AddMorePower

D2.2

Documentation of domain-level ontologies - CHADAs & MODAs

Project number	101091621
Project acronym	AddMorePower
Project title	Advanced modelling and characterization for power semiconductor materials and technologies
Start date of the project	1st January, 2023
Duration	48 months
Call	HORIZON-CL4-2022-RESILIENCE-01

Deliverable type	Report
Deliverable reference number	CL4-2022-RESILIENCE-01, D2.2
Work package contributing to the deliverable	WP2
Due date	30.11.2023
Actual submission date	29th November 2023

Responsible organisation	KAI
Editor	Olivia Pfeiler
Dissemination level	PU
Revision	V0.1

Abstract	D2.4 includes the systematic description and documentation of materials modelling and characterization data created in AddMorePower. To allow interoperability, AddMorePower uses the community standards CHADA and MODA.
Keywords	MODA, CHADA, EBSD experiments, Void Growth Modelling

Funded by the European Union under grant agreement no. 101091621. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

Editor

Olivia Pfeiler (KAI)

Reviewer

Stephanie Anderseck (IKTS)

Contributors (ordered according to beneficiary numbers)

Vedad Babic, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Sebastian Moser, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Manuel Petersmann, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Olivia Pfeiler, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Michael Reisinger, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Martin Diehl, Katholieke Universiteit Leuven
Javier Velo Pérez, Katholieke Universiteit Leuven
Antoine Guitton, Université de Lorraine

Disclaimer

Executive Summary

The AddMorePower consortium is dedicated to developing characterization and modelling methods that can meet the unique needs of upcoming power semiconductor technology generations. To achieve effective and efficient research and innovation, a seamless interoperation between materials characterization, materials modelling, and data science is required. This goal can only be accomplished through the use of FAIR and open data practices.

AddMorePower employs the CHADA and MODA methodologies to achieve FAIR data management. These systematic description and documentation methods are used for materials characterization data and materials modelling data, respectively. They are based on a common terminology, concepts and relationships defined by the community, providing a holistic approach to combine data from various materials characterization and modelling techniques, which allows analysing and modelling of complex structures.

This deliverable presents a MODA for void growth modelling and a CHADA for Electron Backscatter Diffraction experiments. Both contain information about the user case, the model or the sample, the generated raw data, and the post-processed data.

Table of Content

List of Figures

Chapter 1 Introduction

The manufacturing industry is facing new challenges with the advent of Industry 5.0. Innovative solutions are required to meet these challenges. The AddMorePower consortiums focuses its research on developing necessary characterization and modelling techniques to meet the particular needs of upcoming power semiconductor technology generations. One backbone to foster research and innovation in this field is the integration of materials characterization, materials modelling and data science. To enable the fluent interoperation, FAIR and open data practices are needed.

FAIR data management requires harmonized data treatment and harmonized data documentation, not only within the facilities where the simulations and experiments are performed, but across communities. The EMCC and the EMMC developed two methodologies for a systematic description and documentation of materials CHAracterization Data (CHADA) and materials MOdelling Data (MODA). In AddMorePower we make use of the developed concepts and terminology from CHADA and MODA in order to describe the produced data in a harmonized way and to share the gained knowledge in the community.

CHADA (material CHAracterization DAta) is a systematic description and documentation method for material characterization experiments, including user case, raw data generation and post-processing of the data. It enables the systematic investigation of materials. A harmonized experiment documentation is essential for managing material science data and for guiding the development of e.g. new materials that meet specific requirements. CHADA provides the basis for a holistic approach to combine data from different characterization techniques, which enables the analysis and modelling of complex structures and links between different experiments. It is based on a common terminology, concepts and relationships defined by the community [1].

MODA (materials MOdeling DAta) is a systematic description and documentation method that enables the integration of materials data from different sources. A MODA includes the description of the user case, the model or the chain of models, the simulated raw data and the processed data output. It allows for the creation of data-driven models that can be used to predict materials properties and optimize materials design. MODA is based on a common terminology, concepts and relationships between materials data defined by the community [2].

In the first year of the AddMorePower project a MODA describing void growth modelling in a metallization plate of power semiconductors (see chapter Chapter 2) and a CHADA describing the Electron Backscatter Diffraction (EBSD) experiments for two user cases (see chapter Chapter 3) have been developed. Both descriptions are not released to the public yet. In a next step, the responsible AddMorePower partners will get in contact with the EMMC and EMCC in order to review the MODA and CHADA and to officially publish the documents on the respective EMCC and EMCC repositories.

