AddMorePower

D2.1

Data Management Plan

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Abstract	The DMP summarizes the data that will be produced during the AddMorePower project. It describes also the way how data will organized and stored within AddMorePower to achieve FAIR data.
Keywords	Data Management Plan, Characterization Data, Modelling Data, FAIR Data, Data Repository, Data Security

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Disclaimer

Executive Summary

The purpose of the AddMorePower data management plan is to outline a comprehensive approach to material science data management that adheres to the principles of FAIR (Findable, Accessible, Interoperable, and Reusable) data, incorporates ontologies for improved data organization, and utilizes open data repositories for data sharing and preservation.

To achieve the goal of making data FAIR, this plan emphasizes the importance of making data findable by providing descriptive metadata, assigning persistent identifiers, and utilizing standardized vocabularies and ontologies. By implementing these practices, researchers and stakeholders will be able to easily locate and access relevant datasets, enabling the efficient and effective reuse of data for various purposes.

Open data repositories serve as essential platforms for sharing and preserving research data. This plan advocates for the utilization of the NOMAD data repository for material characterization and modelling data. By depositing the processed AddMorePower data in the NOMAD respository, researchers contribute to the broader scientific community, fostering collaboration and enabling data reuse. The repository provides long-term preservation and curation services, ensuring data longevity and accessibility.

Other public data like documentation, scientific articles and general results will be accessible to the public throughout the duration of the project in the form of project progress, news and results. Confidential information will be shared under restriction, only to project partners and the EC and cannot be made openly available.

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Chapter 1 General Information

1.1 Project

The proposed project AddMorePower aims to advance X-ray- and electron-probe related characterization techniques to make them quantitative and automated tools for the power semiconductor industry, and to refine modelling (using MODA) and FAIR data management methods to enhance and efficiently use characterization data (using CHADA). Thereby, AddMorePower will promote the materials integration and development for European power semiconductor technologies, to allow a broader and faster market penetration, while also providing new opportunities for other industries basing themselves on mono- and polycrystalline materials. With the rapid and massive spread of power electronics and power semiconductors to enable the digitalization and the electrification of our society and its supply with sustainable energy, new requirements arise to the conception and integration of semiconductor and interconnect materials. AddMorePower will provide the necessary characterization and modelling techniques that meet the particular needs of the upcoming power semiconductor technology generations:

1. The transition to the new semiconductor materials gallium nitride (GaN) and silicon carbide (SiC), mainly limited by defects in the crystal lattice, for which currently no established characterization workflows exist.

2. The starting 3D-integration also of power devices, posing severe thermo-mechanical challenges to the involved metals and intermetallic materials, which can only be mastered by understanding gained by predictive modelling.

3. The trend towards digitalization and industry 4.0, which requires FAIR (findable, accessible, interoperable and reusable) data at all development and production steps.

The project brings together renowned research institutes with many years of experience in electron- and X-ray characterization, emerging new research groups and company start-ups and researchers with a track record in multi-physics materials modelling as well as data engineering.

1.2 Institutional experiment partners

- Fraunhofer Institute for Ceramic Technologies and Systems IKTS (IKTS)
- KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH (KAI)
- Infineon Technologies Austria AG (IFAT)
- deepXscan GmbH (DXS)
- European Synchrotron Radiation Facility (ESRF)
- Centre National de la Recherche Scientifique (CNRS)
- Ustav fyziky material - Institute of Physics of Materials CAS (IPM)
- Katholieke Universiteit Leuven (KUL)
- Université de Lorraine (UL-LEM3)
- Technikon Forschungs-und Planungsgesellschaft mbH (TEC)

Chapter 2 Data summary

2.1 Purpose of the data

During the AddMorePower project, data will be collected and used to advance X-ray- and electron-probe related characterization techniques as well as modelling and simulation methods for power semiconductor industry.

Apart from research data, other project related data will be produced with the purpose of:

- Sharing information with partners, fostering collaboration and promoting openly shared information.
- Developing and sharing templates, deliverables and guides with partners.
- Disseminating project results to gain visibility within the European community and providing open access to progress and results that are usable and applicable to various industries.
- Control of the quality for deliverables prepared.

