DMP title

Project Name Small-scale modeling of the dissolution behavior of platinum group metal nanoparticles in pyrometallurgical recycling from spent auto-catalysts. - DMP title

Project Identifier 1S07322N

Grant Title 1S07322N

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Description This project aims to develop a multi-scale modeling framework using density functional theory (DFT) and the phase-field method to study the local dissolution behavior of platinum group metal (PGM - Pt, Pd, Rh) nanoparticles in liquid slags containing liquid collector metal droplets. This framework will be used to uncover the dominant dissolution mechanism, leading to new insights into the effects of pyrometallurgical process parameters on the dissolution of these PGM particles, useful for interpreting observations from and optimizing industrial recovery operations. Once the framework is established, it could be applied to different recovery processes as well, increasing its relevance to the industry.

Institution KU Leuven

1. General Information

Name applicant

Héléna Verbeeck

FWO Project Number & Title

1S07322N - Small-scale modeling of the dissolution behavior of platinum group metal nanoparticles in pyrometallurgical recycling from spent auto-catalysts.

Affiliation

- KU Leuven

2. Data description

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

- Generate new data
- Reuse existing 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).

Objectives as stated in the proposal.

The expected measurable outcomes are

1) Interfacial energies of the different components involved in the pyrometallurgical recycling process (PGM nanoparticles, alumina wash coat, collector metal) and reaction kinetics of the dissolution of the Al2O3 carrier materials and the PGM nanoparticles in the slag obtained by performing DFT calculations.

2) A multi-phase-field model that is able to consider the interfacial energies and kinetic properties obtained from DFT calculations.

3) Simulation results will be used to uncover how and in which form the PGMs arrive in the metal droplet and how the recovery efficiency is influenced by the process parameters.

4) Experimental results to validate (parts of) the model.

For 1): using the VASP software and crystallographic information (.cif) and pseudopotentials from existing databases in literature. Two types of data will be created:

a) scripts to start the simulations (e.g. initial positions of the atoms, parametrization of the

simulations...) and scripts to extract the interfacial energies and kinetic properties from the output of the VASP simulations. This will be a collection of MATLAB scripts (.mat format) and VASP (INCAR, POSCAR, KPOINTS, POTCAR) files (converted to .txt files). The total size of all these scripts together will be smaller than 5MB.

b) calculated data. These are numbers that will be stored in .txt files. The total magnitude of these data will be of the order of several kB.

For 2): The multi-phase field model will be developed by using and extending modules of the software development and simulation environment
MOOSE (https://moose.inl.gov/SitePages/Home.aspx). C++ coding will be used. The size of the total program will be of the order of a number of MB. Alternative to the MOOSE code, MATLAB (.mat) scripts and FORTRAN scripts will be developed in an initial stage for 1D simulations. For both, the size will be of the order of a number of MB.

For 3): The outcomes of the simulations are detailed 3D numerical representations of the local structure and conditions as a
function of time (4D numerical data sets). They will be stored in .txt and/or .csv files. The total amount will be of the order of a number of TBs.

a) To obtain the phase-field simulation results, (i.e. the concentration and phase structure as a function of xyz coordinates and time) the MOOSE code developed under (2) will be used, using the interfacial energies and kinetic properties calculated under (1) and existing data from commercial databases TCOX, TCNOBL and MOBNOBL from Thermo-Calc (www.thermocalc.se) as input.

b) Besides the raw simulation data, Matlab scripts for initialization, visualization, and postprocessing of the simulations will be written. The size of these scripts will be of the order of one MB.

For 4):

a) 2D images and movies (ie 2D images as a function of time). Type: .jpeg and .AVI. The volume of these data will be of the order of one TB.

b) Scripts to extract data from the experimental images (typical .txt). The size of these scripts will be of the order of a number of kB.

c) The derived data themselves. These are numerical data. They will be listed in .txt files. The size of these data will be of the order of kB.

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

We intend a theoretical study. Outcomes will be published and the data will be made openly available as much as possible. We do not aim valorisation within this project.

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?

- Yes

For 1) it is allowed to publish data obtained from DFT simulations using VASP and existing pseudopotential and make them openly available if the appropriate references are added to the data or publication.

For 3) It is allowed to publish simulation results obtained with the MOOSE framework and using the commercial databases of ThermoCalc, if the MOOSE software is properly cited and the name and version of the databases is clearly mentioned.

All the other data are primary data or secondary data derived based on primary data obtained in this project.

4. Documentation and metadata

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

1):

1a) The scripts will contain information on the property calculated (the aim of the script), a description of the meaning and format of the expected input and how to generate it, an explanation of the output variables, assumptions on the crystal structure, and orientation of the phases.

1b) The metadata of the files will contain a description of the property(ies) listed, the conditions of the considered systems, compositions, crystallographic information and orientation of the involved phases, version of the VASP code used, name and version of the pseudopotential used, some extra comments related to the calculations if useful (eg use of non-standard VASP options)

2): At the top of the program file, the aim of the program will be described and a description of all input and output will be added, as well as a detailed explanation on how to obtain and generate the required input. The code itself will also be extensively commented to make it as clear as possible.

3):

3a): For every simulation test, raw simulation data will be collected in separate folders, including a txt file with a description of what the data represent and how they were generated. The input files and scripts needed to generate the necessary input data will be saved in the same folder. A special naming, including the type of experiment simulated, temperature, and present components and phases will be used, and a corresponding txt file will be maintained to explain the naming. The scripts used to visualize or post-process the data will be kept in this folder as well.

