Plan Overview

A Data Management Plan created using DeiC DMP

Title: PMP

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Project abstract:

The societal need to conserve materials and energy calls for lighter and stronger metal components. The advantage of metals is their unique combination of plasticity (i.e. formability) and strength, which is governed by their complex structure. This structure is organized hierarchically on several length scales. In contrast to functional materials and polymers, this complexity has led to the common theoretical framework being not physics, but an engineering science: metallurgy. As a result, phenomenological models prevail. The big obstacle to understand the underlying physics is the lack of visualization of the dynamics of the structure. From 2012 to 2019 I have developed a hard x-ray microscope for high-resolution 3D studies. Uniquely, this now allows us to zoom into the material and map grains and dislocations. This will enable 3D movies on all relevant length scales. No competing group will have anything similar within the next 5 years. PMP will exploit this to unravel the physics of plasticity. For the first time, we can directly see the processes involved: the creation of dislocations, their self-organization, and subsequent creation of ever more complex patterns. At the same time, we can deduce the local stress. This will provide answers to longstanding core questions of metal science. Current multiscale models of plasticity are not capable of predicting realistic patterns. The new data will guide theory and allow for direct comparison of models and experiment at all scales. PMP will develop a physics-based multiscale model of plasticity that for the first time can predict which patterns evolve when and where in the metal, and as a result greatly improve predictions of the macroscopic plasticity and strength. If successful, we have created the instrumental and modelling foundation for a new paradigm in structural materials. This will support the ultimate vision of materials and process design in computer models rather than trial and error in the lab.

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PMP

Summary

dataset reference and name

The data collected will be diffraction and tomography images. From these crystallographic orientations, positions, and lattice data of sub grains will be extracted. These data will be obtained both by experiments and simulations.

origin and expected size of the data generated/collected

The amount of data generated in the project is estimated to be several TBs for each synchrotron experiment. The amount of data from other experiments and simulations will be much less.

data types and formats

Experimental data will be stored in the file formats generated by the 3DXRD analysis packages DARFIX as well as custom made software. EBSD and tomography data will be stored in the format generated by the instruments used.
Simulation data will be stored in the format of text files.

Making Data Findable

dataset description: metadata, persistent and unique identifiers e.g., DOI

Data will be collected using the DFXM technique and tomography. DFXM and tomography will be combined at the synchrotron at ESRF and possibly MAXIV.
Additional tomography will be conducted at the imaging centre of DTU.
Crystallographic orientations will also be collected by EBSD using the Zeiss microscope in building 425.
Simulations will be conducted using the crystal plasticity software DAMASK.

Making Data Openly Accessible

which data will be made openly available and if some datasets remain closed, the reasons for not giving access

All data supporting papers published during the project and additional data strictly necessary to reproduce the results will be archived on publicly accessible archives such as https://data.dtu.dk/.
PI will inform DTU IT service about long-term preservation.

where the data and associated metadata, documentation and code are deposited (repository?)

Data generated at DTU are backed up by AIT using DTUs standard procedure for backup of the O: drive/M: drive. Back up of synchrotron data will be discussed with Jan Båtrup when we have the first set.
Access to the data are controlled by access lists managed by DTUBasen allowing the PI to control access to the data.

how the data can be accessed (are relevant software tools/methods provided)?

The data will be shared at the o-drive or at data.dtu.dk.
Data will be structured in one folder for each experiment. Each folder will contain a readme file describing the content of the folder. Log files for synchrotron experiments will also be stored.
Data will be versioned by using date and time as part of the folder / file names.
Data are brought back from the synchrotron on external hard disks (several TB per experiment).
Other data will be stored on the M-drives of participants from DTU Physics and some similar solution for participants from DTU Mechanical Engineering.
A project folder on the O-drive will be used to store raw data and processed data forming the basis of publications.
Data are shared with external partners (Purdue University) using files.dtu.dk.
Data are shared with DTU Mechanical Engineering on the O-drive.

Making Data Interoperable

which standard or field-specific data and metadata vocabularies and methods will be used

There are no metadata standards and metadata will be generated manually.
For codes: a logbook will be made, including info on: the code version, date, input file name.
For experiments: a logbook will be made, including info on: material, responsible, date, equipment, experimental condition, sample ID, sample history, specification of the collected data.

Increase Data Re-Use

what data will remain re-usable and for how long, is embargo foreseen

The data will be kept in the project folder for five years after the project termination. After this period the data will be archived to tape and kept for at least 10 more years.

how the data is licensed

The data will be licenced according to the FAIR principles and use the Creative Commons (CC) copyright licences, and the licence will be described in the attached data license description.

data quality assurance procedures

Data will be documented in logbooks/files with specific details of each experiment/simulation associated with the data.
Readme files explaining the name codes for files and folders as well as the types of data will make the data understandable for secondary users.
Reproducibility of results will be ensured by documenting all relevant information about experiments and simulations.
All data and software used to produce publications, additional data necessary to document and validate development/analysis will be shared.
Trial runs while developing/testing cannot be shared.

Allocation of Resources and Data Security

estimated costs for making the project data open access and potential value of long-term data preservation

The use of tape storage is without any cost for the project.

procedures for data backup and recovery

The data will be stored on tapes and no data are destroyed.

transfer of sensitive data and secure storage in repositories for long term preservation and curation

By using text files and storing the developed software and versions of commercial software