CHADAs and MODAs are living documents. They need to be able to include new insights from the community. The CHADA and MODA presented in this document are the starting point for a harmonized data documentation within AddMorePower. In the following three project years, we will continue our efforts in this direction. The final results will be documented in deliverable D2.4 “Documentation of materials characterization and modelling workflows (R, PU, M48)”.

Chapter 2 MODA for Void Growth Modelling

In this chapter, the MODA for void growth modelling simulated in the project AddMorePower is presented. The MODA is based on the template released by emmc.eu in May 2021 [3] and the common terminology defined in the CEN Workshop Agreement 17284 [2].

MODA authors:

Martin Diehl, Department of Computer Science & Department of Materials Engineering, KU Leuven

Javier Velo Pérez, Department of Computer Science, KU Leuven

Version:

V1.0

Release date:

16.11.2023

OVERVIEW of the SIMULATION			
1	**User Case**	*The metallization plate of power semiconductors plays an important role in the thermal management. During service, it might lose its structural integrity due to void formation and growth.*	
2	**Chain of Models**	**Model 1**	*The mechanical continuum model for static equilibrium is coupled to a crystal plasticity model for plastic deformation in the matrix and a void growth model to study void growth at a grain boundary.*
3	**Publication Peer-Reviewing the Data**	*This simulation has not been published yet*	
4	**Access Conditions**	*DAMASK (https://damask.mpie.de) has been used. DAMASK is free and open source software according to AGPL v3*	
5	**Workflow and its Rationale**	*The aim of this workflow is to investigate the void growth rate in dependency of the internal pressure of the void at a grain boundary. To correctly include the anisotropic plastic flow of metals, a crystal plasticity model is used for the matrix. In the absence of a model for pressure increase, the void is modelled as an elastic material with volume expansion due to temperature increase.*	

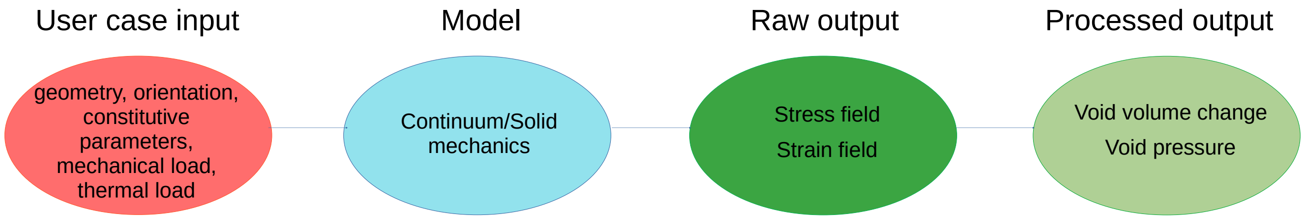
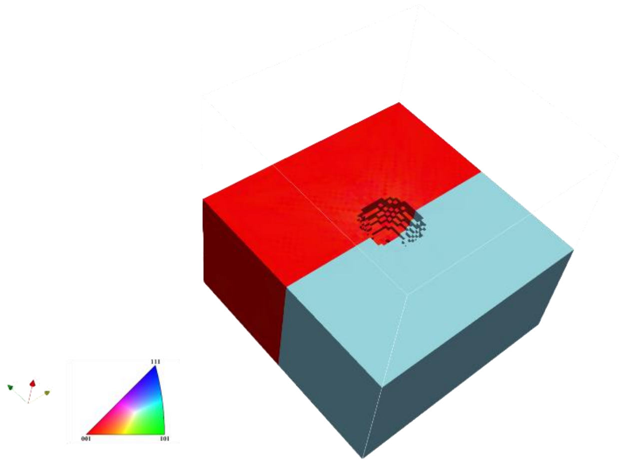


Figure 1: Void growth modelling workflow based on MODA workflow template [4]

