AUTOMATION, DATA DRIVEN AND MACHINE LEARNING METHODS IN COMPUTATIONAL MATERIALS DESIGN

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4th Workshop on Interoperability in Materials Modelling (IntOP2018)

Fraunhofer IWM, Freiburg, Germany

Nov. 6, 2018

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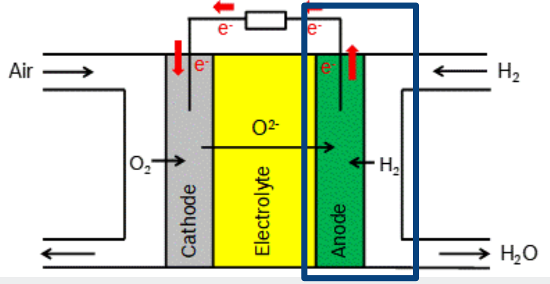
4th Workshop on Interoperability in Materials Modelling

Automation, data driven and ML methods in computational materials design

Outline
Automated DFT simulations – digital materials design
Data-driven microstructure generation – virtual microstructure design
Data-driven materials science – automated extraction of semantic relations

Automated DFT simulations
Modelling SOFC anode aging



Problem

- Ni-YSZ[1] anode degradation qualitatively understood: Ni grains coarsen over time: performance degradation
- Need for quantitative lifetime prognosis > 3000 h, but no validated accelerated lifetime tests

Research objectives:

With combined experimental and simulative multiscale modelling

- Understand relation between anode microstructure evolution and degradation rate
- Propose optimized microstructure

- **Focus on interoperability in modelling chain**

Interface energies Diffusion constants

Ab initio simulation **Thermal grooving exp.**
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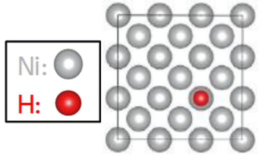
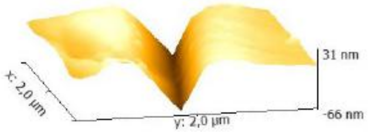
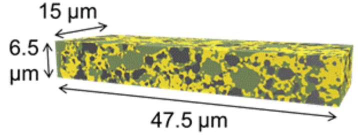




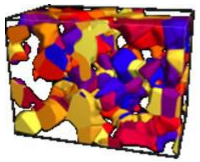
3D microstructure reconstruction of tested cells

Microscopy, µCT
KIT, RJL



3D modelling of microstructural evolution

Phase field simulation
HS Karlsruhe



Long-term performance prediction

Performance model
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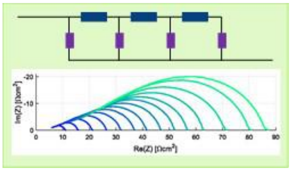


[1] Yttria-stabilized zirconia

PfP KerSOLife100
Funding No. 03ET6101A
Bundesministerium für Wirtschaft und Energie

