General assembly PMD

Digitale **Mo**delle **Graph**en **(DiMoGraph)**

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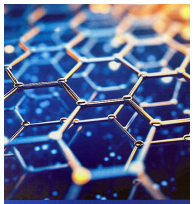
Fraunhofer ENAS

- Motivation
- Experimental progress
- Summary

- Simulation approach
- Ontology
- Use cases

Martin Köhne
Lukas Powalla
Leonhard Niemann
André Hermannsdorfer
Alberto Bollero

Florian Fuchs
Fabian Teichert
Jörg Schuster



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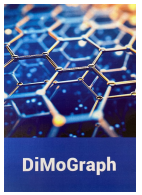
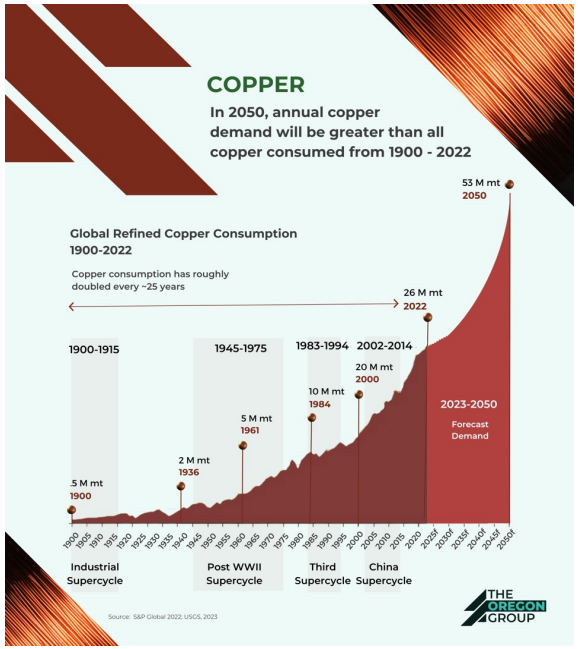
PMD - DiMoGraph
Motivation



Copper demand

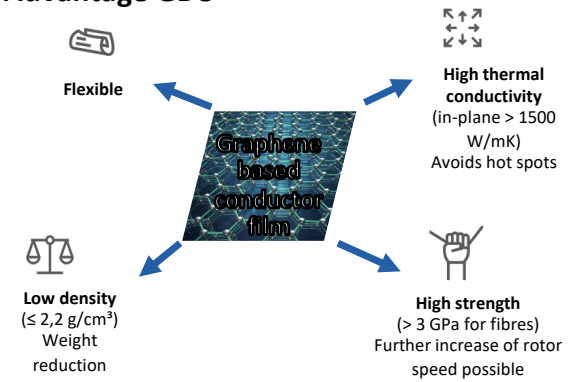


- Copper (Cu) demand will double to 53 million tons/year by 2050
- Current mined Cu production capacity only projected to increase by 20% over the next decade
- Oxygen-free Cu is used in electrical applications
  - +57% increase in demand till 2035
  - Strong increase by transport electrification

→ In long-term Cu price could double or even triple

→ Graphene-based conductors (GBC) as potential Cu replacement

Advantage GBC



Comparison to copper

- Abundancy of carbon is 10x higher
- Carbon deposits are all over the world
  → High security of supply
- Less energy needed for raw material extraction
- Electrical conductivity can reach up to 50% of copper by intercalation of strong Lewis acids.

Future copper demand will surpass mining capacities!

