DigiChrom

Digital tools for improving electroplated layers using the example of chromium(III)-based processes

MATERIALDIGITAL

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Material categories

Metals/Alloys: Chromium

Application areas

General information

Process optimization: Understanding of process-structure-property relation for efficient electroplating**.**
Product development/design: Hard Chrom layer - Goal: obtain a layer with microcracks, which is highly resistant to corrosion. Decorative chromium layer – Goal: obtaining a color fidelity layer with high corrosion resistance.
Quality control: Improve the process stability and capability of chromium plating.

Product Lifecycle

Manufacturing process: Electroplating

Approach

Experiments: Electroplating in trivalent chromium-based electrolytes, Characterization of layers.
Computer Simulations: Simulations of microstructure and mechanical properties with FEM.
ML/Statistical/Big data: Decision trees, CNN, Multiple linear regression, SQL database.
Coupled: Experiments provide large amounts of data, which are analysed using ML. Information for the simulation is generated from the experiments. Results of simulations are incorporated into ML.

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 application ontology, Integration of chemical data, Domains Coating/Layer materials.
Data transformation using ontologies: Transform process and characterization data.
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.

Types of Workflows

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.
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.

Other initiatives/consortia:

Community

Gaia-X: Ecosystem Mobility

Use of PMD-Tools

Ontodocker · PMDco · pyiron · PMD-S · Workflowstore · SimStack

Full project information

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