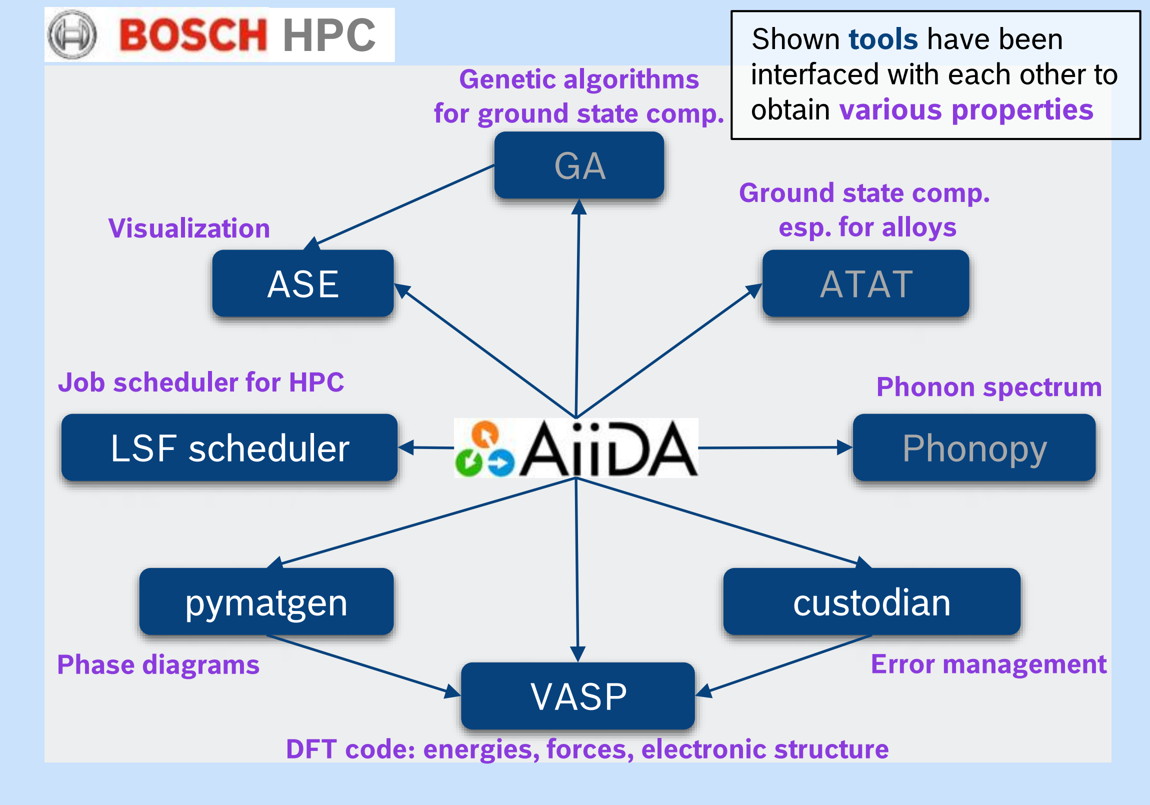
Automated DFT simulations
AiiDA at Bosch

AiiDA – Automated Interactive Infrastructure and Database for Computational Science

- Job manager
- Workflow manager
- Database

Origin of AiiDA

- Joint project between THEOS group / MARVEL Center at EPFL and Research and Technology Center NA at Bosch
- Now Open source project
- Bosch is still actively contributing to its further development



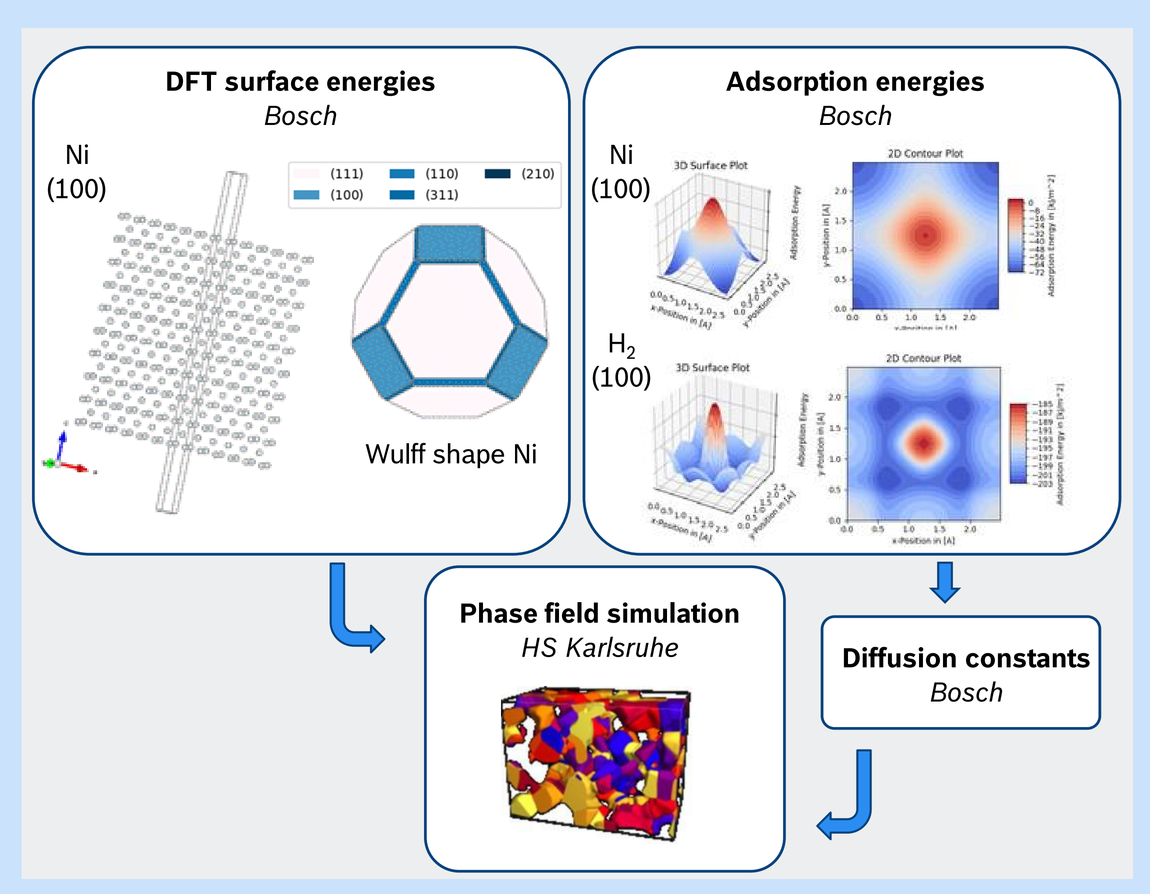
Automated DFT simulations
Use case for linked / coupled workflows

