# DMP title

**Project Name** Linking statistical crystal plasticity modelling of TRIP to the microstructural evolution probed by 3D X-ray microscopy (FWO Senior PDF) - DMP title

**Grant Title** 1281821N

**Principal Investigator** / **Researcher** Matthias Bonisch

**Project Data Contact** Matthias Bonisch

**Description** To enhance the fidelity of computer simulations of the mechanical behavior of transformation-induced plasticity (TRIP) materials a coherent 3D view of the transformation and deformation processes at the grain level would be needed. This project uses cutting-edge in-situ 3D X-ray microscopy to create a detailed view of the 3D microstructural and topological changes across different length scales during deformation of TRIP materials. Informed by the experimental results a novel numerical crystal plasticity model will be developed.

**Institution** KU Leuven

## 1. General Information

### Name applicant

Matthias Bönisch

### FWO Project Number & Title

1281821N

Linking statistical crystal plasticity modelling of TRIP to the microstructural evolution probed by 3D X-ray microscopy

### Affiliation

- KU Leuven

## 2. Data description

### Will you generate/collect new data and/or make use of existing data?

- Generate new data

### Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow and per WP or objective of the project.

- all data listed below are digital (except TRIP steel samples)

| WP | Task | Type of data | Format | Volume | How created |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| WP1 | 1.1 | TRIP steel samples | bulk | 10 mm - 10 cm | cut from larger purchased steel sheet |
| | 1.1 | 1D X-ray diffraction patterns, pole figures | .xy | few MB | lab-XRD on TRIP steel |
| | 1.1 | grain orientation maps | .ang | < 500 MB | Electron backscatter diffraction on heat-treated TRIP steel |
| | 1.2 | macroscopic stres-strain curves | .xls | < 20 MB | mechanical testing |
| | 1.2 | nanoindentation load-displacement curves | .txt | < 50 MB | nanoindentation |
| | 1.2 | heat flow curves | .txt | < 30 MB | differential scanning calorimetry |
| WP2 | 2.1 | 2D X-ray diffraction patterns and radiographs | .tif | 3-5 TB | in-situ 3D X-ray microscopy (3DXRD\|DCT) of TRIP steel |
| | | 3D images of TRIP microstructures including analysis scripts | native 3D image format | 100 - 300 GB | reconstructions based on 2D diffraction patterns |
| | 2.2 | 2D X-ray diffraction patterns | .tif | < 10 GB | in-situ mechanical loading of TRIP steel |
| WP3 | 3.1, 3.2 | source code | .f90, .py | < 50 MB | manual coding of source code |
| | 3.3 | simulation results | .txt | 1-2 GB | output of the new numerical hardening model |

## 3. Legal and ethical issues

**Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registering the fact that you process personal data is a legal obligation.**

- No

Privacy Registry Reference:

Short description of the kind of personal data that will be used:

**Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, add the reference to the formal approval by the relevant ethical review committee(s)**

- No

**Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for what data and which restrictions will be asserted?**

- No

**Do existing 3rd party agreements restrict dissemination or exploitation of the data you (re)use? If so, to what data do they relate and what restrictions are in place?**

- No

## 4. Documentation and metadata

**What documentation will be provided to enable reuse of the data collected/generated in this project?**

- all experiments, procedures and methodologies will be documented in a digital lab-notebook
- all data generated from experiments and simulations will be clearly labelled, described and contextualized
- all raw data will contain metadata detailing parameters and measurement conditions; missing native metadata will be manually documented in the lab-notebook
- all processed data will be clearly labeled for tracability back to its raw data
- source codes will be documented and commented
- simulation results will be accompanied with readme-files explaining how the simulations were configured

**Will a metadata standard be used? If so, describe in detail which standard will be**

**used. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.**

- No

## 5. Data storage and backup during the FWO project

**Where will the data be stored?**

All raw and processed data will be kept on the department's (personal drive on server) and/or universities managed storage facilities (OneDrive, large volume storage). Temporary personal copies can be made for processing purposes.

**How is backup of the data provided?**

The data stored on institutional storage facilities (department or university level) are automatically backed up at least once per day.

**Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available then explain how this will be taken care of.**

- Yes
- No

Personal KUL storage facilities (personal drive, OneDrive) will suffice for the largest part of data (if not all). If more storage capacity is needed, additional capacity will be acquired on the KUL large volume storage.

**What are the expected costs for data storage and back up during the project? How will these costs be covered?**

If KUL large volume storage capacities are required, the estimated associated costs for the duration of the project are 1500 EUR. These will be covered by the FWO bench fee.

**Data security: how will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

Access to the institutional data storage locations is restricted by password and will be granted only to authorized researchers and collaborators.

No sensitive nor confidential data is used in this project.

## 6. Data preservation after the FWO project

**Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state the reasons for this (legal or contractual restrictions, physical preservation issues, ...).**

All data will be preserved for the expected 5 years.

**Where will the data be archived (= stored for the longer term)?**

All data will be archived on the KUL large volume storage.

**What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?**

The estimated costs to archive all data (< 5 TB) on the KUL large volume storage for 5 years is 2860 EUR, which will be covered by the FWO bench fee.

## 7. Data sharing and reuse

**Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?**

- No

**Which data will be made available after the end of the project?**

3D images of TRIP microstructure evolution from WP2 will be shared publicly on Zenodo.

**Where/how will the data be made available for reuse?**

- In an Open Access repository
- In a restricted access repository
- Upon request by mail

- All data (raw, processed, source code, simulation results) stored on a restricted access repositories will be available upon request.
- 3D images will be openly available.

**When will the data be made available?**

- Upon publication of the research results

**Who will be able to access the data and under what conditions?**

Publicly available 3D images will be accessible for anyone.

Data available upon request from the access-restricted repositories will be shared freely for research purposes or after a contractual agreement between both parties.

**What are the expected costs for data sharing? How will the costs be covered?**

None. The databases we will use (Zenodo) are fully funded and provide their service at no cost.

Sharing data stored in the instititutional repositories will not incur costs in addition to the storage costs themselves.

## 8. Responsibilities

**Who will be responsible for data documentation & metadata?**

Matthias Bönisch

**Who will be responsible for data storage & back up during the project?**

**Who will be responsible for data storage & back up during the project?**

Responsible for transfer to institutional repositories: Matthias Bönisch

Responsible for storage & backup of institutional repositories: KUL IT

**Who will be responsible for ensuring data preservation and reuse ?**

Responsible for transfer to long-term institutional data storage repositories: Matthias Bönisch

Responsible for ensuring long-term data preservation on institutional repositories: KUL IT

**Who bears the end responsibility for updating & implementing this DMP?**

Matthias Bönisch