DigiMatUS

Digitialization of materials research on thin-film materials using the example of high-resolution piezoelectric ultrasonic sensors

Project duration: 01.04.2023 – 31.03.2026

Material categories

Nanomaterials: Metal thin films, piezoelectric based AlN-, AlScN- thin films

Application areas

General information

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, crystallinity, orientation, and piezoelectric prop.
Quality control: Predict film properties from process parameters.

Approach

Experiments: Process properties of magnetron sputtering. Film and transducer properties.
Computer Simulations: Acoustic simulations of fabricated transducers, electrical simulations for impedance matching networks, AI-driven simulation of process parameters.
ML/Statistical/Big data: Neuro-symbolic integration, informed machine learning, data-efficient learning.
Coupled: Acoustic properties of transducers are dependent on the film properties. Film properties are directly dependent on process parameters. Parameter settings derived from AI-driven prediction system will be used for sputtering processes.

Centrality of FAIR

Findability: CoatO ontology registered at a suitable service. Ontology classes identified by PID.
Accessibility: Conceptual model mapped to CoatO. Implemented as a data interface by multiple partners.
Interoperability: CoatO written in OWL, follows FAIR principles, based on ISO/IEC 21838-2:2021.
Reusability: CoatO uses open license & version control. Development process meets best practices.

Aspects of digitalization

Semantic Interoperability

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.

Types of Workflows

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

Data-federation

IT Architecture

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.

Use of PMD-Tools

Ontodocker
PMDco
pyiron
PMD-S
Workflowstore
SimStack

Full project information

https://material-digital.de/download/2024-10-08_Projektubersicht_DigiMatUS.pdf