2.1 MODA – Physics-based Model

MODEL 1

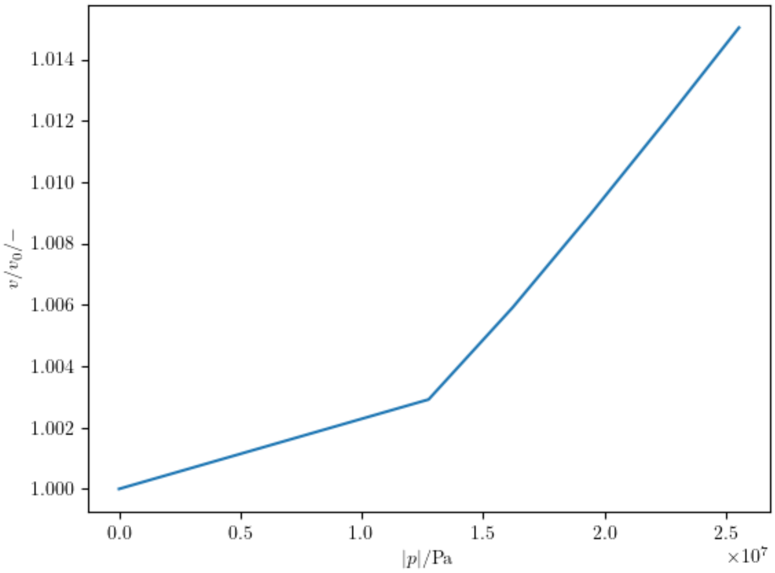
Void growth at grain boundary

1	Aspect of the User Case/System to be Simulated	
1.1	Aspect of the User Case to be Simulated	*Prediction of void growth rate in dependence of the internal pressure.*
1.2	Material	*Electrochemically deposited thin film polycrystalline copper metallization (<20µm) and organic trace impurities*
1.3	Geometry	*Bicrystal with spherical void. Shown below is a cut along the x-direction, the grain boundary is along the z-direction. Colour code is according to the inverse pole figure (IPF) along the z-direction.* 
1.4	Time Lapse	*500s*
1.5	Manufacturing process or in-service conditions	*The stress on the sides of the volume element is set to 0.0 MPa*
1.6	Publication on this data	*n/a*

2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	**MODEL TYPE AND NAME**	*Continuum model/Solid Mechanics.*	
2.1	**MODEL ENTITY**	*The entities in this material model are finite volumes/grains.*	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION** **PE**	**Physical Equation**	*Conservation of linear momentum ("Cauchy's first law of motion"):* div(***P***) = ***0*** *The static mechanical equilibrium is presented in a large strain formulation.* *A multiplicative decomposition of the deformation gradient* ***F*** *is used:* $\mathbf{F} = \mathbf{F}_e\,\mathbf{F}_i\,\mathbf{F}_p$ *In the matrix,* $\mathbf{F}_p$ *evolves according to a crystal plasticity law. In the void, the diagonal components of* $\mathbf{F}_i$ *are increased linearly with time.*
		Physical Quantities	***div*** *: Divergence operator* ***P*** *: First Piola-Kirchhoff stress tensor* $\mathbf{F}_e$ *: Elastic deformation gradient* $\mathbf{F}_i$ *: Lattice distorting, inelastic deformation gradient* $\mathbf{F}_p$ *: Lattice preserving, inelastic deformation gradient*
2.3	**MATERIALS RELATIONS**	**Relation**	*Linear* ***elasticity*** *(in the void)* - Generalized Hooke's law **S = C : E** - Elastic constants ***Elasto-viscoplasticity*** *(in the matrix)* - *Plastic velocity gradient (per system* $\alpha = 1\,..\,N$*)* $L_p = \Sigma_\alpha \dot{\gamma}_\alpha (s_s^\alpha \otimes n_s^\alpha)$ - *Phenomenological crystal plasticity* - *Shear in a slip system* $\dot{\gamma}^\alpha = \dot{\gamma}_0 \left\lvert \frac{\tau^\alpha}{\xi.\alpha} \right\rvert^n sgn(\tau^\alpha)$ −*Deformation resistance* $\dot{\xi} = h_0 \left(1 - \frac{\xi}{\xi_\infty}\right)^a sgn\left(1 - \frac{\xi}{\xi_\infty}\right)$
		Physical quantities/ descriptors for each MR	***C*** *: fourth-order elasticity tensor (****C*** *=* C_{ijkl} *, with only three independent components* C_{11}*,* C_{12}*,* C_{44} *for cubic crystals)* ***E****: Green-Lagrange strain tensor:* $\mathbf{E} = \frac{1}{2}\,\mathbf{F}_i^T(\mathbf{F}_e^T\,\mathbf{F}_e - \mathbf{I})\mathbf{F}_p$ *--* ***I*** *is the identity tensor* ***N*** *: number of slip systems* ***s****,* ***n*** *: Unit vectors along the shear direction and shear plane normal* γ *: Shear strain (*γ_0 *: reference shear strain)* τ *: Resolved shear stress* n *: Rate exponent* ξ *: Deformation resistance (initial* ξ_0*, saturation* ξ_∞*)* *a : Hardening exponent* ***Other****: crystal orientations*
2.4	**SIMULATED INPUT**	*n/a*	