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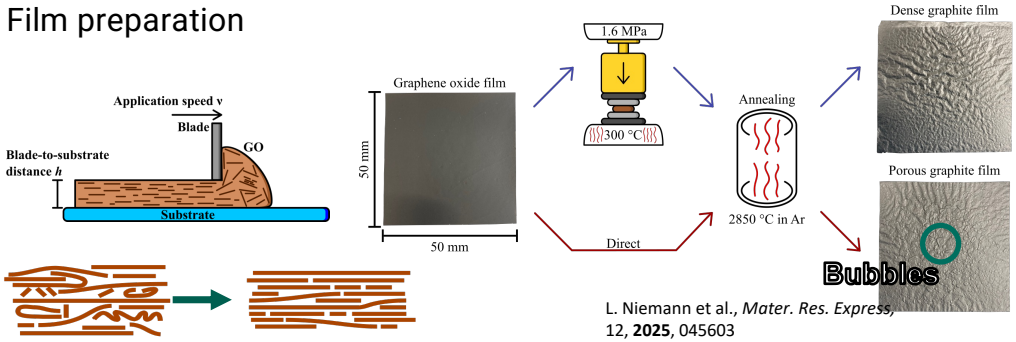
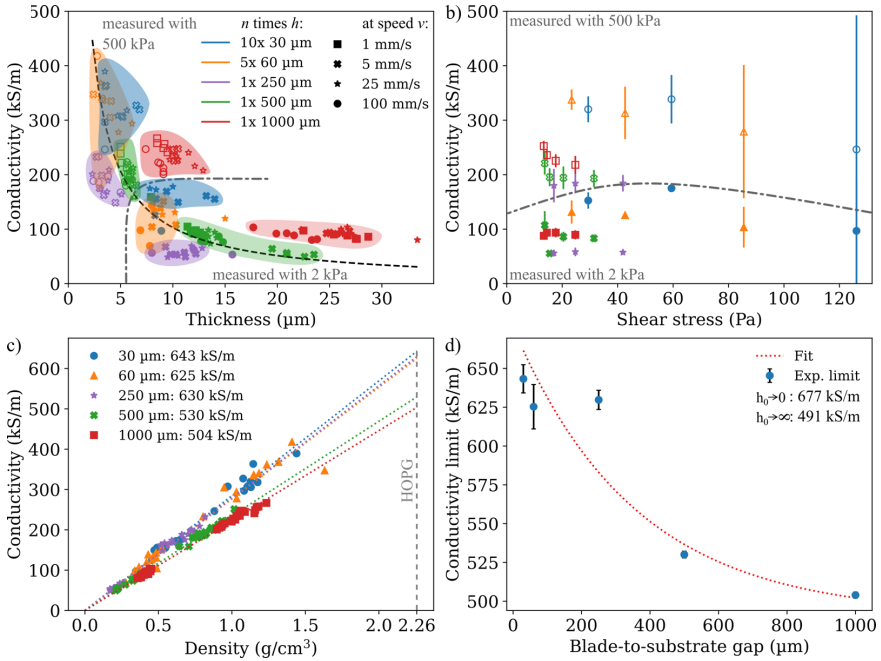
Experimental progress

Improve graphite flake networks by blade-coating

Film preparation



L. Niemann et al., *Mater. Res. Express*, 12, **2025**, 045603



- Final electrical conductivity after doping depends on conductivity of starting material
- Electrical conductivity usually independent of object dimensions
  → Here: Dependency on the thickness
- Shear stress does not influence conductivity
- Blade-to-substrate gap seems crucial for high electrical conductivity

Small blade-to-substrate gap forces mechanically flakes to align parallel to each other.

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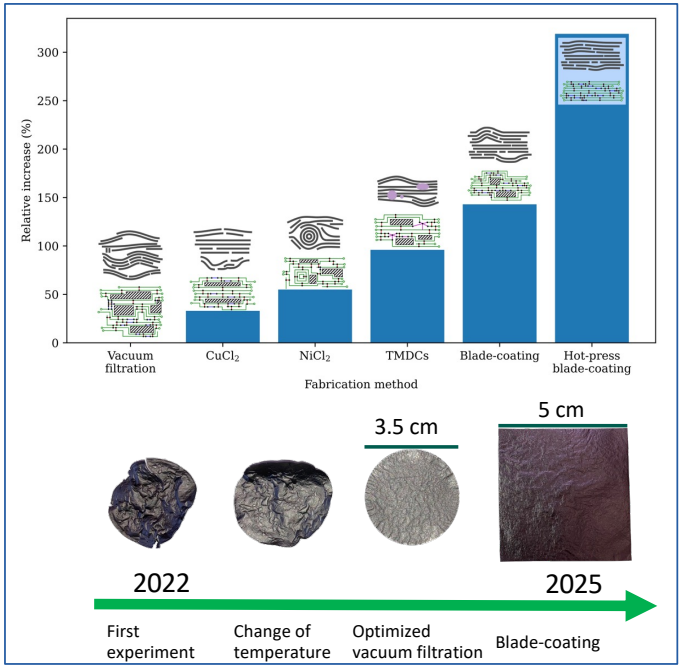
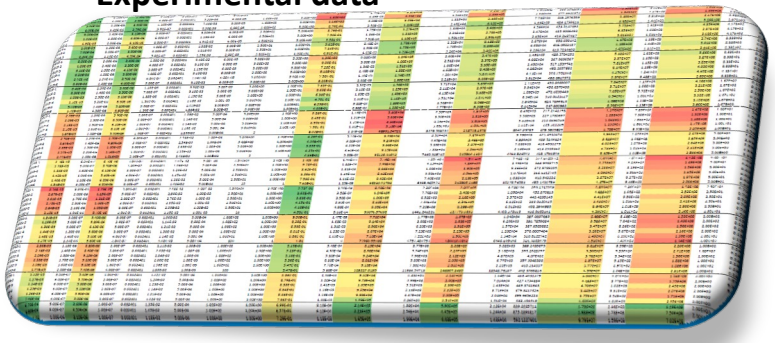
Experimental progress

