Breaking the strength-ductility paradox by stacking fault energy design

A Data Management Plan created using DMPonline

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Project abstract:

The Holy Grail in tailoring structural materials is to develop materials with a targeted combination of high strength and high ductility. In general high strength is accompanied by low ductitility and vice versa: the strength-ductility trade-off or paradox. Changing the deformation mechanism in metals from dislocation movement (SLIP) to mainly TRIP or TWIP effect, the paradox could be by-passed. A design parameter to tailor TRIP/TWIP vs. SLIP is the stacking fault energy (SFE). The present project will combine ab initio modelling to calculate the SFE in plastically anisotropic multi component materials with in-situ TEM and XRD to determine the SFE experimentally, and validate the models. Subsequent crystal plasticity modelling and thermodynamic modelling predicts alloy compositions for optimal high strength-high ductility. F.c.c. multi-components alloys as austenitic stainless steels and high entropy alloys will be investigated.

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Data Collection

What type of data will be collected?/How will the data be collected?/Which file formats are the data in?

- images for various types of microscopy (.TIFF),
- raw data from diffraction experiments in laboratories and at synchrotrons (.RAW)
- analyzed data will be saved in Origin and Excel files
- modelling results from first principles (VASP)
- modelling results from thermodynamic modelling (ThermoCalc)
- modelling results from crystal plasticity (mathlab)

File formats are given above as far as currently know.

What are the estimated amounts of data?
Estimated amount of data <2Tbyte

How will the data be structured?
Data will be structured after the various project participants (1 Post Doc + 1 PhD) and the various materials to be investigated.

How will the data be versioned?
Data will be versioned chronologically.

Are there any limitations on the use of existing data
No limitations after publication, unless patenting options emerge.

Are there any ethical or legal issues to be considered?
No ethical issues. Legal issues are covered by NDA among project partners.

Are there other external requirements?
No.

Data Storage

Where are the raw data and results stored?
Raw data and results will be stored on the individual M: drives of project participants and the O: drive with access for all DTU project participants.

How are the data backed up?
Back up is taken care of. Data area backed up by AIT using DTUs standard procedure for backup of the M: and O: drive.

How is access control managed?
Access to the data are controlled by access lists managed by DTUBasen allowing the PI to control access to the data.

How are data shared within the project?
Sharing among project participants via O: drive; sharing with external partners via files.dtu.dk.

Sensitive data is projected by passwords.

Documentation

Are there metadata standards?
All project participants are requested to keep a log book of their experimental research activities and appropriate ReadMe files for modelling results.

What metadata will be included?
At the end of the project the physical log book will be stored by the PI and a digital copy will be stored on the O:drive (not to be shared, only accessible for the PI). ReadMe files accompany the results on the O: drive.

How will the metadata be generated?
Metadata is generated manually by the project participants.

How will data be documented?/How will the data be understandable for secondary users?
Data will be documented and made understandable for secondary users by ReadMe files.

How will reproducibility of results be ensured?
Reproducibility will be ensured by detailed description of how the laboratory experiments and modelling activities were achieved. The reproducibility of experimental results is verified by repeating the tests (as always!)

Data Sharing

Which data will be shared?
Published experimental and modelling results and supplementary (unpublished) experimental results that corroborate the work, will be shared.

Which tools/software are needed to view/visualize/analyze the data?
The published data will be accessible through software that is universisally available.

Which data cannot be shared?
Data that will be used for possible patents will not be shared.

Who will have access to the data?
Access is given to colleagues in the field after dialogue with the PI (not to commercial enterprises)

When will data be shared?
Data can be shared after publication.

Where will data be shared?
Sharing through DTU data: data.dtu.dk

How will the data be made discoverable?
Discoverable via DOI.

Long-term Preservation

This will be considered in the future.