3	**Solver and Computational translation of the specifications**	
3.1	**Numerical Solver**	*Spectral solver using FFT (DAMASK_grid with forward backward difference scheme)*
3.2	**Software tool**	*DAMASK (license AGPL v3)* *https://damask.mpie.de* *https://doi.org/10.1016/j.commatsci.2018.04.030*
3.3	**Time step**	*0.2 seconds (50 times steps for a total of 10 simulation seconds)*
3.4	**Computational Representation**	**Physics Equation, Material Relations, Material** *The deformation gradient is split into an average part and a fluctuating part. The fluctuating part is adjusted until the resulting stress is in mechanical equilibrium*
3.5	**Computational boundary conditions**	*The boundary conditions are given in terms of the volume average on a periodic domain*
3.6	**additional Solver Parameters**	*Derivative approximation: FWBW_Difference* *Field equations are solved using fully implicit time stepping* *Equilibrium of the mechanical stress field is ensured by evaluating the Root Mean Square (RMS) value of the divergence of the stress field*

2.2 MODA – Post Processing

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	*The volume change of the void (v/v_0) is plotted as a function of the absolute pressure (p) in the void.* 
4.2	**METHODOLOGIES**	*1) First, the Cauchy stress is calculated from the deformation gradient* ***F*** *and the second Piola-Kirchhoff stress* ***S****. Then, the absolute pressure p of the Cauchy stress is calculated.* *2) The determinant of the deformation gradient is calculated to obtain the change in volume in the void v/v_0.* *Both quantities are averaged over the volume of the void. All relations are standard in continuum mechanics.*
4.3	**MARGIN OF ERROR**	*The post processing is exact.*

Chapter 3 CHADA for EBSD experiments

In this chapter the CHADA for Electron Backscatter Diffraction (EBSD) experiments performed for two user cases of the project AddMorePower is presented. The CHADA is based on the common terminology defined in the CEN Workshop Agreement 17815 [1] and on the template released by M. Sebastiani et al. in April 2019 [5].

MODA authors:

Vedad Babic, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Sebastian Moser, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Manuel Petersmann, KAI- Kompetenzzentrum Automobil und Industrieelektronik
Michael Reisinger, KAI- Kompetenzzentrum Automobil und Industrieelektronik

Version:

V1.0

Release date:

17.11.2023

OVERVIEW of the Characterization		
1	**Samples**	Sample #1: Stressed or un-stressed polyheater test chip. For a detailed description see: Aichinger et al 2010 - In-situ Polyheater - a reliable tool for performing fast and defined temperature switches on chip [6] and Moser et al. 2019 - A novel setup for in-situ monitoring of thermo-mechanically cycled thin film metallizations [7]. Sample #2: GaN on Si structures Testing Environment is in vacuum (1E-5 – 1E-6 mbar)
2	**Chain of methods**	SEM imaging is used to find the area of interest after which the EBSD acquisition is started.
3	**Data publication**	• S. Moser, M. Kleinbichler, S. Kubicek, J. Zechner, M. J, Cordill, *Electropolishing – a practical method for accessing voids in metal films for analyses*, Applied Sciences *11*, no. 15: 7009, 2021, doi: https://doi.org/10.3390/app11157009 [9] • L. Hucht, *Correlation of pore formation and microstructural characteristics by linking SEM and EBSD data - application to the Cu metallization of power devices*, Master Thesis, *University Duisburg-Essen*, Duisburg-Essen, 2022 [10] • Related EBSD paper: S. Bigl, S. Wurster, M.J. Cordill, D. Kiener, *Advanced characterisation of thermo-mechanical fatigue mechanisms of different copper film systems for wafer metallizations,* Thin Solid Films, Vol. 612, pp. 153-164, 2016, doi: https://doi.org/10.1016/j.tsf.2016.05.044.[11]