Output on atomistic scale

- Surface energies of Ni w/ different surface orientations: material parameter 1 for extended phase field simulation[1]
    - Validation w/ experimental data (weighted average)
- Adsorption energies of Ni / H_2 on Ni surface: input for calculation of diffusion constants
    - Diffusion constants: material parameter 2 for phase field

Current status workflow and linking

- Manual data transfer to partners required
- Workflow not automated
- **Open simulation platform would enable process automation**



[1] Instead of total diffusion, volume and surface diffusion calculated individually at HS Karlsruhe

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Data-driven microstructure generation
Speed-up in materials development

Motivation

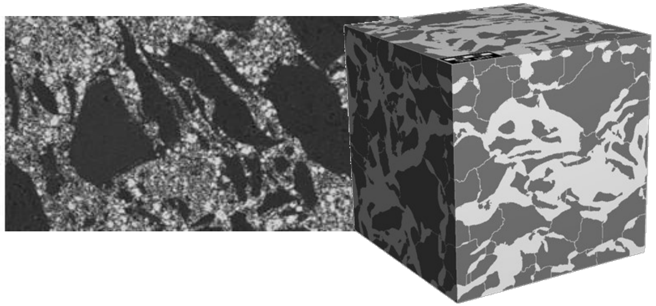
- Properties of heterogeneous materials depend strongly on microstructure
- Optimizing microstructure by trial-and-error very lengthy and expensive because of the long experimental chain (sample manufacturing, analyses, measurements)
- Explore potential of data-based methods for accelerating materials development on micro-scale.

Use cases

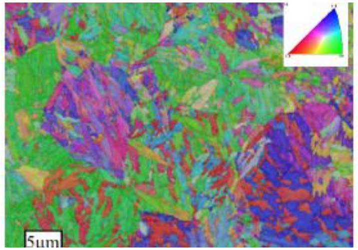
Fuel cell anode (SOFC)
porous Ni-YSZ composite

Source: KIT, PfP KerSOLife100
Funding No. 03ET6101A

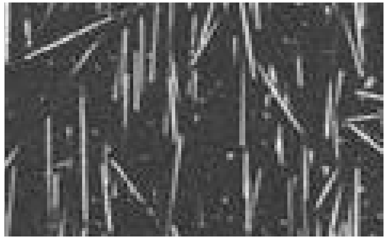
Ceramic composite material
glass particles in precursor matrix



Martensitic steel
nested grain structure



Short glass fiber reinforced thermoplastics (SFRT)