Impact of processing on electr. conductivity



- Ordering of flakes
  - Reduced porosity
  - Improvement of conductivity
- Hot-press densification with strong impact on conductivity
- Blade-coating needs no additives

Experimental data



Improvement of graphene oxide flake based graphite conductors by progress in flake orientation

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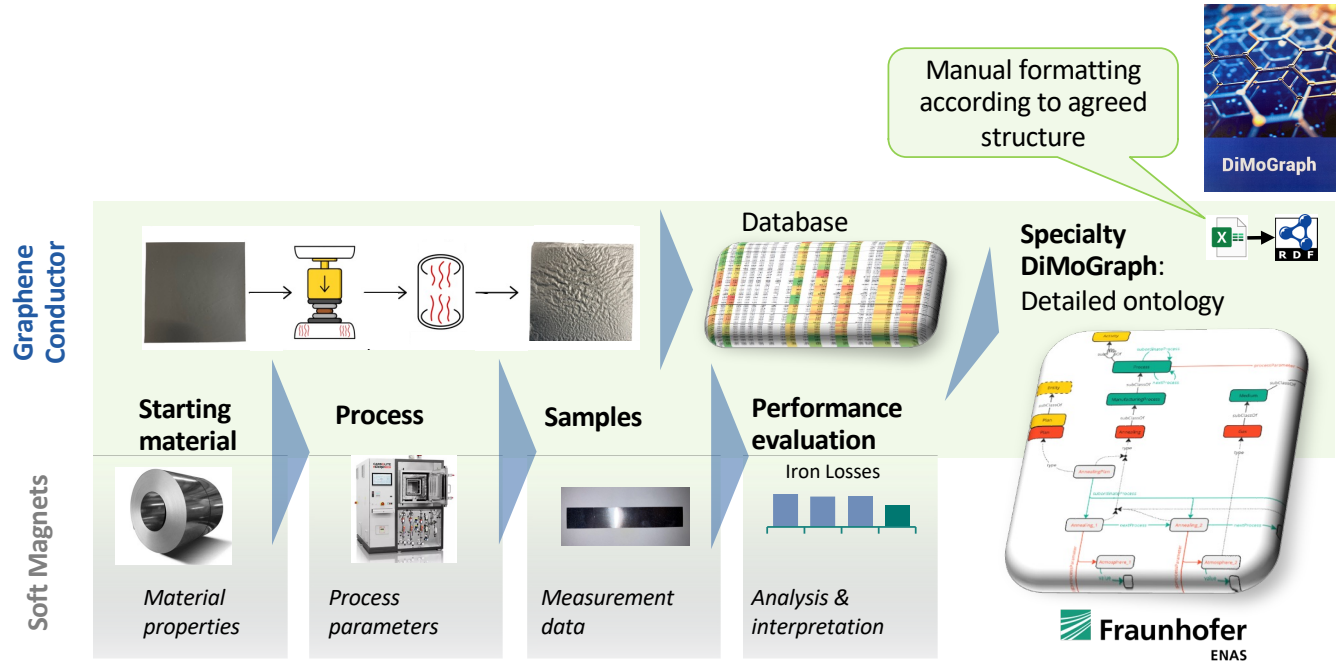
Summary

Results

- Detailed ontology for fabrication of graphene oxide based graphite films
- Integrate simulations and their refinement via machine learning
- Insight into possibilities of Digital material research:
  - Speed up data analysis
  - Make historical data usable
- Ongoing application:
  - Soft magnets:
    Magnetic properties analysis



Conclusions

- Ontology enables deep understanding of all process steps and their holistic interactions
- Manual creation of an ontology is possible, but inefficient.
- Large benefit (understanding, structuring, speed, IP generation …) is expected for complex datasets.

DiMoGraph paved the way into Digital Materials Research

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Thank You ☺

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Lukas Powalla

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Alberto Bollero

Department of Advanced Technologies and Micro Systems, Robert Bosch GmbH

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