2.2 Description of the data

Primary research area

Applied Materials Science

Short description of the data

The data include measurements and meta data from X-ray- and electron-probe characterization techniques for material science, as well as simulated data from materials modelling methods.

AddMorePower will produce also data that are not related to lab measurements and simulations, e.g. resulting from surveys, interviews, conf calls and meetings.

Type of the data

The AddMorePower project will produce different type of data: numeric data like individual measurement results or time series, images from e.g. SEM based methods, as well as data extracted from images (categorical and numerical) or data from non-technical work.

2.3 Data storage and file conventions

An overview of the data generated within the AddMorePower project (formats, size and volume) are shown in Table 1, Table 2 and Table 3.

Table 1: File formats used for the data generated within AddMorePower

Technique / Source	Data Format
X-ray tomography data	- Collected raw data format: .tiff, .txrm - Microscope settings and imaging parameters: .xmp, index - Meta data format: .h5. - Processed data (reconstruction, analysis) format: .tiff, .mrc
multi-scale DFXM	.hdf5
multi-mode XRM	.hdf5
X-BIC	.hdf5
Porosity maps / segmentations	.tiff, .png, .csv, .txt
In-situ experimental data	.txt, .txrm, .tiff, .dm3
SEM 2D & 3D	- 2D SEM images raw data format: .tiff, .png - 2D SEM images processed data format: .tiff, .csv - 2D SEM meta data formats: .tiff, .json, .csv
EBSD	- EBSD maps raw data format: .oipx, .h5oina, .ebsp - EBSD maps processed data format: .atex, .tiff - EBSD raw data: .H5oina, .ctf, .crc - Project file for EBSD software: .oipx (requires directory with .dat files) - Kikuchi pattern for each pixel: .tiff - Exported images: .tiff, .png, .jpeg - Sample meta data: .json - Quantitative EBSD evaluation (MTEX): .json
EDX	- Project file for EDX software: .oipx (requires directory with .dat files) - Exported images: .tiff, .png, .jpeg - Sample meta data: .json - EDX map data (.csv)
ECCI	- Images: .tiff - Sample meta data: .json - Quantitative ECCI evaluation (dislocations): .json
TEM	.tiff, .jpeg, .dm3 (Gatan)
Modelling & simulation data	- Input: .yaml, .vti, .msh (text based) - Raw data: .hdf5 (binary) - Processed: .vrk, .pdf, .txt - Output data format: .txt, .jepg, .png, .bmp, .vtk, .gif, .avi, .mat, .f90, .py, .cpp - WBPJ
Raman	.txt

Technique / Source	Data Format
Data generation for communication and project management activities	- Website and social media data: Twitter and LinkedIn data (incl. download of files, interview recordings, sharing progress and contact information) - Format: .pdf, .jpg, .mp4
Documentation	- Microsoft Office incl. datasheets and shared documents for collaborative work, guides and templates. - Format: .docx, .xlsx, .pptx
Dissemination and exploitation	- dissemination and exploitation plan - Format: .docx., .jpg, .pdf
Deliverables	- Format: .docx, .pdf

Table 2: Expected size of the raw data generated within AddMorePower

Technique / Source	**Expected size** (average value per data file)
X-ray tomography data	- 1.7 GB - reconstruction: 2.3 GB (reco tif), 4.2 GB (reco mrc) - average per collected raw file incl. meta data approx. 3,4 MB.
multi-scale DFXM	~10 GB
multi-mode XRM	~50 GB
X-BIC	100 MB
Porosity maps/ segmentations	Several GB
In-situ experimental data	200 kB
SEM 2D & 3D	SEM micrographs: ~5 MB per micrograph
EBSD	- EBSD maps: ~50 MB per map - HR-EBSD maps: ~500 GB per map
EDX	Few MB
ECCI	Few MB
TEM	1MB - 100MB
Modelling & simulation data	- ½ to 50 GB (typically 1 GB to 10 GB per simulation - ~10 GB for input our source files
Raman	Few GB raw data

