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## Data Article

# Datasets for the analysis of dislocations at grain boundaries and during vein formation in cyclically deformed Ni micropillars



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## ABSTRACT

The dataset together with the corresponding Python scripts and Jupyter notebooks presented in this article are supplementary data for the work presented in Samaee et al., 2019 [1]. The data itself consists of two parts: the simulation data that was used in [1] to analyze the effect of a particular grain boundary on curved dislocations and the precession electron diffraction (PED) strain maps together with post-processed data for analyzing details of the observed dislocation vein structures. Additionally, the complete stress tensor components, which are not shown in [1], have also been included. The data sets are accompanied by Python code explaining the file formats and showing how to post-process the data.

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## Specifications Table

Subject	Materials Science (General)
Specific subject area	Combining transmission electron microscopy and simulations for the investigation of dislocation in single crystal and bicrystal Ni micropillars.
Type of data	Image Data files
How data were acquired	FEI Tecnai G2 (200 kV FEG) Transmission Electron Microscopy (TEM), nanobeam precession diffraction (PD) patterns, DigiSTAR (NanoMEGAS), TOPSPIN software.
Data format	Raw Analyzed Filtered
Parameters for data collection	The PED strain map was obtained from Pillar G1, all simulation data was obtained from finite element simulations.
Description of data collection	For obtaining the PED strain maps an electron probe of size ~4 nm was used with a step size of 40 nm and a precession angle of 0.5°. The samples were aligned along the [100] zone axis. Simulation data is based on anisotropic elasticity calculations using the finite element method, where the dislocation is represented through its equivalent eigenstrain.
Data source location	For the microscopy work: Electron Microscopy for Materials Science (EMAT), Department of Physics, University of Antwerp Antwerp Belgium
Data accessibility	For this article; additional code is available from a software repository hosted on GitLab at: <a href="https://gitlab.com/computational-materials-science/public/publication-data-and-code">https://gitlab.com/computational-materials-science/public/publication-data-and-code</a> Name of the repository: 2019_MSE-A__Samee-et-al__Dislocation-structures-and-the-role-of-GBs
Related research article	Vahid Samaee, Stefan Sandfeld, Hosni Idrissi, Jonas Groten, Thomas Pardoen, Ruth Schwaiger, Dominique Schryvers, Dislocation structures and the role of grain boundaries in cyclically deformed Ni micropillars, Materials Science and Engineering A, 769, 2020, 138295 [1]

**Value of the Data**

- The dataset shows digitized PED strain map data, which can be further analyzed
- Both experimental and simulation data can serve as reference data for other works
- The datasets will be useful for related research on dislocation structure formation for further comparisons and cross linking
- The accompanying Python scripts show how to handle digitized PED strain data
- The datasets consist of files that contain additional raw data, i.e., stress tensor components, that have not been presented in Ref. [1]. This is useful for, e.g., verification or comparison with data obtained from other methods, or for further analysis of the physical situations presented in Ref. [1].

**1. Data**

**The first dataset** which is contained in the directory 'PED-strain-maps' consists of the following files:

- *Fig. 7a\_tem\_image.png*: a TEM micrograph showing dislocation vein structures
- *strain\_xx.txt, strain\_yy.txt, strain\_xy.txt*: the digital PED strain maps in text files as x-y data with a space as column separator.

In order to show how to read in the data and how it can be further post-processed, we included two Python scripts (see the file README.md for further instructions on how to run the code). '01\_plot\_2D\_data.py' demonstrates how to read and how to produce the plot Fig. 7 in Ref. [1].

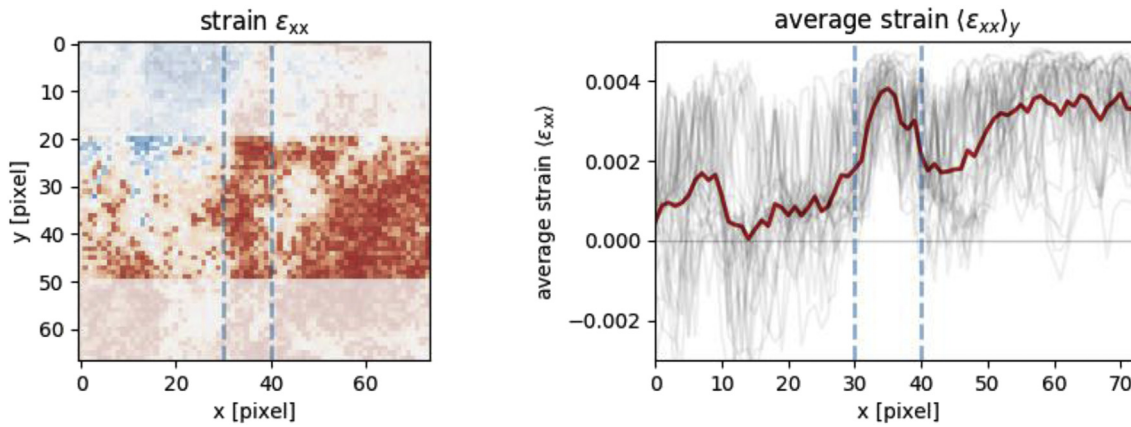
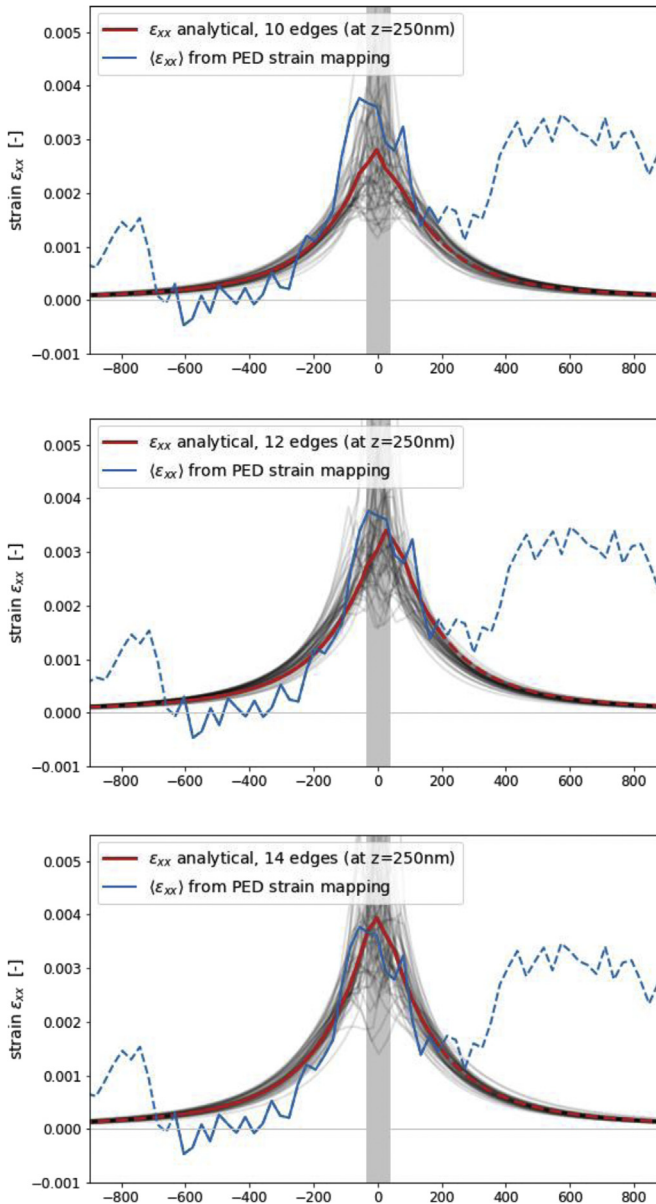