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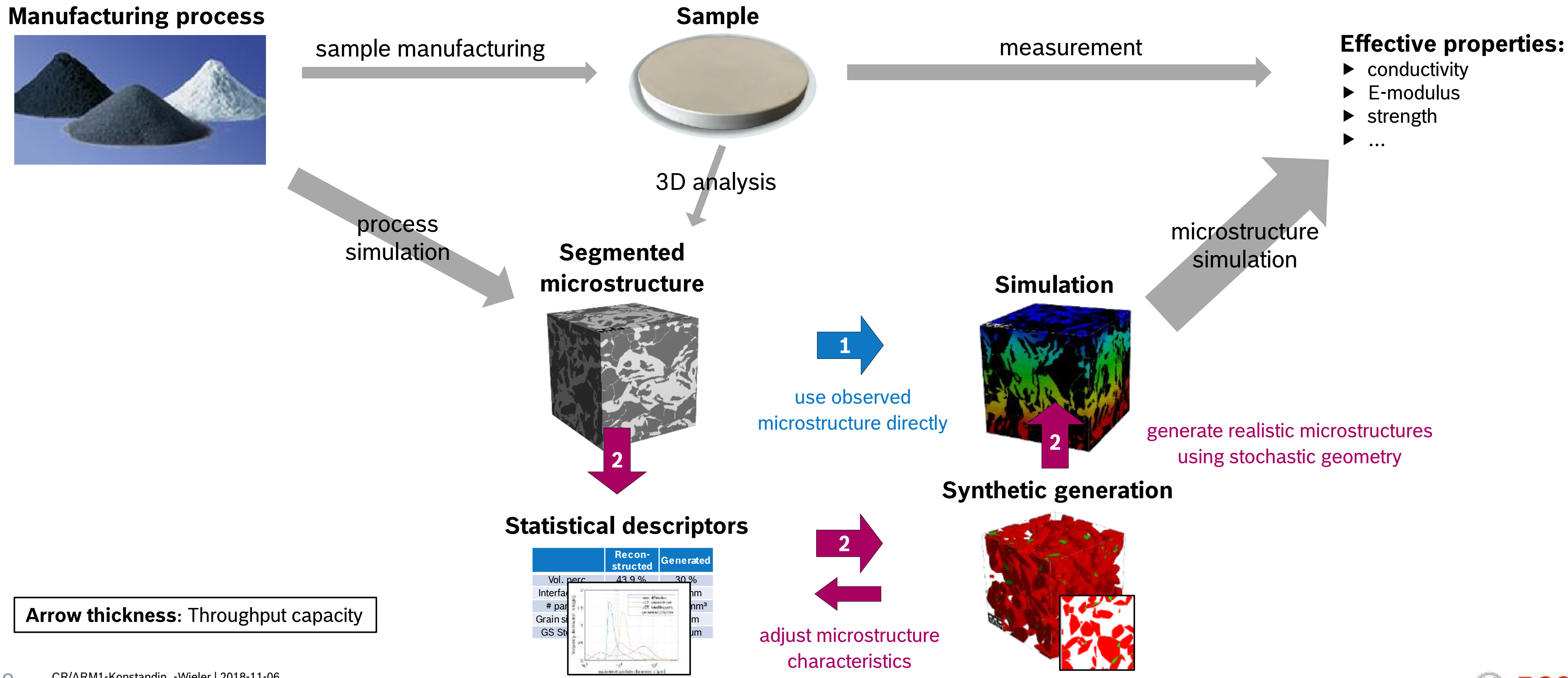
Data-driven microstructure generation
Current status: process of materials development



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Data-driven microstructure generation
Perspective: use potential of data-based approaches

