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Deformation behavior of nano-porous polycrystalline silver. Part II: Simulations

S. Zabihzadeh [a, b], J. Cugnoni [c], L.I. Duarte [d], S. Van Petegem [a], H. Van Swygenhoven [a, b, *]

[a] Photons for Engineering and Manufacturing, SYN, Paul Scherrer Institut (PSI), CH-5232 Villigen, Switzerland
[b] Neutrons and Xrays for Mechanics of Materials, Institute of Materials, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
[c] Ecole Polytechnique Fédérale de Lausanne (EPFL), LMAF-STI, Lausanne, CH-1015, Switzerland
[d] ABB Switzerland Ltd. Corporate Research, CH-5405, Baden-Daettwil, Switzerland

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ABSTRACT

Three-dimensional finite element simulations of nano-porous silver structures are performed to understand the correlation between the porous morphology and the mechanical behavior. The nanostructures have been obtained from ptychographic X-ray computed tomography. The simulations allow distinguishing between the interplay and role of the ligament size, the pore morphology and the porosity, and therefore provide a better comprehension of the experimental observations. We show that the proposed model has a predictive character for mechanical behavior of nano-porous silver.

1. Introduction

The mechanical response of porous materials can be modeled with finite element (FE) simulations [1]. Several models exist to generate these structures such as the periodic Kelvin cells [2] and the Weaire-Phelan cells [3] generated with the surface Evolver program developed by Brakke [4] or the Voronoi Diagram [5]. It is however also possible to generate a micromechanical model directly from the microstructure obtained by tomography techniques [1]. To capture the effects of heterogeneity and structure of the porous network three-dimensional (3D) simulations are required. Recent developments in high-resolution 3D imaging techniques, such as focus ion beam (FIB)/scanning electron microscopy (SEM) or X-ray tomography launched a larger interest in performing 3D simulations on the actual microstructure of the porous materials [6–12]. Using high-resolution 3D images obtained from serial-block face scanning electron microscopy [13], Carr et al. [9] studied the influence of aging on the porosity, the pore distribution and the elastic modulus of sintered micro silver paste. It was reported that aging does not influence the global density and the elastic modulus of the material. However, aging increases the heterogeneity in the pore distributions and results in a clustering of pores leading to a local decrease of the elasticity next to the high porous regions. Our previous [14] experimental work on nano-porous sintered silver layers showed a strong dependency of the mechanical behavior on the microstructure. To allow a better understanding, 3D (FE) microstructure-based simulations are performed. The statistically representative volume elements or RVE were obtained by ptychographic tomography, a technique providing a higher resolution than X-ray nano-tomography [15]. By comparing the simulation results with in-situ and ex-situ tensile tests the deformation mechanisms are discussed.

2. Experimental setup and simulation methodology

2.1. Sample fabrication

Eight thin layers (25 ± 5 μm) of porous polycrystalline silver layers are produced during pressure assisted sintering. The samples are called as S1–S8 and are sintered in the temperature range of 210–300 °C, pressure range of 4–12 MPa during 3–10 min. More details about sample fabrications are found in first part of the paper [15]. S1 and S8 are samples sintered respectively at lowest and highest extremes of sintering conditions.

* Corresponding author. Photons for Engineering and Manufacturing, SYN, Paul Scherrer Institut (PSI), CH-5232 Villigen, Switzerland.
E-mail address: helena.vs@psi.ch (H. Van Swygenhoven).

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2.2. In-situ tensile testing

The in-situ mechanical tests are carried out at the powder diffraction station of MS beam-line of the SLS [16]. For the in-situ experiments, an X-ray beam with energy of 20 KeV and a size of $400 \times 200\ \mu m^2$ is selected and the diffraction patterns are recorded with the MYTHEN II microstrip detector [17]. The diffraction peaks are fitted with a split Pearson-VII function plus a linear function (for background noise) and information about full-width-at half-maximum (FWHM), integral width (iw) and peak position (θ) are extracted. Finally, Williamson-Hall (W–H) method based on Gaussian-Cauchy distribution [18] is applied for deconvolution of the peak broadening caused by the grain size and root-mean-square (RMS) strain [14,19,20]. RMS strain is defined as the spread of the lattice strain from the averaged value inside a grain, calculated from FWHM, and is an estimation of the internal strain inside the material. A dog-bone shaped geometry with width of $2000 \pm 5\ \mu m$, thickness of $25 \pm 5\ \mu m$ and gauge length of $1500\ \mu m$ is selected for tensile experiments and strain is measured using digital image correlation (DIC) method. The specimens are deformed during continuous tensile test at room temperature and with a strain rate for $0.015\%.s^{-1}$ for ex-situ and $0.01\%.s^{-1}$ for in-situ experiments.

