DigiChrom project overview

MATERIALDIGITAL

Project duration: 01.12.23 - 30.11.26

MSE - Material

Metals/Alloys: Chromium

MSE - Application areas

Process optimization: Better understanding of process-structure-property relationship for more efficient electroplating.

Product development/design: The aim is to obtain a layer with microcracks, as this layer is highly resistant to corrosion.

Quality control: Improve the process stability and capability of chromium plating.

MSE - Product Lifecycle

Manufacturing: Galvanic deposition

MSE - Material properties

Mechanical: Tensile strength, Hardness, Young's modulus (Nanoindentation)

Crystallographic: Particle distribution, Cracks, Grain size and orientation

Corrosion: Chemical Potential, NSS, Anodic polarisation, tarnish

Chemical: Layer Composition, Concentration, pH

Kinetic: Hydrodynamics, Deposition rate

Other: Wear resistance, Colour, Gloss, Adhesion

Coupled: All properties are the result of the microstructure and layer composition, which depend on the process parameters.

MSE - Approach

Experiments: Electroplating in trivalent chromium-based electrolytes, Characterization of the deposited layers.

Computer Simulations: Simulations of microstructure and mechanical properties with FEM.

Machine Learning/Statistical/Big data: Machine learning (Decision trees, Convolutional Neural Networks), Multiple linear regression, SQL database.

Coupled: The experiments provide large amounts of data that are stored in SQL and then analysed using machine learning and multiple linear regression. In addition, information for the simulation is generated from the experiments. The results of the simulation are then also incorporated into the machine learning.

MSE - Material scales

Coarse-grained atomistic: Grain size and orientation

Microscale: Microstructure, Cracks, Particle distribution

Continuum/Macro-scale: Layer properties

General - Centrality of FAIR

Interoperability: The project involves 9 partners who generate different data. All of this data will be stored in an SQL database and used together for machine learning. The project could serve as an example of cooperation in electroplating and act as a kind of branch solution.

General - Types of data

Raw data: Experimental data, time series data, Images, Simulation data, Chemical composition are all included in the project.

Processed data: Merging, mapping the data in SQL database with additional calculations are in included in the project.

Analysed data: Data are statistically analysed for normal distribution, correlation, and regression. Both classical mathematical methods and machine learning are used.

General - Documentation and publishing of data

Electronic Lab notebooks: eLabFTW

Code repositories: GitHub

Publication in data focused journals: J. Electrochem. Soc, J. Appl. Electrochem., Coatings

Other: Microsoft Azure Cloud Explorer

General - Proprietary/Non-proprietary

Both: Process parameters, Electrolyte composition (proprietary), experimental data (mostly non-proprietary)

Ontologies - Aspects of digitalization

Procedures for ontology development: Development of application ontology, Integration of chemical data, Domains Coating/Layer materials.

Data transformation using ontologies: Transform process and characterization data.

Publishing/disseminating knowledge graphs: Publishing knowledge graphs about process-structure-property relationship in electroplating.

Workflows benefitting from knowledge graphs: Digitalization and merging of experimental data, lab book and characterization data.

LLM integration: Easier access to the data and evaluations.

Ontologies - Levels of structured data handled

Human-readable documentation: Excel data, lab book

Partially structured data: Data from simulations, Measurement data, machine data (plating control software)

Ontologically described data (RDF data): Data processed using application ontology

Ontologies - Existing ontologies used

MSE ontologies: PMDco 2.0.7

Ontologies for units: CHEBI:24431

Domain-specific ontologies: Application Ontology DigiChrom, PMD TTO

Ontologies - Tools for ontologies

Editors and Collaborative tools: Protégé

Visualization tools: WebVOWL, Miro

Utility python libraries: langchain

Other: Microsoft Azure Fabric

Workflows - Types of workflows

Data acquisition from experiments: Coating experiment, equipment controls are automated, Chemical analysis, Characterization of the layers, excel data as output.

Post-processing/analysis of raw data: Preparation of raw data from experiments for semantic annotation using Microsoft Azure Fabric, python. Statistical analysis about normal distribution, correlations, and regression.

Provenance within experimental processes: Generate enough data for a detailed model of the process-structure-property relationship.

Machine-learning: Analysis of the data and create a model of the process-structure-property relationship. Analysing of pictures regarding cracks.

Computer simulation pipelines: Simulations for e.g., nanoindentation and determining mechanical properties of chromium layers.

Workflows - Workflow priorities

Other: Digitalization of the experimental data. Merging and mapping of the data form different source and provide the data for ML.

Workflows - Workflow challenges

Data formats: Each measurement device has it one format and export (text, csv, tsv etc.).

User interfaces: Easy access to the data and evaluations.

Semantic representation: Linking the data with sufficient semantics.

Other: Achieve a common understanding (electroplating <-> data science).

Workflows - Levels of workflow implementations

User friendly interfaces: The additional effort for digitization should be low in order to increase acceptance.

Workflows - Use of PMD workflow store

To find reusable workflow modules

Find interoperable set of workflow modules

Publish own workflows/modules

Workflows - Tools for workflows

Workflow management: Microsoft Azure Fabric Pipelines

Simulation/CAD tools: Abaqus

Utility python Libraries: Pyiron, Scipy, Psycopg2, Langchain, Pandas

ML/LLMs: AcademicCloud, ChatGtP, LLAMA

Other: Microsoft Azure Fabric, PostgresSQL

IT & Security - Computational demands

Local workstation

Usage of HPC resources

Usage of cloud resources: Commercial Cloud Azure

GPU cluster access

IT & Security - Data-federation

With project partners: Easy access to data and evaluation, protection of the proprietary data.

IT & Security - Software user interface

Executable: Frontend for access to data and evaluations.

IT & Security - Data encryption

Certification: For the access to proprietary data.

Community - Other initiatives/consortia:

Gaia-X: Ecosystem Mobility

Use of PMD-Tools

Workflowstore **PMDco** **pyiron**