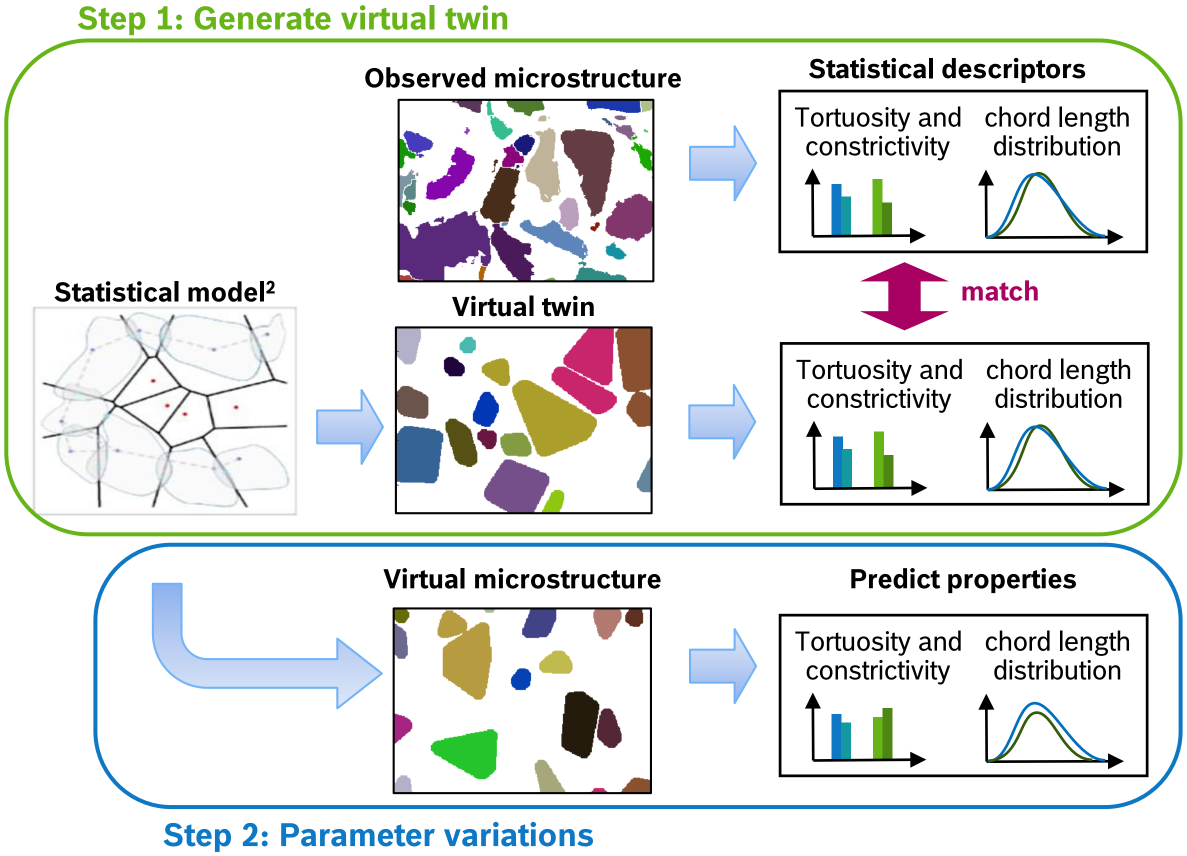
Limitation of current approach

- Many manufactured samples required for statistical microstructure reconstruction
- Simulations do not provide design rules for microstructure optimization → trial and error

Idea of data-driven microstructure generation

- Predict effects of variations in microstructure
- For realistic microstructures: need for data-based generator[1]

- **Virtual microstructure design can speed-up and reduce costs of materials development significantly**
- **Marketplace platform beneficial for linking of tools and use of database**



[1] using databases and/or AI methods w/ data of previously / virtually reconstructed microstructures
[2] Source: Westhoff et al., Computational Materials Science 126 (2017) 453–467, Ulm University, Institute of Stochastics

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Data-driven materials science

Access unstructured data, uncover hidden knowledge and make predictions

Project scope

- Automated knowledge based analysis of literature, patents and websites

Advantages

- Vast amounts of available unstructured data and knowledge made accessible
- High efficiency by structured data compared to pdf-document collection
- Hidden knowledge can be extracted, new knowledge can be predicted.

Results: Relation extraction

10.1016/j.cis.2010.05.006	Mn2Bi2W20	Hc	Oe	193
10.1016/j.carbon.2014.05.064	Fe3O4	Hc	Oe	250
10.1016/j.ceramint.2014.08.071	La0.7Sr0.3MnO3	Hc	Oe	20
10.1016/j.carbon.2013.05.044	14% Ni–B	Tc	K	172
10.1016/S1572-0934(11)04001-7	CeCu2Si2	Tc	K	0.5
10.1016/S1572-0934(11)04003-0	CePt3Si	Tc	K	0.75
10.1016/j.ceramint.2014.08.071	La0.7Sr0.3MnO3	magnetoresistance		0.58
10.1016/S0007-8506(07)61219-0	samarium-cobalt	remanence	mT	890
10.1016/j.carbon.2009.05.022	α-Fe2O3	remanent magnetization	emu/g	0.203
10.1016/S0007-8506(07)61219-0	neodymium-iron-boron	remanence	mT	1100
10.1016/j.ceramint.2014.08.117	Mg0.96Tb0.04Fe2O4	Lattice constant		8.367
10.1016/S0009-2614(99)00026-3	La1.56Eu0.04Sr0.4CuO4	Lattice parameters		5.318