Table 3: Estimation of the raw data volume generated within AddMorePower

Technique / Source	Raw data volume estimation
X-ray tomography data	- Average volume data per data measurement (tomography) approx. 3GB and in-situ/sample mapping – 1GB. - 50 GB (25 * 2GB) - reconstruction: 63 GB (reco tif), 113 GB (reco mrc) - Estimated volume of generated data volume in whole project approx. 4- 5TB.
multi-scale DFXM	200 GB
multi-mode XRM	1 TB
X-BIC	Few GB
Porosity maps / segmentations	1 TB
In-situ experimental data	5 MB
SEM 2D & 3D	SEM micrographs: About ~100 GB during the project.
EBSD	- EBSD maps: ~ 500 GB during the project. - HR-EBSD maps: ~ 5 TB during the project.
EDX	Few GB
ECCI	Few GB
TEM	1-5 TB
Modelling & simulation data	1TB + Full field simulations: Total expected ~ 500 GB + 100GB
Raman	< 5 GB

2.4 Measures of quality assurance which are taken for AddMorePower data

The measures of quality assurance which are taken for AddMorePower data are listed in Table 4.

Table 4: Measures to ensure high data quality in AddMorePower

Technique / Source	Measures
X-ray tomography data	Adjust focus with focal series, improve brightness and image quality by calibrating beam optics to produce most round and bright spot, adjust rotational axis visually to ensure full area of interest is visible during experiment. dXs: mentioned above and additionally to calibrate X-ray beam path and defined resolution the siemens star calibration target is imaged.

Technique / Source	Measures
multi-scale DFXM	As a service provider we permanently improve these tools. Parameters like strain can easily be calibrated with Si standards
multi-mode XRM	As a service provider we permanently improve these tools. Parameters like strain can easily be calibrated with Si standards
X-BIC	An imaging tool that provides essentially strongly contrasted images for qualitative comparison
Porosity maps / segmentations	Based on the selected procedure, the calibration protocols e.g of reference sample will be established.
In-situ experimental data	Calibrate force sensor with known samples
SEM 2D & 3D	SEM is calibrated once a year by the constructor.
EBSD	EBSD system calibration is checked before each measurement
EDX	EDX system validation performed every 3 months
TEM	Measurement validation performed every 3 months to ensure values are within +/-5% of target values.
Modelling & simulation data	DAMASK has an extensive test suite.
Raman	Raman spectrometry of crystalline materials can be used for strain determination in near surface areas. Calibration standards for the relevant materials in this project are available

Chapter 3 FAIR Data

The EC guidelines on FAIR principal data management sharing approach are used within the AddMorePower project to ensure the DMP goals and ensure no additional issues to occur.

3.1 Making data findable

Persistent identifiers

The AddMorePower processed data will have Digital Object Identifiers (DOIs) as persistent identifiers (PIDs).

Meta data

At a minimum meta data that are automatically captured by instruments will be curated at each AddMorePower partners and linked to the raw data. The AddMorePower consortium will spend effort to save additional meta data and auxiliary data, such that other parties understand the data (that is, to understand their collection or creation, analysis, and research results obtained on its basis) and can re-use it.

3.2 Making data accessible

3.2.1 Repositories

During the project, all kind of data that need to be shared within the consortium is stored at an iShare repository where all partners have access to.

During and after the project, processed AddMorePower data (including metadata, documentation and, if applicable, relevant code) will be stored or archived in and publicly shared via the NOMAD (https://nomad-lab.eu/) repository, which is a standardized repository within the material science community.

Open data (scientific articles, conferences) will be shared on social media channels (website, Twitter and LinkedIn) and on the AddMorePower website.

Published documents and shared data will be useful for broad public, EC, civil society, while the confidential data will only be shared among the project partners.

3.2.2 Data

Access to project data

Public data will be accessible to the public throughout the duration of the project in form of project progress, news and results (scientific articles, conferences). Confidential information will be shared under restriction, only to project partners and the EC and cannot be made openly available (DoA, GA).

Access to processed data and processed data sharing

Processed data resulting from AddMorePower-funded research will be made accessible to everyone i.e. open data, without embargo period. The Principal Investigator may request an embargo period in accordance with the AddMorePower data policy.

License to be applied to the open data

The processed AddMorePower data and meta data are available under the CC-BY-4.0 Creative Commons license (https://creativecommons.org/licenses/by/4.0/).

Access to raw data and raw data sharing

Access to raw data resulting from AddMorePower-funded research will be managed by each AddMorePower facility individually. Details are given in Table 5.

