# DigiMatUS project overview


Project duration: 01.04.2023 - 31.03.2026

## MSE - Material

**Nanomaterials:** Metal thin films and piezoelectric aluminium nitride based (AlN, AlScN) thin films on glass and sapphire substrates

## MSE - Application areas

**Process optimization:** Process and synthesis parameters, simulation of process.
**Product development/design:** Faster development cycles for thin film processes.
**Material prediction**: Find thin films with desired properties, especially crystallinity, orientation, and piezoelectric properties.
**Quality control:** Predict film properties from process parameters.

## MSE - Product Lifecycle

**Refining/Processing:** Investigate dependence of process parameters on thin film properties, prediction of process parameters for specific film properties.
**Product development:** Shorten development cycles for thin film / multilayer deposition processes.

## MSE - Material properties

**Mechanical:** Film roughness, Film density
**Thermodynamic:** Particle energy, plasma density
**Crystallographic:** Film texture, film orientation
**Structural:** Film adhesion
**Other:** Piezoelectric properties, optical properties, acoustic properties

## MSE - Approach

**Experiments:** Process properties of vacuum based deposition processes (magnetron sputtering). Film properties (e.g. structural, crystallographic, or electric properties) and transducer properties.
**Computer Simulations:** Acoustic simulations of the fabricated transducers, electrical simulations for impedance matching networks, AI-driven simulation of process parameters.
**Machine Learning/Statistical/Big data:** Neuro-symbolic integration, informed machine learning, data-efficient learning.
**Coupled:** Acoustic properties of the transducers are highly dependent on the film properties on the glass substrates, especially the orientation and piezoelectric properties. Film properties are directly dependent on process parameters. Parameter settings derived from AI-driven prediction system will be used for sputtering processes.

## MSE - Material scales

**Microscale:** Thin films
**Mesoscale:** Thin films
**Continuum/Macro-scale:** Transducers

## General - Centrality of FAIR

**Findability:** The CoatO ontology will be registered at a suitable registration and indexing service. Ontology classes are identified by unique and persistent identifiers.
**Accessibility:** We created a conceptual model of the domain which is mapped to the CoatO. This conceptual model has been implemented as a data interface by multiple partners and is actively used to access data used to train AI systems.
**Interoperability:** CoatO is written in OWL and follows FAIR principles and is based on ISO/IEC 21838-2:2021. The metadata for data on process and film properties is aligned with this ontology.
**Reusability:** CoatO is published under an open license and under version control ensuring provenance. The development process meets ontology development best practices.

## General - Types of data

**Raw data:** Process parameters, measurement data
**Processed data:** Analytics data, trend data
**Metadata-focused:** CoatO Ontology

## General - Documentation and publishing of data

**Code repositories:** GitHub

## General - Proprietary/Non-proprietary

**Mostly proprietary data**

## Ontologies - Aspects of digitalization

**Procedures for ontology development:** Development of thin film ontology for magnetron sputtered thin films and film properties based on BFO.
**Data transformation using ontologies**: Data is transformed from partner-specific representations into a CoatO-aligned format.
**Publishing/disseminating knowledge graphs:** The ontology-aligned datamodel enables the generation of RDF-based triples which integrate data from different sources and partners.

## Ontologies - Levels of structured data handled

**Undocumented data:** Partner-specific spreadsheets.
**Human-readable documentation:** Reports.
**Partially structured data:** Excel sheets with collected data, measuring device outputs, database.
**Ontologically described data (RDF data)**: Produced as part of the project.

## Ontologies - Existing ontologies used

**MSE ontologies:** Perspective integration of PMDCo (v3+)
**Ontologies for units:** UO
**Domain-specific ontologies:** ChEBI
**Other ontologies:** BFO

## Ontologies - Tools for ontologies

**Editors and Collaborative tools:** Protégé
**Validation tools**: Hermit
**Formats and Languages:** OWL, RDF
**Utility python libraries:** py-horned-owl
**Other:** Robot, OWL API, Horned OWL

## Workflows - Types of workflows

**Data acquisition from experiments:** Depositions, material properties and transducer performance as data acquisition for simulations and machine learning.
**Post-processing/analysis of raw data:** Python scripts.
**Machine-learning:** Pytorch Lightning training loop and scheduling
**Computer simulation pipelines:** Post-processed data for acoustic simulations of transducers.
**Other:** Case-based reasoning

## Workflows - Workflow priorities

**Automation of workflows:** Raw data evaluation and transformation by customized python scripts

## Workflows - Workflow challenges

**Integration of tools:** Integration of diverse experimental tools.
**Automation:** Due to diverse sputter tools and infrastructure, sophisticated general automization can be time consuming.

## Workflows - Levels of workflow implementations

**Script jobs:** Python scripts

## Workflows - Publishing of workflow-related elements:

**Workflow modules:** If design is of general interest for community.
**Complete workflows:** If design is of general interest for community.

## Workflows - Use of PMD workflow store

**To find reusable workflow modules**
**To find complete workflows**
**Publish own workflows/modules**

## Workflows - Tools for workflows

**Simulation/CAD tools**: LtSpice, AWR Microwave Office
**Experimental software**
**Utility python Libraries**: scikit-rf, scipy, sqlalchemy, psycopg2, alembic, pandas, numpy
**Tools for ontologies/RDF data**: Protégé, Robot, py-horned-owl
**ML/LLMs:** PyTorch
**Languages:** Python, Fortran

## IT & Security - Computational demands

**Local workstation**
**GPU cluster access**
**Other:** GPU-server

## IT & Security - Data-federation

**Within own institution:** Internal data infrastructures.
**With project partners:** Exchange between experimental and theoretical / simulation partners.
**PMD-S:** To be decided on basis of data security.

## IT & Security - Software user interface

**Executable:** Python library for process parameter prediction.

## IT & Security - Tools for IT-architecture and security

**Data back-ends:** SQL data interfaces

## Use of PMD-Tools

**Workflowstore**

**PMDco**