orientation and the cellular structure during plastic deformation. We observe that despite the stochastic structure, surprisingly, the slip system activations in the honeycombs are almost identical to their corresponding bulk single crystals at the early stage of the plastic deformation. On the other hand, however, the yield stresses of the honeycombs are nearly independent of their crystallographic orientations. Similar mechanical response is found in compression testing of nanoporous gold micro-pillars aligned with various crystallographic orientations. The macroscopic stress tensors of the honeycombs show the same anisotropy as their respective bulk single crystals. Locally, however, there is an appreciable fluctuation in the local stresses, which are even larger than for polycrystals. This explains why the Taylor/Schmid factor associated with the crystallographic orientation is less useful to estimate the yield stresses of the honeycombs than the bulk single crystals and polycrystals, and why the plastic deformation occurs at smaller strains in the honeycombs than their corresponding bulk single crystals. Besides these findings, the observations of the crystallographic reorientation suggest that conventional orientation analysis tools, such as inverse pole figure and related tools, would in general fail to study the plastic deformation mechanism of monocrystalline cellular materials.

1. Introduction

This study is inspired by the recent development of bulk nanoporous gold (NPG), especially by its applications as actuators and sensors [1–4]. Early studies on the mechanical properties of NPG using nanoindentation [5–8] and micro-pillar compression [6,9] revealed a size effect of the NPG, *i.e.* the smaller the ligament size is, the stronger is the NPG. It is observed that when the ligament size approaches 10 nm, the yield stress of the ligament (the beam connecting the nodes) reaches its theoretical yield strength suggested by the micro-pillar NPG compression test [9]. Despite the high yield strength, NPG has been proven to be brittle as shown by tensile tests on millimeter-size samples [10], where no apparent plastic deformation was observed in the stress–strain curve. Especially, as the size of the ligament becomes small, the NPG undergoes a ductile-to-brittle transition [11,12]. Recently, it has been shown that the ductility of NPG can be significantly improved by optimizing the dealloying process which enables realizing crack-free NPG bulk samples [13]. The analysis and interpretation in these investigations are mostly based on the analytical models developed for macroscopic cellular materials (e.g. Gibson and Ashby [14]) and the knowledge of gold nano-wires and micro pillars [15–22]. To account for the size effect, these analytical models employed in the previous experimental studies have been extended by including the Hall–Petch effect [8] or strain gradient effects [23]. Due to the large length scale difference between the sample size (μm to mm) and the ligament size (nm) [9,10,13] in addition to the complex cellular structure, the direct observation of the deformation

* Corresponding author.
E-mail address: d.ma@mpie.de (D. Ma).

http://dx.doi.org/10.1016/j.actamat.2015.11.016
1359-6454/

mechanisms of NPG is very challenging. Though efforts have been made by using transmission electron microscopy (TEM) and scanning electron microscopy (SEM) [13,24–27], a comprehensive structure–property relation of NPG has not been established. Hence, numerical modeling can be an alternative to improve the understanding of the relation between the cellular structure and its mechanical response upon external loading. By using continuum models, the elastic and plastic deformation of metallic nanoporous materials have been investigated [28–31] where the main focus was to use more realistic cellular structures from experimental observations aiming at a better prediction of the elastic modulus and yield stress. In these studies, the constitutive description considers the base materials of the cellular materials as isotropic. However, as exemplified by Jin et al. [13], the mean grain size of NPG is typically orders of magnitude larger than the ligament size, *i.e.* within one grain, each ligament and each node connecting the ligaments all share the same crystallographic orientation. Hence, using isotropic models is not adequate to correctly describe the elastic and plastic anisotropy of the crystalline materials, particularly for single crystals under complex boundary conditions [32,33].

In this study, we make the first attempt to address the interplay between the cellular structure and the mechanical anisotropy of the base material by using crystal plasticity simulations. The primary aim is to reveal the possible impact of the anisotropy on the mechanical properties of the single crystalline cellular materials, as well as invoking new experimental and computational investigations. Instead of directly addressing three-dimensional (3D) foams, in this paper, on the modeling side, we only focus on two-dimensional (2D) honeycombs, and we confine ourselves to studying the dependence of the plastic deformation of single crystalline stochastic honeycombs on the crystallographic orientation, as illustrated in Fig. 1. The corresponding elastic behavior is presented and discussed in another publication [34]. Besides the crystal plasticity simulation, we also conducted NPG micro-pillar compression tests aligned with various crystallographic orientations.