Table 5: Access to raw data and raw data sharing at AddMorePower partners

Organization	Access to raw data & raw data sharing
IKTS	FORDATIS (https://fordatis.fraunhofer.de) is the Fraunhofer research data repository that enables easy and transparent publication of data, while still complying with the scientific guidelines for high quality reproducible research.
KAI	KAI doesn't have its own public raw data storage. However, after clearance process by top management sharing relevant and selected raw data on open repositories is planned.
IFAT	IFAT doesn't have its own public raw data storage. However, after clearance process by top management sharing relevant and selected raw data on open repositories is planned.
DXS	Sharing of the measurement raw and processed data will be established according to the project data policy.
ESRF	ESRF beamline data are published via the ESRF data portal and organized according to the ESRF data policy. Data have a default embargo period of 3 years. The Identity is managed by the ESRF Single Sign On (SSO) platform. The implementation of Access Control Lists (ACLs) on the ESRF file systems allows fine-grained access control to directories and files depending on the user's identity. Access to embargoed data via the on-line catalogue (https://data.esrf.fr) of the ESRF is restricted to registered users only. Open data are accessible to all i.e. no login required.
CNRS	There is no possibility currently, but CNRS will learn from the other AddMorePower partners during the project how to share raw data.
IPM	There is no possibility currently, but IPM will learn from the other AddMorePower partners during the project how to share raw data.
KUL	KU Leuven has some means but they need further evaluation during the project.
UL-LEM3	There is no possibility currently, but data can be requested upon demand at the principal investigator.

3.3 Making data interoperable

To make AddMorePower data interoperable, the AddMorePower partners are encouraged to use state-of-the-art data formats for meta data management, like Nnexus, .HDF5, hdm5, ChemML, CIF, VASP, Molpro, NOMAD Metainfo or .ome. Furthermore, all partners will make sure to increase consistent data organization, e.g. via data model proposed as proposed by the Open Microscopy Environment and by generating taxonomies and ontologies based on the CHADA and MODA concepts to describe data and context information.

3.4 Increase data re-use

All AddMorePower partners aim to increase data re-use by establishing or improving their existing data re-use strategy in the framework of the project. Currently, some partners have already strategies in place, like:

- Making data and metadata accessible to the community via an own repository after an embargo period (e.g. ESRF: https://data.esrf.fr, Fraunhofer: https://fordatis.fraunhofer.de)
- Release code + material configuration as documented and maintained open source software.
- Versioning paper-specific input files etc. and share them on demand.
- Store data after the departure of non-permanent employees, along with a signature and share them on demand.

3.5 Project guidelines

To increase data re-usability, a consistent data organization with common guidelines is required at each AddMorePower partner, but also over all partners. Currently, the AddMorePower partners have their own guidelines (see Table 6 and Table 7). During the project the AddMorePower partners will align on good practices and aim to harmonize the data organization to establish general guidelines for the whole project team.

Table 6: Guidelines for a consistent organization of the data at partner level

Organization	Guidelines
IKTS	Data sets are organized by project, experiment and date. Furthermore, IKTS plans to establish a reliable scheme to ensure consistent data organization guided by internal standards.
KAI	KAI initiated already guidelines how to store characterization data and meta data. Currently, meta data are stored in .json files. Within AddMorePower KAI will extend the research on consistent data organization and by generating taxonomies and ontologies based on the CHADA and MODA concepts. Furthermore, KAI will extend the identified best practice for data organization also to simulation data.
IFAT	Characterization and modelling data are stored according to internal guidelines.

Organization	Guidelines
DXS	dXs develops and optimizes software for the control and operation of X -ray microscopes. The generated data is properly stored and organized by project, session, sample name and date. The processed data is stored according to the same nomenclature of session, sample and date. The generated metadata is stored in .h5 as original data and is never modified.
ESRF	On ESRF beamlines data are written by the control system (BLISS) and organized according to a well-defined schema to conform with the ESRF data policy. Data are organized by proposal, session, sample, and datasets. See https://bliss.gitlab-pages.esrf.fr/bliss/master/data/data_policy.html for details.
CNRS	Currently, there is no guideline. It will be discussed within the lab during the AddMorePower project.
IPM	Currently, there is no guideline. It will be discussed within the lab during the AddMorePower project.
KUL	- General code: Stored on gitlab.kuleuven.be - Paper: Latex, specific code - Input data stored on gitlab.kuleuven.be - Raw data/simulation stored on workstation/super computer (with backup)
UL-LEM3	Currently, there is no guideline. It will be discussed within the lab during the AddMorePower project.
TEC	TEC is managing and creating postings on the project website, aligned with FAIR principles.