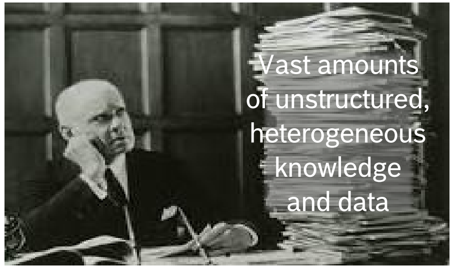
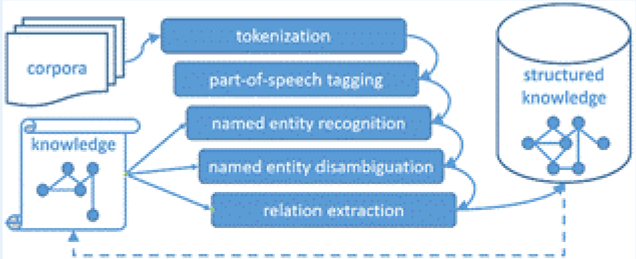
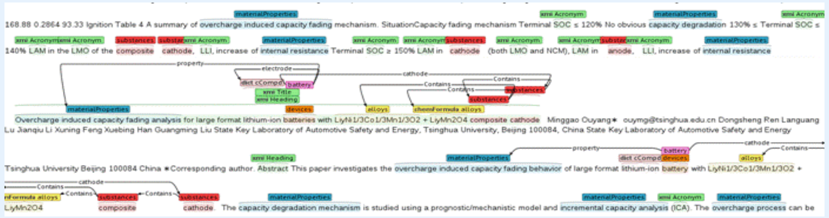


Image: Courtesy of Computer History Museum

Text mining: From vast amounts of unstructured data to a structured knowledge





Example: annotated text after entity/relation extraction

Pipeline for extraction of entities (e.g. materials, ...), relations and frames (is a, reacts with, is part of, ...) from unstructured, heterogeneous texts (e.g. literature, patents, websites, ...).

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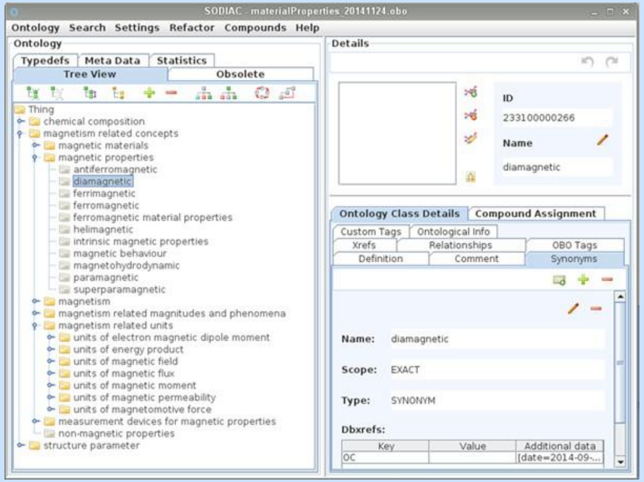
Data-driven materials science
Application: text mining for magnetic materials

Objective

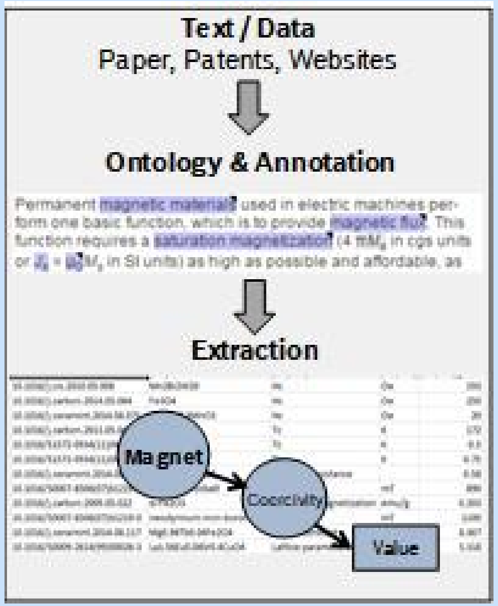
- Efficient extraction of design rules for hard magnets from publications, patents and websites