4	**Access conditions**	Data processing: At ULM: • EBSD - ATEX - Free for non-commercial use, http://www.atex-software.eu/ • HR-EBSD - ATEX - Commercial, http://www.atex-software.eu/ At KAI: • EBSD - MTEX - Open source: https://mtex-toolbox.github.io/ • HR-EBSD - CrossCourt4 - Commercial, BLGVantage http://www.hrebsd.com/wp/crosscourt/
5	**Workflow of the characterization**	The sample is mounted on the stage within the vacuum chamber of the SEM. The electron beam is set up and the beam alignment is conducted. The area of interest is found by imaging in the SEM. Subsequently, the stage is tilted to 70 degrees tilt and the EBSD detector is inserted into the chamber. EBSD scan settings are chosen, i.e. grid size and step size. When everything is prepared, the scan starts, meaning that in an automated manner the probing electron beam is scanned from grid point to grid point of the previously determined grid. For each grid point, the response of the electron beam impinging the sample surface is detected with a dedicated EBSD detector. Due to its large area, the EBSD detector captures a considerable part angular distribution of the backscattered electrons, and hence diffraction related information. The raw EBSD detector information, image data showing Kikuchi diffraction patterns, is used for post-processing. In conventional EBSD it is Hough transformed to determine crystal structure, phase and individual crystal orientations on the sample, whereas in HR-EBSD it is directly evaluated using cross-correlation techniques to determine orientation data. This data is subsequently cleaned up, removing uncertain data points. The orientation and phase data can be used for texture analysis or after applying grain reconstruction algorithms, grain size analysis. Furthermore, analysis of the plastic deformation within the sample can be performed.

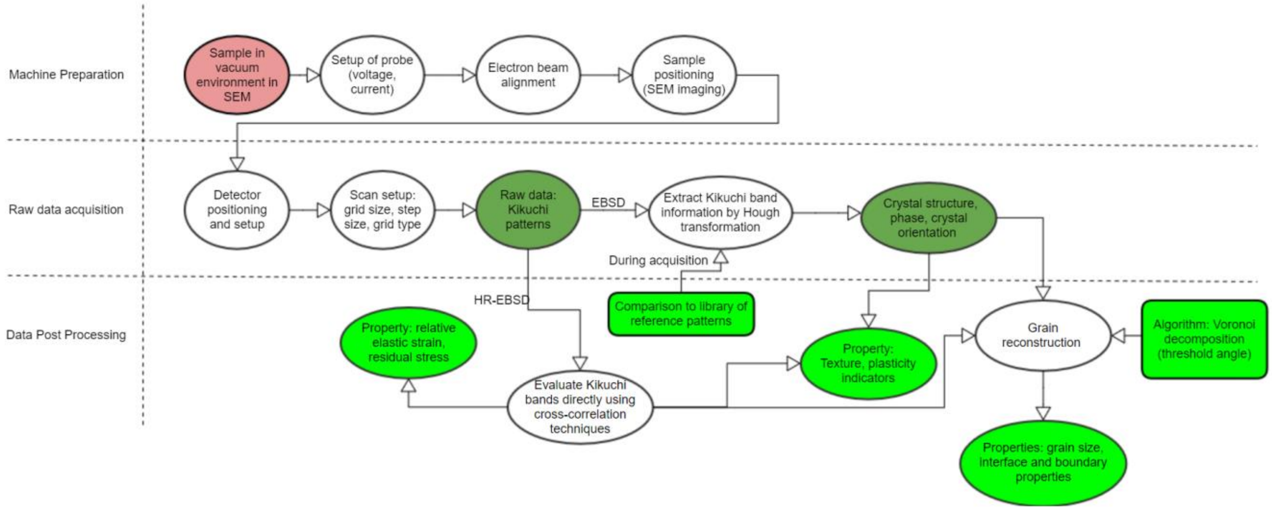


Figure 2: EBSD characterization experiments workflow in linked characterization methods style [8]

