Towards an ontology-based digital twin for graphene-based conductor materials

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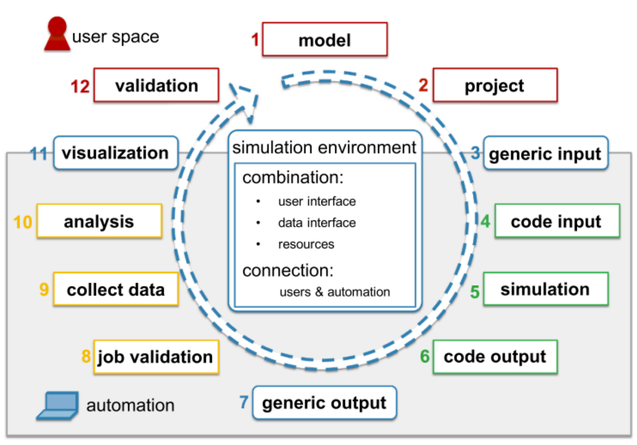
Digital models, ontology, workflows

Platform MaterialDigital (PMD)

- Development of a material ontology for a knowledge-based storage format
- Store data on a platform in a standardized format
- View, compare, analyze, and process data on interactive web application



J. Janssen et al., *Computational Materials Science* **163**, 24 (2019)

Ontology & knowledge graph

- Ontologies: prov-o + pmdco + application ontology + qudt
- Software: Protégé, Python + owlready2
- Include relevant material properties, process parameters, and model parameters
- Create database
- SPARQL queries to filter the database

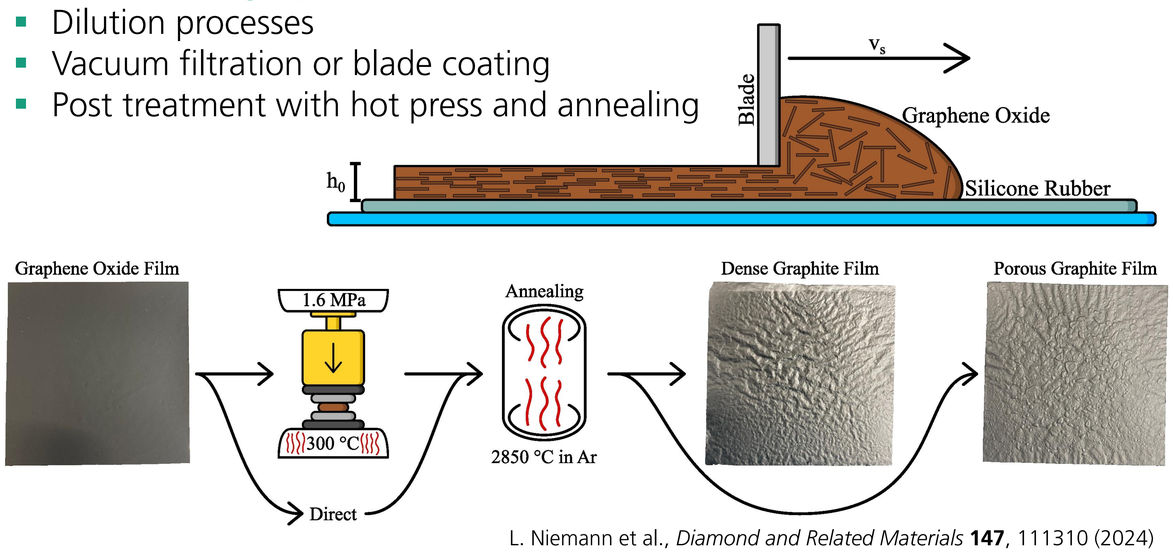
Simulation workflows

- Connect software tools with ontology to store simulation results in knowledge graph
- PMD workflow store based on pyiron

Use case: digitalized lab book

Production of graphene-based materials

- Dilution processes
- Vacuum filtration or blade coating
- Post treatment with hot press and annealing



L. Niemann et al., *Diamond and Related Materials* **147**, 111310 (2024)

Various measurements

- Eddy current, viscosity, shear stress, thickness, mass

Digital description

- Standardized formats: Excel --> json --> rdf
- Interactive app to enter, change and store data
- Scripts for automatic data visualization

Graphene conductor database

Blade coating | Hot press | Annealing | **Samples** | Analyze data | Individual SPARQL query

Samples: 90

Select sample: GIC-022-1

Add new sample

Delete selected sample

Production | Graphene oxide film | Graphene film

Production

property	value
production process	vacuum filtration
hot press	--
annealing	A-1

Change

Annealing

step	atmosphere	heating rate	temperature	duration
1	H2/Ar			
2	Ar			
3	Ar			
4	Ar			

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Graphene-based conductor materials