It should be emphasized that the simulation and the experiment conducted in this study do not match one-to-one for the following reasons: (1) obviously the geometries in terms of the cellular structure are different, *i.e.* 2D honeycombs in the simulation and 3D foams in the experiments. (2) the boundary conditions are also different, *i.e.* in the simulation, plane strain compression is applied, and in the experiments, unaxial compression is applied. (3) As mentioned above, NPGs exhibit a size effect [9] which is not included in the constitutive law implemented in the current simulation approach. On the other hand, it has been shown that the slip system activation in gold micro-pillars still follows the Schimd law as in bulk samples [19]. The employed crystal plasticity model in this study is capable of tackling the kinematic evolution of the crystals during plastic deformation. Thus, the simulation and experiments still can be qualitatively compared in terms of the crystallographic orientation effect on the mechanical response of the monocrystalline cellular materials.

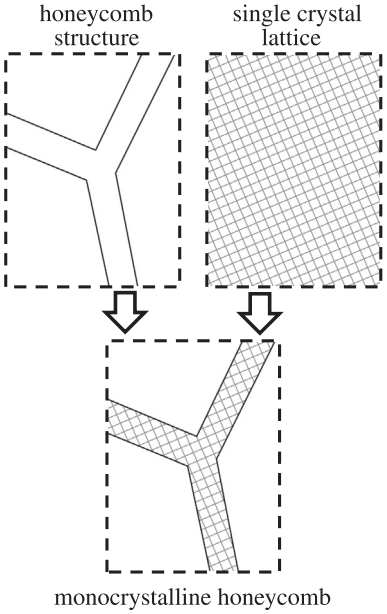

Fig. 1. A schematic of the motivation of this study which is to investigate the interplay between the cellular structure and the crystallographic orientation.

This paper is organized as follows: in Section 2, we first describe the experimental procedure of the compression tests on NPG micro-pillar, followed by the description of crystal plasticity model and the simulation setup in Section 3. The experimental results of the compression tests on NPG micro-pillar are to be shown in Section 4; and in Section 5, we present the simulation results of the monocrystalline honeycombs, including the stress–strain curves, the slip activities, and the crystallographic reorientation; the results presented in Sections 4 and 5 will be discussed in Section 6; finally, Section 7 summarizes this study.

2. Methodology of micro-pillar compression tests on nanoporous gold

Microcompression experiments were performed on nanoporous Au (NPG) with 70% porosity with open foam structure. The specimen was prepared from an as-drawn Au_{30} Ag_{70} alloy wire. First, slices were cut from the wire, then polished and annealed at 950° C for 100 h to allow for grain growth. Nanoporous Au was synthesized from the annealed alloy slices using free corrosion in HNO_3 (65%) for 72 h to remove the Ag. The Ag content in the dealloyed specimens was determined to be less than 1 at.% by EDX analysis in the SEM. Measurements of the dimensions show that less than 1% shrinkage occurs during dealloying, and combined with the sample weights before and after dealloying, are consistent with a relative density of the dealloyed specimens of 30–31%. SEM images of the NPG specimens reveal ligament diameters of approximately 50 nm and cell sizes of approximately 75 nm. The crystallographic orientations of the grains were determined using electron backscatter diffraction (EBSD) in an SEM at 20 keV. The out of plane orientations were recorded both using Miller indices and graphically in an inverse pole figure.

The compression tests were performed on pillars of 3 μm diameter and 6 μm height that had been cut out of single grains in the polished surfaces of the NPG samples using focused ion beam milling with 30 keV Ga [9]. Pillars were cut into several grains. The grains are easily identified in the SEM micrographs by the grooves that formed at the boundaries during the anneal. The micro-pillars were uniaxially compressed at a loading rate of 50 μN/s using a flat punch in a nanoindenter (MTS G200 XP) [9,19]. The measured forces and displacements were converted to engineering stresses and strains using the pillar diameter dimensions [9,19]. The flow stresses were estimated by the intercept of the initial linear elastic slope and the slope in the plastic region.

3. Modeling and simulation methodology

In this study, crystal plasticity (CP) [35,36] is applied. In this section, the spectral based method to solve the mechanical equilibrium and compatibility conditions is first briefly mentioned, followed by the formulation of the employed CP constitutive