DMP title

Project Name COMPRESSIVE FAILURE OF UNIDIRECTIONAL COMPOSITES: EFFICIENT COMPUTATIONAL MICROMECHANICS AND EXPERIMENTAL VALIDATION - DMP title

Project Identifier 3E210588

Grant Title 1231322N

Principal Investigator / Researcher Christian Breite

Description In COCOMI, I will develop computational micromechanics tools to predict longitudinal compressive failure of unidirectional composites under quasi-static and fatigue loading. Deep learning will be used to efficiently identify the weakest locations in a virtual coupon (hot spots). During a research stay, a convolutional neural network will be developed and trained for this purpose based on coarse finite element (FE) models. The FE models will use microstructures generated by a newly developed 3D microstructure generator, which is trained based on deep learning of computed tomography (CT) data. Once the hot spots have been identified, only a few refined FE models will be required to detect where the kink band initiation will be triggered, which then leads to compressive failure. This procedure will be applied to both quasistatic and fatigue compressive loading, and predictions will be based on input parameters that are objectively measured on the actual constituents. Experimental validation will be performed based on compressive strength, compression-compression fatigue life and the actual micromechanisms observed in CT data.

Institution KU Leuven

1. General Information

Name applicant

Christian Breite

FWO Project Number & Title

1231322N

COMPRESSIVE FAILURE OF UNIDIRECTIONAL COMPOSITES: EFFICIENT COMPUTATIONAL MICROMECHANICS AND EXPERIMENTAL VALIDATION

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. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

Type of Data	Format	Volume	How created
X-ray computed tomography volumes	.tif	4 TB	XCT core facility – KU Leuven
Synchrotron computed tomography images	.tif, .h5	60 TB	Synchrotron radiation facilities (ESRF and SLS)
Optical Images	.tif	1 TB	*In-situ* using optical cameras for mesoscale DIC
ABAQUS simulation files	.inp, .odb	5 TB	Using ABAQUS finite element simulation software

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)

- Yes

The KU Leuven Committee for Ethics on Dual use, Military use & Misuse has approved my research under reference number D-211005.a.

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?

1. For the X-ray computed tomography volumes: Sample type, layup and dimensions, source and detector specifications, load and displacement for each *in-situ* scan, scan settings (voltage, current, exposure time, number of projections, number of averaging procedures, voxel size, source to object distance, source to detector distance).
2. For the synchrotron computed tomography volumes: Sample type, layup and dimensions, source and detector specifications, load and displacement for each *in-situ* scan, scan settings (voltage, projections, exposure), propagation distance, beam type, camera specifications.
3. For the optical images: Sample type, layup and dimensions, camera specifications, image acquisition rate, region of interest, subset size, step size.
4. For the ABAQUS simulation files: There will be comments in the ABAQUS / Python scripts about specific features implemented in the models. The .inp files store all input information in terms of material properties, behaviours and geometric features of the model. Together with the scripts this provides enough information to enable reuse of the models.

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.

- Yes

Metadata generation is performed automatically for the computed tomography operations (1) and (2), e.g., generation of the scan settings.txt file through the CT acquisition software.

For the optical images, manual metadata will be created by myself and the researchers I supervise, incorporating the data stated in section 4.1.

For TIFF file extensions, I follow the ISA-Tab standard.

For the CT data, I follow the NeXus standard.

For the ABAQUS simulation files the meta data is automatically added to the files (software manufacturer standard), which is readable with ABAQUS simulation software.

5. Data storage and backup during the FWO project

Where will the data be stored?

For all data, I will use external hard disk drives (HDDs) while creating a data backup on our research group NAS systems.

How is backup of the data provided?

Since the start of the project (01/10/21), we have purchased a separate 48 TB NAS which can be expanded to 96 TB on demand for the exclusive purpose of storing the generated data of this project. The NAS system is operated in 2-drive-failure save mode. Furthermore, selected data have a separate copy in our research group (Composite Materials Group) shared folder and in the my personal OneDrive folder as well as on internal hard drives of the my main workstation.

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

There is enough space on our HDDs, NAS, shared folder and OneDrive personal folder. The available storage is expected to be sufficient to include the data generated within the three years of this postdoctoral study. The purchase of additional HDDs or NAS could be an option in the future but is judged as non-essential at this moment.

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

We primarily expect a moderate cost of purchasing HDDs.

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

I have the HDDs under my possession. I can allow access to selected individuals if desired. Only I have access to my personal OneDrive folder. Only authorised personnel (within our group) has access to our local NAS systems and shared drive. This systems are password protected.

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 retained for an expected 10-year period after the end of the project.

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

External HDDs and NAS.

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

No costs are anticipated (excluding the moderate cost of HDD replacements).

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?

While the complete dataset is anticipated to be too large for open access availability, exemplary sub-datasets are expected to be made available after the end of the project or/and upon publication of the research results.

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

- In an Open Access repository

I have already stored two datasets, similar to what I will create in COCOMI, on Mendeley Data, for which I have also published two data articles in Data in Brief Journal. I will do the same (storing on Mendeley Data and publishing data articles) for the current project.

Storing data in Zenodo is also an option and will be considered.

When will the data be made available?

- Upon publication of the research results

I will try to make the data publicly available during the project along with publication of the results.

Who will be able to access the data and under what conditions?
Both Mendeley Data and Data in Brief article are open access. Therefore, the data will be accessible for public.

What are the expected costs for data sharing? How will the costs be covered?
Mendeley Data provides 10 GB of free space which should be sufficient for our purposes.
Any anticipated costs related to data sharing and publications will be paid from the bench fee.

8. Responsibilities

Who will be responsible for data documentation & metadata?
Christian Breite

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

Who will be responsible for ensuring data preservation and reuse ?
Christian Breite together with my supervisor Yentl Swolfs

Who bears the end responsibility for updating & implementing this DMP?
My supervisor, prof. Yentl Swolfs, bears the end responsibility of updating & implementing this DMP.