Fig. 1. Output from the script `02_plot_averaged_data.py` which shows how to use the dataset for post-processing.



**Fig. 2.** Resulting normal strain distributions for three different numbers of dislocations. Each of the thin gray lines is the result of one random dislocation configuration while the red line is the ensemble average; the blue line shows the experimental data.

The second Python script shows how to post-process the strain data, e.g., by averaging as shown in Fig. 1. Further documentation of the data formats is available in the included Jupyter notebook.

**The second data set** is contained in the directory “Strain-analysis” and consists of the images shown in Fig. 2. The data shown in each of these images is obtained by running 50 simulations (i.e., strain field evaluations) with dislocations at random positions. Additionally, ensemble averages of the strain data were computed and shown as thick red lines. The data in Fig. 2 shows the difference in strain distribution resulting from systems with 10, 12, and 14 dislocations and supports the analysis and discussion in section 3.3 and Fig. 7 in Ref. [1].

The **third data set** is located in the directory 'Dislocation-at-GB' and contains tensorial stress data along different lines through the bicrystal as indicated by the three lines A, B, and C in Fig. 9 in Ref. [1]. In addition to the stress distribution shown in Fig. 10 of [1] the datasets furthermore contain all possible stress tensor components, which might be potentially useful for other researches. The included Jupyter notebook documents and demonstrates how to import the "pickled" data (the file with the ending '\*.pkl' were originally exported from pandas dataframes). The following data files are included: each directory ('along\_y\_inside\_G2', 'intersection\_of\_slip\_plane\_with\_GB', and 'through\_grains\_along\_x) contains 4.pkl files with stresses for the 4 different grain configurations as shown in Fig. 10 in Ref. [1]. Each of the three directories is for one of the plot lines are labeled with "A", "B", and "C" in Fig. 9 in Ref. [1].

The complete data sets and the python code are additionally available from the public area of the GitLab account <https://gitlab.com/computational-materials-science> which also will have updated version of the code. GitLab also has a viewer that is able to show the content of the Jupyter notebooks.

## 2. Experimental design, materials, and methods

In this work, precession electron diffraction (PED) was used to analyze strain fields linked to the dislocation veins. Electron precession was carried out using a "DigiSTAR" (NanoMEGAS) system attached to an FEI Tecnai G2 (200 kV FEG) TEM. A precession angle of  $0.5^\circ$  was used resulting in an electron probe size of  $\sim 4$  nm. A step size of 40 nm was used for the scanning of the samples. The sample was aligned along the [100] zone axis in order to increase the accuracy of the strain measurements in two orthogonal directions. An off-axis high speed optical camera focusing on the fluorescent screen was used for recording of diffraction patterns. These patterns were then analyzed by the TOPSPIN (NanoMEGAS) software to generate the strain maps.

Finite element simulations for the bi-crystalline system were performed using the commercial software COMSOL Multiphysics® [2]. The slipped area of the dislocation was presented by an equivalent eigenstrain "layer" following the procedure outlined in Ref. [3]. The data points in the data set were obtained at points of equal distances where the quadratic finite element shape functions of were used to interpolate and to differentiate the nodal displacement values. Then, the resulting stress tensor components were transformed to the respective local coordinate systems of the two grains, before the data was written to the file contained in the data set.

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## Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## References

- [1] Vahid Samaee, Stefan Sandfeld, Hosni Idrissi, Jonas Groten, Thomas Pardoen, Ruth Schwaiger, Dominique Schryvers, Dislocation structures and the role of grain boundaries in cyclically deformed Ni micropillars, *Mater. Sci. Eng. A* 769 (2020) 138295.
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