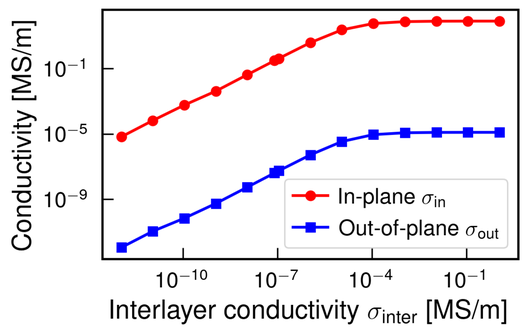
Material properties

- Stack of disordered graphene flakes
- High electrical conductivity
- Influenced by packing density, number of layers, flake size and orientation, microscopic conductivity

Use case: network simulation model

GraConSi

- Own network simulation tool
- Nodal analysis to calculate the conductivity (in-plane, out-of-plane)
- Workflow automatized with pyiron



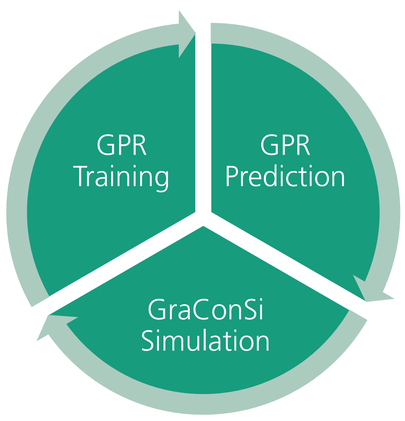
Digital description

- Semantic data description
- Store all input / output data in ontology / knowledge graph
- Workflow automatized with pyiron

Use case: data-driven surrogate model

Surrogate model

- Gaussian process regression (GPR)
- Fast, sufficient accuracy
- Uncertainty quantification



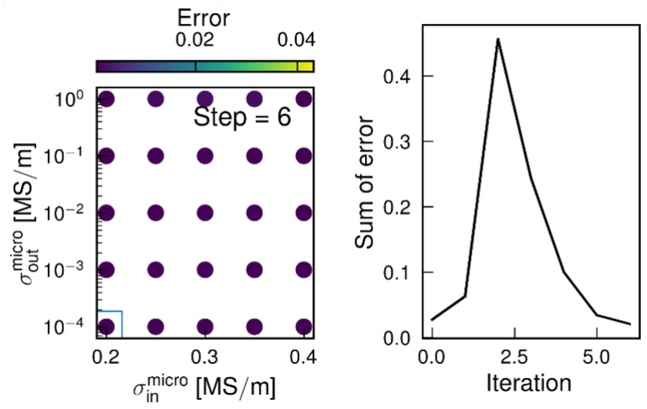
GPR training

Iteratively add new data points

(1) Predict properties with GPR

(2) Perform GraConSi simulation for data with highest uncertainty

(3) GPR training with new data



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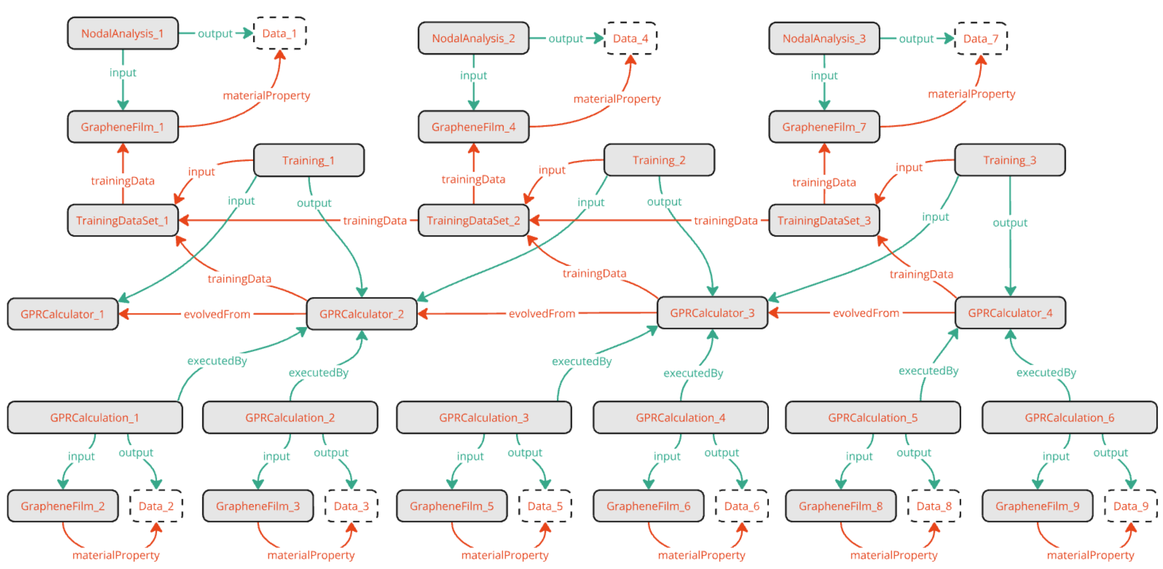

This work has been funded by the *Bundesministerium für Bildung und Forschung* via the project *DiMoGraph*.

Bundesministerium für Bildung und Forschung

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