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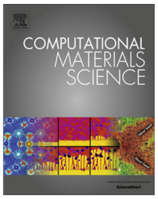

# Deformation mechanisms in nanoporous metals: Effect of ligament shape and disorder

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ABSTRACT

The current work presents a numerical modelling approach for investigating the effect of ligament shape and disorder on the macroscopic mechanical response of nanoporous gold (NPG). The approach starts from a 'single ligament' analysis with respect to three fundamental deformation modes, bending, torsion, and compression, that depend on the ligament shape. It can be shown that the predictive capability of the highly computationally efficient beam model is sufficient for a large variation in ligament shapes. Using a representative volume element (RVE) composed of such ligaments, different degrees of disorder are included. For both the single ligament and RVE models, the cylindrical beam serves as a common reference to compare the results when varying the ligament shape. From the comparison of the RVE elastic response with the single ligament results and the further analysis of statistical information from the elements in the RVE, it is found that bending is the major deformation mode for perfectly ordered RVEs, whereas torsion gains importance for increasing RVE disorder. The effect of compression of the ligaments can be neglected in general. It is concluded that the transition to torsion deformation due to disorder is the cause of the strongly reduced lateral expansion during compression deformation of NPG.

## 1. Introduction

Nanoporous gold (NPG) made by de-alloying can be produced as macroscopic objects that exhibit a bi-continuous network of nanoscale pores and solid 'ligaments' [1]. The solid fraction of the porous body is approximately 30% [1,2]. Recent studies explored the use of NP metals, especially NPG, made by de-alloying as a functional material for catalysis, actuation and sensing [3–5]. Mechanical performance is relevant to each of these fields. It is therefore necessary to gain a fundamental understanding of the mechanical behavior of such a material. Experimental tests on the compression, tension, fracture, and indentation of NPG reflect the current interest in this material [6,7]. Numerous experimental studies reported that in addition to the relative density, the strength of NPG strongly depends on its average ligament radius [8–10], that is, the macroscopic strength of NPG increases with decreasing ligament size [2,11–14].

There is no doubt that one of the most interesting features that NPG materials possess is the famous 'size effect' [9,14], i.e., different macroscopic mechanical responses have been observed for different ligament sizes, specifically different ligament radii, for the same solid fraction. However, the fundamental reason for this effect is still under debate.

It would be rational to state that the macroscopic mechanical response of an NPG material is mostly influenced by two aspects: the constitutive material law and the geometrical/structural properties of the ligament network. Concerning the constitutive law, extensions to classical continuum plasticity models, e.g., as applied in [7,15], have been suggested for including size effects by splitting the volume and the surface into separate models [16] or in the form of a gradient extended crystal plasticity theory [17]. In this way, a size-dependent elastic modulus or size-dependent plasticity can be predicted. The latter is computationally expensive, so until now, relatively simple honeycomb-like 2D-structures have been studied.

Choosing an arbitrary average ligament size, the size effect reduces to a given Young's modulus and yield strength captured with the material parameters of a conventional plasticity model. Microscopic features such as surface effects are ignored. In this way, attention is drawn towards the influence of the shape-related parameters of NP materials as has been analyzed previously in several works [7,15,18–21]. One could argue that the determination of the size effect for NP materials, typically making

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use of models translating macroscopic stress into local stresses acting in the ligaments, requires the knowledge of the relationship between the shape-related properties and the macroscopic mechanical response.

Motivated by previous publications [7,15,18–21], where all ligaments were assumed to be cylindrical and of the same size, Pia and Delogu [18] conducted a statistical analysis for quadratic beams, focusing on the relationship between the morphological features of the ligaments and the mechanical responses of the NP materials. In their study, a simplified polynomial equation (Eq. (1)) was applied to describe the geometrical profiles of different ligament variations extracted from scanning electron microscopy (SEM) micrographs. Based on these statistical morphology data, a phenomenological model based on Timoshenko's beam bending theory was developed to describe elastic bending. Their work brought further insight towards revealing the influences on the elastic response produced by the ligament geometry of NP materials.

$$r = nx^2 + m \tag{1}$$

In Eq. (1), $r$ denotes the ligament radius and $x$ is the axial coordinate with $x = 0$ being the ligament's center. The shape of the ligament is defined as $n = (r_{end} - r_{mid})/(l/2)^2$ and $m = r_{mid}$, where, $r_{end}$ is the radius at the ends, $r_{mid}$ is the radius in the middle of the ligament, and $l$ is the length of the ligament.

