
"Elucidating the mechanism of third phase formation: a combined neutron/X-ray scattering and computational modeling approach

A Data Management Plan created using DMPonline

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Project abstract:

To combine molecular dynamics simulation and statistical mechanical theory (Manchester) with the experimental program in the Japanese Atomic Energy Authority (Japan) to elucidate the structure of the 3rd phase, sometimes formed in nuclear extraction processes.

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Manchester Data Management Outline

- No
- Not applicable
- Yes – leading a collaboration
- Acquire new data

The project involves the creation of new simulations for which pre-existing data are not required.

- University of Manchester Research Data Storage Service (Isilon)
- < 1 TB
- Not applicable
- < 5 years
- No sensitive or personal data

We will have no such information.

- Not applicable
- No
- Not applicable
- No

Andrew John Masters

Question not answered.

Data Collection

Numerical data, such as molecular co-ordinates generated by a simulation.

It will be created by a molecular dynamics simulation code. The data will be lists of numbers, stored typically in a binary format. The volume of data to be stored will be typically 10 - 100 MByte.

Documentation and Metadata

All necessary documentation as to the use of our simulations will be published online, along with useful metadata to help other potential users. Access will be free. All publications will contain required meta-data and documentation in supplementary documentation.

Ethics and Legal Compliance

No ethical issues are anticipated, but if they arise, we will seek advice from the University of Manchester.

This will be managed via University of Manchester institutions (e.g. UMIP).

Storage and Backup

On hard-discs on the University of Manchester's Computer Shared Facility.

There is no restricted access to our data. Storage of data and access to it will be managed by the investigators, taking advice from the University of Manchester's Research IT team.

Selection and Preservation

We anticipate that we will generate no data of long-term value. The project is about general physical behaviour, such as the symmetry of a phase. In case we do need to retain any data long-term, we will seek advice from Manchester's Research IT.

Again we foresee no need for long-term preservation of data. In the unlikely event this is needed, we will again make use of the University of Manchester's long-term storage facilities.

Data Sharing

Data will be made freely available on request. Our website and supplementary information provided in our papers will also give free access to data. All our publications will be free access. Data will also be stored on the FactSage thermochemical data base.

No

Responsibilities and Resources

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Only the data management resources already provided by the University of Manchester.