2.3. Simulation methodology

The general framework of the microstructure-based simulation is similar to the work done by Maleki et al., 2016 [23]. First, the high-resolution 3D reconstructed images obtained from the ptychography measurements [15] are segmented for the silver phase using the ITK-SNAP software, then they are meshed using the software VoxelMesher developed at the Laboratory of Applied Mechanics and Reliability Analysis (LMAF) group of École polytechnique fédérale de Lausanne based on the algorithm presented in Ref. [21]. A quadratic ten-node tetrahedron is selected as the meshing element. Details about the X-ray ptychography measurement and analyzed porous structure of the samples are found in Ref. [15]. Fig. 1 displays a representative 3D image of the segmented silver phase for a pillar with diameter of 4 μm. The FE package used in this work is Dassault Simulia Abaqus Standard using an implicit integration scheme (using the standard direct Newton-Raphson nonlinear solver). A mesh convergence analysis was performed to verify the stagnation of the solution with mesh refinement levels (convergence within 0.5%).

To model the loading, a displacement controlled mixed static-kinematic boundary condition is selected. This boundary condition is chosen based on the work of Cugnoni and Galli (2010) [22] on particle-reinforced composite materials; one end of the object is kept fixed in the loading direction while a displacement ramp up to 1% effective strain is imposed on the other end parallel to the tensile direction, the perpendicular lateral faces are left stress-free. More details about these boundary conditions are explained in Ref. [23]. A RVE approach [22,23], is applied for the homogenization to determine the smallest volume representative for the continuum behavior. The bulk material properties of the silver skeleton, including its elastoplastic behavior, are identified using an inverse homogenization approach on a selected sample; S5. The accuracy of the model is further verified by comparing the simulation with experimental results obtained from ex-situ tensile deformation with a strain rate of $0.015\%.s^{-1}$ performed at room temperature on a wide set of sintered silver layers. In what follows all simulations results are compared with experiments performed at a strain rate of $0.015\%.s^{-1}$ except stated otherwise.

2.4. Representative volume element

Due to heterogeneity of the porous structure, the FE simulation of the porous materials should be performed in three dimensions [24]. 3D simulations are however expensive in terms of computational time. To overcome this issue a homogenization approach is applied to minimize the required volume for the simulations. In this work the RVE approach proposed by Cugnoni and Galli [22] is employed. RVE refers to the smallest volume extracted from the bulk of a heterogeneous material which is large enough to be representative of the behavior of the whole sample while it is small enough to be simulated or measured in a reasonable time and cost [25]. According to De Gol et al. [26] an appropriate size of the RVE for an object with porosity in the range of 25–30% is estimated to be around of 8–9 times the averaged pore size. For this work, sample S5, which has a porosity of 29% and pore size in the 200–400 nm range, is selected as the reference sample for RVE identification and a cube is considered as the proper shape due to the overall isotropy of the microstructure. Details on the porous structure of sample S5 are found in Ref. [15]. The RVE size is verified by studying the convergence of the results when changing the size of the cube, by verifying the position invariance of the solution and by comparing the scatter within multiple realizations. Therefore, three different cubes with side length of 2.5 μm, 3 μm and 4 μm are

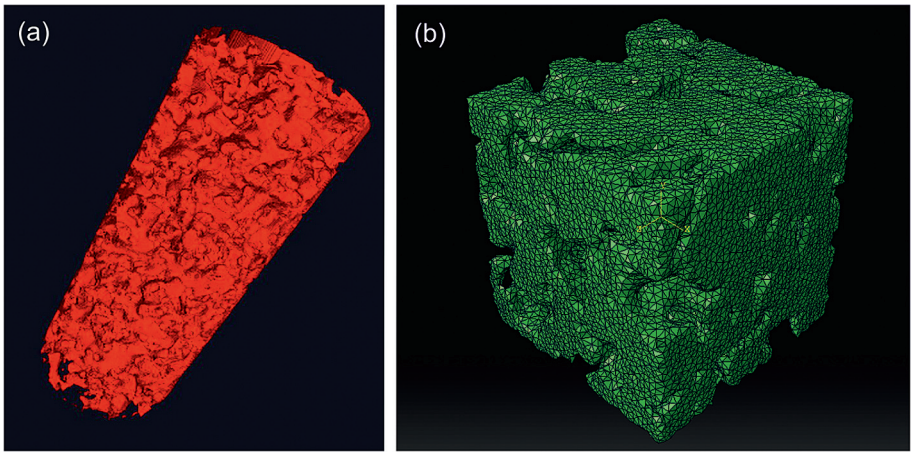

Fig. 1. (a) 3D rendering of a representative pillar with diameter of 4 μm segmented for the silver phase using the ITK-SNAP software, (b) feature-preserving FE mesh model of a 3-μm-length cube extracted from the pillar presented in (a).