Table 7: Data naming guidelines at partner level

Organization	Guidelines
IKTS	Data names include experimental features, sample name and experiment type, but a completely consistent naming scheme over all data sets must still be established. A new guideline based on CHADA and MODA concepts will be defined within AddMorePower.
KAI	KAI will generate an internal guideline for naming the data in AddMorePower by using taxonomies and ontologies based on the CHADA and MODA concepts.
IFAT	Data are named according to internal guidelines.
DXS	Currently naming is done according to acquisition setting, date and time. It can be improved/modified according project requirements/nomenclature (e.g. CHADA and MODA)
ESRF	Metadata follow the Nexus conventions (https://nexusformat.org). Currently almost 1000 Nexus compliant metadata tags have been defined for the ESRF data repository (cf. https://gitlab.esrf.fr/icat/hdf5-master-config/-/blob/master/hdf5_cfg.xml). This file also defines the mapping between the Nexus tag and how it is stored and displayed. The Nexus tags are stored in the .hdf5 file format.

Organization	Guidelines
CNRS	Currently, there is no guideline. It will be developed within the AddMorePower project.
IPM	Currently, there is no guideline. It will be developed within the AddMorePower project.
KUL	HDF5-based file format with standardized names and meta data.
UL-LEM3	Currently, there is no guideline. It will be discussed within the local team.

Chapter 4 Allocation of resources

FAIR is a central part of AddMorePower data management; it is considered at every decision in the AddMorePower data management plan. FAIR data processes ensure that data are used as efficient as possible. Making data FAIR is therefore not a cost that can be separated from the rest of the project. In total, the AddMorePower partners allocated 59 PMs (details see Table 8) in the AddMorePower project to work on data management and related topics. These resources in conjunction with activities outside of the AddMorePower project will bring material science data management at each partner to the next level.

Table 8: Data management costs of the project

Organization	Cost and resource estimation
IKTS	In WP2 IKTS will invest 10 PMs in data management
KAI	FAIR Data storage and data management is currently a focus topic at KAI and is driven by a total of 3 headcounts over the course of the next 3.5 years. 12 PMs of it within the AddMorePower project.
IFAT	In WP2 IFAT will invest 1 PM in data management
DXS	At the current state human resources for data management in WP2 is planned with 2 PMs in total.
ESRF	In WP2 ESRF will invest 12 PM in data management
CNRS	In WP2 CNRS will invest 6 PM in data management
IPM	In WP2 IPM will invest 1 PM in data management
KUL	In WP2 KUL will invest 6 PM in data management
UL-LEM3	In WP2 UL-LEM3 will invest 3 PM in data management and will invest 1000 € for upgrading the NAS.
TEC	In WP2 TEC will invest 6 PM in data management

Chapter 5 Data security

5.1 Measures or provisions that are in place to ensure data security

iShare is the main repository used by the consortium, secured with log in system and managed by Infineon. Internal managing and versioning of the system are assured.

Technikon, as the project management team of AddMorePower, is responsible for data management shared and created within the project and the data shared at the project website.

Managing und versioning of public data shared via the NOMAD repository is managed by NOMAD.

5.2 Long term preservation of public data

The data shared on project website will be preserved and remain re-usable for 5 years after the project end.

The data shared on the NOMAD repository will be preserved and remain re-usable for 10 years.

5.3 Back ups of the data

Table 9 lists how each AddMorePower backups data generated within the project.