3.1 CHADA – Sample

1. SAMPLE		
1.1	**User**	Human operator with expertise, knowing how to operate both the SEM and EBSD system.
1.2	**User case (sample specifications)**	• User case #1: (KAI) Semiconductor device ("Polyheater") with a dedicated copper metallization structure (≙ ROI) to be investigated ○ The device itself has dimensions of 2x3 mm^2 in lateral directions and 120 µm in thickness ○ The ROI has dimensions of typically 500x700 µm^2 in lateral directions and 5-20 µm in thickness. ○ The surface within the ROI can be either as-fabricated, roughened (due to thermomechanical testing), or prepared by e-polishing (typically performed after thermo-mechanical testing for surface smoothing). ○ A detailed description of the samples can be found in the paper from Aichinger et al 2010 [7]. • User case #2: (ULM) Silicon-based wafer piece with an epitaxial GaN layer to be investigated ○ The wafer pieces have typical dimensions of 1x1 cm^2 and 775 µm in thickness. ○ surface as deposited In both cases, the sample is fixed on a sample holder using conductive silver paste or clamping.
1.3	**Specimen**	User case #1: Copper metallization structure that is integrated onto a Polyheater microelectronic chip (no conductive coating required) User case #2: GaN on Si
1.4	**Testing environment**	SEM chamber: high vacuum (1E-5 – 1E-6 mbar)
1.5	**Material**	• electrochemically deposited thin film polycrystalline copper metallization (≤ 20µm) • GaN/AlGaN heterostructure on Si

3.2 CHADA – Method

2.	**METHOD**	
2.1	**Sample/probe physics of interaction**	The electron beam impinges on the sample surface and subsurface, where it interacts with the probed sample material. The backscattered electrons are detected in the EBSD-detector creating Kikuchi diffraction patterns. They are automatically analysed to extract the crystal structure, phase, and orientation information and stored together with the SEM image of the EBSD scanned area.
2.2	**Volume of interaction**	The scattering interaction is limited to the surface and subsurface layers of the sample. The volume of interaction, in particular the depth of interaction, strongly depends on the probing parameters such as the acceleration voltage.
2.3	**Equipment setup**	Probe alignment and setup, sample positioning.
2.4	**Calibration**	During installation of the EBSD system.
2.5	**Probe**	Electron beam, accelerated by a voltage in the range of 1-30 kV. The electron beam is further characterized by its current.
2.6	**Detector**	Solid state detector using either a **C**harge **C**oupled **D**evice (CCD) sensor or a **C**omplementary **M**etal-**O**xide-**S**emiconductor (CMOS) sensor for detecting diffraction patterns of back-scattered electrons.
2.7	**Signal**	Back-scattered electrons
2.8	**Time lapse**	Depending on sample quality - scan size and step size - from minutes to hours (dwell time per pixel in ms range)
2.9	**Testing input parameters**	Electron beam voltage and current, SEM working distance, sample tilt, detector orientation and insertion distance
2.10	**Main acquired channels**	1. Kikuchi patterns 2. Orientation data

3.3 CHADA – Raw Data

3	**RAW DATA**	
3.1	**Raw Data**	Unindexed: Kikuchi diffraction pattern images for each pixel. May serve as direct input for alternative methods such as "HR-EBSD" (image registration between patterns). Indexed (software processed): corresponding crystal structure, phase, and orientation data (3x3 matrix per pixel).
3.2	**Data acquisition rate**	~1000 points per second (depending on detector and recording mode)

3.4 CHADA – Data Processing

4. DATA PROCESSING		
4.1	**Main data filtering processes**	• Removal of data points based on mean angular deviation (MAD), a quality metric used by Oxford Software, which basically relates to the uncertainty in translating Kikuchi patterns to orientations. • Removal of small grains, which might be due to misindexing. • Smoothing or filtering of the orientation data (after grain reconstruction) to reduce noise.
4.2	**Main data analysis procedures**	• Grain reconstruction based on phase and orientation data, to analyse grain size distribution. • Texture analysis by simply analysing the acquired orientations. • Analysis of local misorientations - plastic deformation - kernel average misorientation (KAM).
4.3	**Main processed channels**	Orientation and phase data.
4.4	**Data processing through calibrations**	n/a
4.5	**Properties (elaborated data)**	Grain size and shape characteristics, plastic deformation indicators, texture, interface characteristics, deformation.

