A dataset combining microcompression and nanoindentation data from finite element simulations of nanoporous metals

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Abstract

Nanoporous metals with their complex microstructure represent an ideal candidate for method developments that combine physics, data and machine learning. They allow to tune the solid fraction, ligament size and connectivity density within a large range. These microstructural parameters have a large impact on the macroscopic mechanical properties. This makes this class of materials an ideal science case for the development of strategies for dimensionality reduction, supporting the analysis and visualization of the underlying structure-property relationships. Efficient finite element beam modeling techniques are used to generate ~200 data sets for macroscopic compression and nanoindentation of open pore nanofoams. A data base is provided that uses consistent settings of structural and mechanical properties on the microscale for which the elastic-plastic macroscopic compression behavior and the hardness is predicted. Ligament geometries of two different initial solid fractions are chosen, for which the structural randomization, the connectivity density, the yield stress and the work hardening rate are randomly varied in large ranges. This database allows deriving the microstructure-properties relationships of nanoporous metals by means of dimensionality reduction, data mining and machine learning.

1. Description of Data

1.1. Simulation data

The simulation data are provided in the data set **"SimulationData.zip"**. These data are computed with the help of micromechanical FE-beam models and symmetric boundary conditions following [1–3]. The variation of the ligament shape is implemented in form of the parabolic-spherical ligament as described in [4,5] in combination with the nodal correction as proposed by [6]. For description of the nanoindentation model, the reader is referred to [7], published in connection with this dataset.

The simulation dataset contains three files named "G21.dat", "G33.dat" and "G11-G44.dat". The coding of the geometry numbers "G" with indices "ij" follows [5]; corresponding ligament geometries G_{ij} are listed in Table 1. In this table, r_{end} and r_{mid} denote the radii of the ligament at the end and in the middle, respectively. The relative density (initial solid fraction before randomization and cutting of the structures) is denoted by φ_0 and is computed under the supposition that the ligaments are organized in a diamond unit cell with unit cell size $a = 1$ and ligament length $l = 0.433$ [1].

For each data set, the headings of the columns are organized in the same way, providing the input and output data of each simulation in the rows below the headings, sorted by the job number j. The headings translate to math notation as defined in Tables 2 and 3. In Table 2, further microstructural features are defined by the parameters $0 \leq A \leq 0.3$ and $0 \leq \zeta \leq 0.3$, which denote the randomization [2] and the cut fraction [3], respectively. The material behavior on the local level (ligament; solid phase – subscript s) is assumed as elastic-plastic deformation behavior with linear isotropic work hardening. The elastic properties for gold are set to $E_s = 80$ GPa and Poisson's ratio $\nu_s = 0.42$. The plastic material parameters are randomly varied in the ranges $20\ \text{MPa} \leq \sigma_{y,s} \leq 1000\ \text{MPa}$ and $1\ \text{GPa} \leq E_{T,s} \leq 10\ \text{GPa}$.

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Simulation results are denoted according to Table 3, where we distinguish between macroscopic elastic and plastic properties. The values are obtained from the homogenization of the representative volume elements (RVE) for the compression and indentation model. Similarly to the microscale, the macroscopic properties are denoted by Young's modulus E, Poisson's ratio ν, yield stress σ_y, work hardening rate E_T, plastic Poisson's ratio ν_p, and nanoindentation hardness H. Details on how they are determined from the simulations can be found in [7].

Table 1. Ligament shapes defined by parameters r_{mid} and r_{end}. Coding of the shapes G_{ij} for possible combinations of r_{mid} and r_{end} is given with resulting solid fractions φ_0.

	$\frac{r_{mid}}{r_{end}} = 0.5$		$\frac{r_{mid}}{r_{end}} = 0.75$		$\frac{r_{mid}}{r_{end}} = 1.0$		$\frac{r_{mid}}{r_{end}} = 1.25$	
r_{end}	Geometry	φ_0	Geometry	φ_0	Geometry	φ_0	Geometry	φ_0
0.1	G_{11}	0.0816	G_{12}	0.1252	G_{13}	0.1784	G_{14}	0.2421
0.125	G_{21}	0.1232	G_{22}	0.1825	G_{23}	0.2635	G_{24}	0.3661
0.15	G_{31}	0.1736	G_{32}	0.2524	G_{33}	0.3574	G_{34}	0.4871
0.175	G_{41}	0.2342	G_{42}	0.3202	G_{43}	0.4565	G_{44}	0.6131

Table 2. Description of headings in files "G21.dat", "G33.dat" and "G11-G44.dat": Simulation Inputs (micro-structure and mechanical properties)

	Ligament shape			Microstructure		Solid phase properties	
Job	rend_l	r_sym	phi	A	zeta	sy	ET
j	r_{end}/l	$\frac{r_{mid}}{r_{end}}$	φ	A	ζ	$\sigma_{y,s}$	$E_{T,s}$

Table 3. Description of headings in files "G21.dat", "G33.dat" and "G11-G44.dat": Simulation Outputs (effective macroscopic properties).

	Macrosc. elastic prop.		Macroscopic plastic properties			
Job	E_RVE	nu_RVE	sy_RVE	ET_RVE	nup_RVE	H_RVE
j	E	ν	σ_y	E_T	ν_p	H

1.2. Python code for principal component analysis

The python codes for the principal component analysis is provided with the file **"PCA-Python.zip"**. The principal component analysis (PCA) is applied in conjunction with a multi-layer perceptron (MLP) algorithm using the scikit-learn package [8]. Running the script for the PCA of the macroscopic compression PCA-RVE.py in the same folder where the data sets "G21.dat", "G33.dat" and "G11-G44.dat" are located, the code produces the images "*.png", provided with the file **"PCA-images.zip"**. These images allow to compare the result of the PCA with decreasing number of components (*PCA NC=…) with the machine learning approximation of the original data (*RAW NC =...) for all output variables or a selected output variable from Table 3.

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1.3. Results of principal component analysis

The results of the principal component analysis as described in Section 1.2 are provided in the zip file **"PCA-results.zip"**. For each variable a file "*RAW NC=*-annfit.dat" is created together with PCA files for decreasing number of components ("*PCA NC=*-annfit.dat"). These files contain two columns, where the first is the target of the ML training (desired output - d) with the RAW/PCA inputs and the second is the corresponding ML output (ann_prediction). A plot of ann_prediction versus d allows assessing, if the content of information in the presented inputs is sufficient to predict the desired output. The better the data organized along the 45° diagonal line, the better the presented information is, i.e. it is more sufficient and complete to describe and approximate the problem. The evolution of the absolute mean error is provided as table in the file (*-PCA-Err.dat).

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