Table 9: Data back ups at each AddMorePower partner

Organization	Raw data storage & backups
IKTS	Data from finished projects are regularly preserved as a back-up on a separate storage facility for at least 10 years. Ongoing project data is saved daily on a backup for up to a year back. Archived data and daily backups are stored safely in a separate facility.
KAI	KAI conforms to Infineon's data retention rules and utilizes Infineon's data storage solutions (see IFAT). Within the AddMorePower project KAI will set up databases (e.g. data lake) specifically intended for long term raw data storage (e.g. 10 years).
IFAT	Infineon has data retention rules and data storage solutions. For technical data a period of six years is specified. In standard file shares data is stored and back-ups are made as long as there is an active owner. On standard file shares data is backed up twice a day. Furthermore, the disaster recovery plan defines that files are stored in two separate data centers.
DXS	All data at dXs are saved locally saved and backed up on the NAS server. dXs plans to establish data storage on tape for longer timescales.

ESRF	Beyond 2 months the data is migrated to tape storage and remains accessible via the ESRF data portal. Two copies are stored on separate tape systems. Writing data back from tape to disk is fully automatic when access to the data is requested via the data portal (data.esrf.fr). Writing data back from tape to disk can also be done manually by the system administrators. All raw data at ESRF are archived for 10 years. Processed data are archived on request. The ESRF plans to keep the data archived on tape for ten years or as long as economically affordable (the retention time may depend on the volume of data generated). Meta data is kept forever. Our data policy does currently not define what happens to the data after ten years.
CNRS	n.a.
IPM	n.a.
KUL	All centrally stored data is backed up. Internal backup follows the data management plan of the research group.
UL-LEM3	Light data are stored on university servers and kept for five years after the end of the project. Heavy data are stored internally for 2 years after the end of the project. Light data is backup on 3 distinct sites. Heavy data has no backup except RAID5 NAS protection. A confirmation is required before erasing the data.
TEC	n.a.

Chapter 6 Ethics

The data created in AddMorePower does not contain personal or sensitive data. Personal data from partners will not be shared.

AI (machine learning) methods will be used within AddMorePower to support the interpretation of data obtained from simulations and experimental characterization. The combined expertise in the field of data science/artificial intelligence and materials science will be used to critically assess the outcome of the employed AI techniques. These techniques will not raise any ethical issues.

Chapter 7 Other issues

We use the Data Stewardship Wizard (DSW) with its *ESRF* (ID: esrf:esrf:0.1.31) knowledge model to make our DMP. More specifically, we use the https://dmp.esrf.fr DSW instance where the project has a direct URL: https://dmp.esrf.fr/projects/723b30b0-502a-4060-a37e-3d9ed76993bc.

Support funded research

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List of Abbreviations

Table 10: List of abbreviations

Abbreviation	*Explanation*
3DXRD	*3D-Xray Diffraction*
AB	*Advisory Board*
ACL	*Access Control List*
CA	*Consortium Agreement*
CHADA	*Characterisation Data Generalization*
CL	*Cathodo Luminescence*
DAMASK	*Düsseldorf Advanced Material Simulation Kit*
DFXM	*Dark Field Xray Microscopy*
DMP	*Data Management Plan*
DoA	*Description of Action (Annex 1 of the Grant Agreement)*
DOI	*Digital Object Identifier*
DSW	*Data Stewardship Wizard*
EB	*Executive Board*
EBIC	*Electron Beam Induced Current*
EBSD	*Electron BackScatter Diffraction*
EC	*European Commission*
ECCI	*Electron Channeling Contrast Imaging*
EDX	*Energy-Dispersive Xray*
FAIR	*Findable, Accesible, Interoperable, Reusable*
GA	*Grant Agreement*
GaN	*Fgallium Nitride*
HR-EBSD	*High Resolution EBSD*
IMR	*Interim Management Report*
MODA	*Materials Modelling Generalization*
NAS	*Network Attached Storage*
NDA	*Non-Disclosure Agreement*
PID	*Persistent Identifier*
PM	*Person Month*

PR	*Periodic Report*
SEM	*Scanning Electron Microscopy*
SSO	*Single Sign On*
STEM	*Scanning Transmission Electron Microscopy*
SXDM	*Scanning Diffraction Xray Microscopy*
TEM	*Transmission Electron Microscopy*
TRCL	*Time resolved CL*
TXM	*Transmission Xray Microscopy*
WP	*Work Package*
X-BIC	*Xray Beam Induced Current*
XRM	*XRay Microscopy*