When considering the work of Pia and Delogu [18] as an important element describing the relationship between the ligament geometrical properties and the macroscopic mechanical response, another equally important element to consider is the network construction of the NP materials. Based on the 'ball-and-stick' beam model proposed by Huber et al. [7], Roschning and Huber [15] conducted a thorough investigation on the influences of the randomization parameter ($A$) of network randomization on the mechanical response of an RVE. It was found that the Young's modulus ($E$), yield strength ($\sigma_y$), and elastic Poisson's ratio ($\nu_E$) are heavily influenced by $A$. This is mainly because $A$, as the major structural parameter across the whole RVE, is responsible for describing the length variation and curvatures of the ligaments that control the deformation mechanisms within the ligament network.

The works of [7,15,18] were the pioneering efforts for analytically characterizing the effects of the geometrical and structural properties of NP materials on the mechanical responses of NP materials. This inspired a further study combining both approaches into one comprehensive work. It is worthwhile to note that most of the work studying the mechanical behavior of NP metals is based on macroscopic compression. Samples can be produced in mm to cm scale in a quality allowing large plastic deformation in such tests [22]. It has been assumed in [7,18,19,23] that during macroscopic compression, bending is the dominant deformation mechanism and that the effects of axial tension and compression within the ligaments can be neglected.

NP materials show immediate brittle failure in experiments under macroscopic tension. So far, the only way to prevent this is by infiltration with a polymer. It has been shown recently that such a material can be deformed in four-point bending to considerable strains [24]. However, there exist theoretical studies, such as [25], that investigated the scaling laws of an NPG under macroscopic tension. In addition, in the MD simulations presented in [25], progressive necking and rupture were observed, but the stress-strain data before that point could be used to fit the Gibson-Ashby model. The resulting scaling law contains an additional term, which is linear for the Young's modulus. This underlines the relevance of tension deformation within the ligaments, which reflects the increasing alignment of the ligaments during macroscopic tensile deformation.

The present work establishes the relationship between the geometrical and structural properties and the corresponding mechanical responses, beginning with the analysis of single ligaments. The ligaments serve as building blocks with variable geometrical properties defined by a few parameters. In an extension to [18], the mechanical response is investigated not only for bending but also for three fundamental loading cases, i.e., bending, torsion, and compression, depending on the geometrical parameters. This is followed by analyses of compressing ordered and disordered NPG networks composed of a large number of such ligaments within an RVE with regard to the elastic modulus and yield strength. This brings the discussion to the structural level, following [7,15]. A close correlation between the single ligament geometry and the macroscopic mechanical response of the RVE is revealed, and the contributions from bending, torsion, and compression on the deformation mechanisms are discussed.

## 2. Single ligament analysis

### 2.1. Model setup

#### 2.1.1. Geometry determination

The finite element analysis (FEA) code ABAQUS/Implicit [26] is used for this analysis. Both beam and solid elements are applied for the single ligament analysis. The objective of applying a computationally more expensive solid model is to examine the applicability and accuracy of the beam model that offers excellent computational efficiency for a spectrum of typical ligament geometries and loading conditions. In the following, $r$ and $l$ denote ligament radius and ligament length, respectively, as illustrated in Fig. 1a. According to Eq. (1), the ligament radius of the cylindrical ligament is denoted as $r(n = 0) = r_0$, and the aspect ratio of a ligament is defined as $r_0/l$, i.e., the cylindrical ligament serves as a common reference for all ligament geometries throughout this work.

A shear deformable beam element has been compared with a solid element using a Kalvin unit cell [27], validating the modelling capability of the beam element for open cell foam structures with a solid fraction $\varphi$ ranging from 2% to 9% for polyester urethane and aluminum foams. However, unlike the thin beam with a small aspect ratio $r_0/l \approx 0.1$ as used in [27], ligaments with a larger $r_0/l$ ratio of approximately 0.25 are typical for NPG materials [7,15]. This leads to the question of whether the beam element is capable of capturing the main characteristics of the thick ligaments with sufficient accuracy, i.e., deviations should be below the uncertainties in the experiments on NPG.

Fig. 1b shows that the ligament shape varies significantly in a real material. To analytically describe the ligament shapes, a quadratic equation (Eq. (1)) is implemented, following Pia and Delogu [18]. Ligaments with varying shapes can be characterized using the dimensionless parameter $n \cdot r_0$. For $n \cdot r_0 > 0$, the ligament shape is concave, while for $n \cdot r_0 < 0$, the ligament has a convex shape. While [18–20] exclusively studied the case of $n \cdot r_0 > 0$, the geometries found in [28] by analyzing the 3D FIB tomography of polymer-infiltrated NPG suggests extending the analysis to $n \cdot r_0 < 0$. Such convex ligaments are supposed to originate from the pinching-off and retracting of ligaments during heat treatment and coarsening, leaving a mass concentration, also called a "dangling" ligament.

The solid fraction $\varphi$ is the major parameter for describing the structure-property relationship of NP materials [2,29]. The calculation of $\varphi$ for RVE in the current paper can be found in [15], which is derived from the ball-stick model of the diamond