3b): The scripts will contain information on the meaning and format of the expected input and how to generate it, and an explanation of the aim of the script and which kind of output is generated.

4):

4a): Images and movies will be collected in separate folders per simulation test including a txt file with a description of the experimental conditions (type of experiment, name of equipment used, date, temperature profile, material compositions, pO2 of the atmosphere in the furnace, ..., irregularities noticed during the experiment). A special naming, including the date, type of experiment simulated, temperature, and present components and phases will be used and a txt file will be maintained explaining the naming. Also, the scripts (from 4b) used to visualize or post-process the data will be kept in this folder.

4b): The scripts will contain information on the meaning and format of the expected input and how to generate it, and an explanation of the aim of the script and which kind of output is generated.

4c): The metadata of the files will contain a description of the property(ies) listed, type of

experiment and experimental conditions applied, compositions of the involved phases, and extra comments (eg irregularities noticed during the experiment). A clear reference of the folder and file names of the experimental data (4a) will be given.

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

To our knowledge, there is no standard available yet for the kind of data that we will generate. Therefore, the metadata as specified under 4.1 will be applied. Only for the input files for the VASP and MOOSE software, the format is specified by the software, but even then we will add extra metadata information on top of the file as specified in 4.1 explaining in words the aim, geometry and initial conditions of the simulation.

5. Data storage and backup during the FWO project

Where will the data be stored?

All data will be stored in archive space at the VSC-KU Leuven (https://icts.kuleuven.be/sc/english/research/HPC). There is a possibility to stage part of the data for fast access. Also, people from outside can get access upon request. Besides that, most of the data will also be stored on the pc of the researcher (Héléna Verbeeck) involved in the project.

How is backup of the data provided?

The archive on the VSC-KU Leuven foresees a daily backup.

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

All the required storage & backup capacity are available on the archive of the VSC-KU Leuven.

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

The cost will be 70 euro per Terrabyte per year. This cost is foreseen in the project.

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

The data are not confidential. To prevent unauthorized persons would change the data, the following measures are taken:

- the personal computers of KU Leuven personel require a KU Leuven user number and password to access the data
- for the data archived at the VSC we can define read/write restrictions; write permission will only be given to the researcher active on the project; read permissions can be given to outsiders interested in the data

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, ...).

We will keep all the data archived at the VSC compute infrastructure for a period of 5 years after the end of the project.

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

The data will be stored on the VSC-KU Leuven archive.

Furthermore, for 1a) and 4b), scipts will also be published as additional material together with publications or in an open repository (Zenodo or a repository advised by the journal). 1b) and 4c) will be listed in publications as well.

For 2), the phase-field simulation code will be made available through GitHub under the GNU Lesser General Public License.

What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?
Data can be archived on the VSC KU Leuven for €70/TB/year. The price includes staging space to where the data can be copied temporarily to use it in computations. We expect that by the end of the project we will need approx. 2 TB (cost of max €140/year). Since this project will most probably feed into future related projects, we will foresee budget allocation in these projects for long-term storage of the data.

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

For 1a) it is allowed to publish data obtained from DFT simulations using VASP and existing pseudopotential and make them openly available if the appropriate references are added to the data or publication.

For 3) It is allowed to publish simulation results obtained with the MOOSE framework and using the commercial databases of Thermo-Calc, if the MOOSE software is properly cited and the name and version of the databases are clearly mentioned.

All the other data are primary data or secondary data derived based on primary data obtained in this project.

Which data will be made available after the end of the project?
All data, except those generated in 3a, 3b, and 4a will be fully publicly available after the project. The large data sets of 3a, 3b, and 4a will be archived on the VSC KU Leuven until 5 years after the project and can be accessed upon request. This permission is needed, not to protect the data, but because we have to give the outsider temporary access to the VSC and to stage the data temporarily to a place where fast access is possible.

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

- In an Open Access repository

Furthermore,
1a, 4b: Scripts will also be published as additional material together with publications or in a repository under CC-BY license, eg in Zenodo (if we find a more specific repository, this will get the preference) or in a repository advised by the journal.
1b, 4c: Will also be listed in publications and/or can be published in the NIST material repository (https://materialsdata.nist.gov/) where data are published under a CC-BY license and get a doi.
2: The phase-field simulation code will be made available through GitHub under the GNU Lesser General Public License.
3, 4a: If the large data sets stored on the VSC KU Leuven archive are made available upon request, this will be done under CC-BY license.

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?
The full dataset will be available and can be used by anyone and for any purpose, provided that they give appropriate credit, i.e. reference to the related publications and/or doi of the data set.

What are the expected costs for data sharing? How will the costs be covered?
There are no extra costs associated with the data sharing. Zenodo and NIST are free of charge.

8. Responsibilities

Who will be responsible for data documentation & metadata?
Only one researcher is involved in the project (Héléna Verbeeck). She will be responsible for

documentation of all data generated through or based on VASP simulations (1a+b), for all data generated through or based on the MOOSE simulations and for the MOOSE code (2, 3a+b), and for the documentation related to the experimental data (4a+b+c).

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

I (Héléna Verbeeck) will be responsible for putting the data I generate within this project on the VSC KU Leuven archive space.
The VSC-KU Leuven team maintaining the VSC-KU Leuven archive is responsible for the daily backups.

Who will be responsible for ensuring data preservation and reuse ?

The supervisor (promotor), Nele Moelans, is responsible for ensuring data preservation and reuse of all data generated during the project.

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

The end responsibility for updating and implementing the DMP is with the supervisor (promotor), Nele Moelans.