Chapter 4 Summary and Conclusion

CHADA and MODA are methodologies for fostering innovation and research in materials manufacturing for Industry 5.0. The integration of materials characterization, modelling, and data science through these methodologies enables the sharing of insights and knowledge that can be used to develop better materials and manufacturing processes. By implementing CHADA and MODA, the community can benefit from:

1. Greater understanding of materials structure and properties across the whole community
2. Better prediction of materials behaviour
3. Improved materials design and development
4. Optimized manufacturing processes
5. Increased efficiency and productivity
6. Reduced costs
7. Accelerated innovation and research

Standardized terminology and classification are crucial to create taxonomies and ontologies for materials modelling and characterization. They are the formal basis for harmonized metadata with which models and databases can be linked. Additionally, they ease communication, dissemination, storage, retrieval and mining of data about materials modelling and characterization across the community.

The CHADA and MODA presented in this document are the starting point for a harmonized data documentation within AddMorePower. The final results will be documented in deliverable D2.4 “Documentation of materials characterization and modelling workflows (R, PU, M48): Documentation of the developed and implemented workflows based on the community standards CHADA and MODA”.

Chapter 5 List of Abbreviations

Abbreviation	Translation
AlGaN	Aluminium Gallium Nitride
ATEX	Analysis Tools for Electron and X-ray diffraction
CCD	Charge Couples Device
CHADA	Materials Characterization Data
CMOS	Complementary Metal-Oxide-Semiconductor
DAMASK	Düsseldorf Advanced Material Simulation Kit
EBSD	Electron Backscatter Diffraction
EMCC	European Materials Characterization Council
EMMC	European Materials Modelling council
FWBW	Forward backward difference scheme
GaN	Gallium Nitride
HR-EBSD	High Resolution Electron Backscatter Diffraction
IPF	Inverse Pole Figure
KAI	Kompetenzzentrum Automobil- und Industrieelektronik
KAM	Kernel Average Misorientation
kV	kilovolt
MAD	Mean Angular Deviation
MODA	Materials Modelling Data
ms	milliseconds
MTEX	Free Matlab toolbox for analyzing and modeling crystallographic textures by means of EBSD or pole figure data
RMS	Root Mean Square
ROI	Region of Interest
SEM	Scanning Electron Microscopy
Si	Silicon
ULM	Université de Lorraine

Chapter 6 Bibliography

[1] *CWA 17815 – Materials characterisation – Terminology, metadata and classification*, October 2021

[2] *CWA 17284 – Materials modelling – Terminology, classification and metadata*, October 2018

[3] Emmc.eu, *MODA template*, 2021.

[4] Emmc.eu, *MODA workflow template*, 2021.

[5] M. Sebastiani, C. Charitidis, E. P. Koumoulos, *CHADA docx detailed forms*, Zenodo, 2019, doi: https://doi.org/10.5281/zenodo.2637419

[6] T. Aichinger, M. Nelhiebel, S. Einspieler, T. Grasser, *In-situ Polyheater - a reliable tool for performing fast and defined temperature switches on chip*, IEEE Transactions on Device and Materials Reliability, vol. 10, no. 1, pp. 3-8, 2010, doi: 10.1109/TDMR.2009.2033467.

[7] S. Moser, G. Zernatto, M. Kleinbichler, M. Nelhiebel, J. Zechner, M. J. Cordill, R. Pippan, *A Novel Setup for In Situ Monitoring of Thermomechanically Cycled Thin Film Metallizations*. JOM 71, 3399–3406, 2019, doi: https://doi.org/10.1007/s11837-019-03695-2

[8] M. Sebastiani, C.Charitidis, E. P. Koumoulos, *Main Introduction to the CHADA concept and case studies*, Zenodo, 2019, doi: https://doi.org/10.5281/zenodo.2636609

[9] S Moser, M Kleinbichler, S Kubicek, J Zechner, M. J, Cordill, *Electropolishing – a practical method for accessing voids in metal films for analyses*, Applied Sciences 11, no. 15: 7009, 2021, doi: https://doi.org/10.3390/app11157009

[10] L. Hucht, *Correlation of pore formation and microstructural characteristics by linking SEM and EBSD data - application to the Cu metallization of power devices*, Master Thesis, University Duisburg-Essen, Duisburg-Essen, 2022

[11] S. Bigl, S. Wurster, M.J. Cordill, D. Kiener, *Advanced characterisation of thermo-mechanical fatigue mechanisms of different copper film systems for wafer metallizations*, Thin Solid Films, Vol. 612, pp. 153-164, 2016, doi: https://doi.org/10.1016/j.tsf.2016.05.044.