Results

- Text mining method from drug discovery transferred to material science w/ external partner
- Structured hard magnets knowledge created as ontology for semantic text processing
- **~10,000 magnetic material properties** from more than **2 million publications** extracted



Ontology for hard magnets



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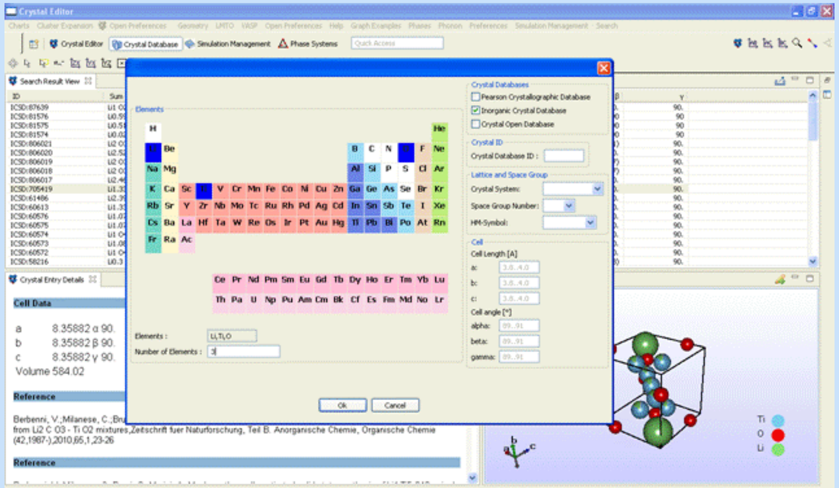
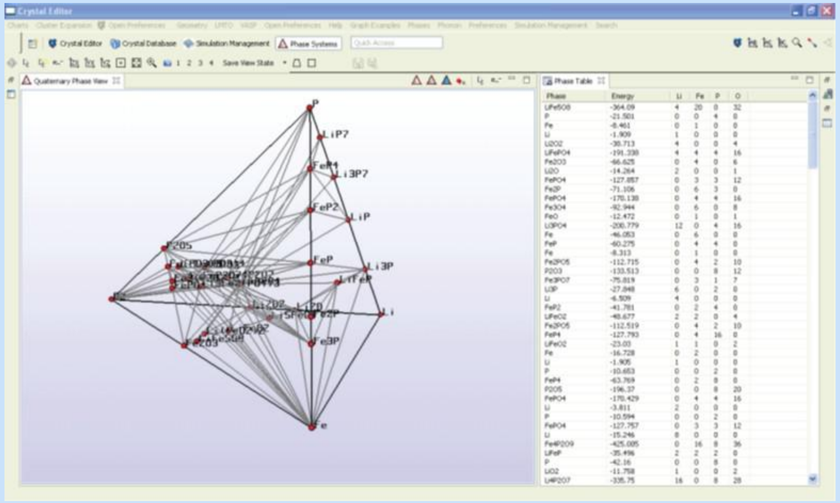
Data-driven materials science
Combination with other data sources

- Integration of different data sources into a data warehouse to unify access
  - Literature data from text mining results
  - Crystal Structure Databases: ICSD[1], COD[2], Pearson[3]
  - Ab-initio databases: Materialsproject, AFLOW[4], OQMD[5]

- Specific hard-magnetic data sources
  - Ab-initio results from LMTO[6] calculations (Prof. Elsässer, FhG IWM)
  - Results from own experiments





[1] Inorganic Crystal Structure Database, [2] Crystallography Open Database,
[3] Crystal Structure Database For Inorganic Compounds, [4] Materials Property Database,
[5] Open Quantum Material Database, [6] Linear muffin-tin orbital (Ab-initio method, alternative to DFT)

Materials data warehouse (market place platform) forms a basis for automated workflows and using AI methods