

EvalSpek-ML: Disassembling linear combinations into their constituent parts

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Big Data Analytics – Connection Workshop

2023-02-23

Summary

$$D(x) = \sum_{i=1}^N a_i \cdot (d_i * R)(x) + B(x)$$

$D(x)$ total dataset

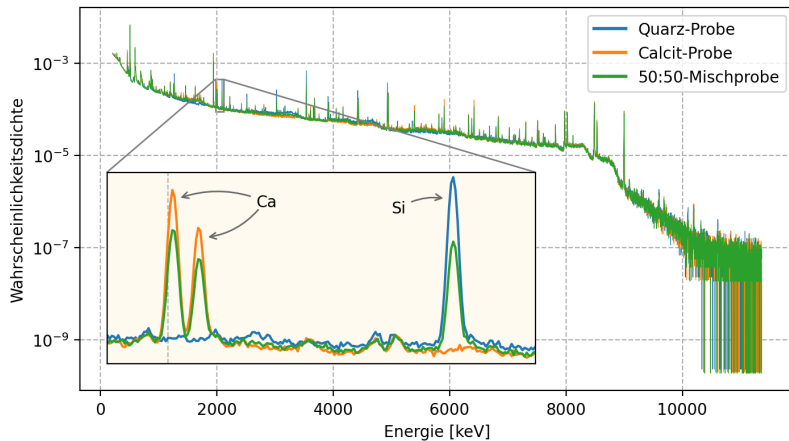
a_i prefactors: $a_i \in [0, 1]$; $\sum_{i=1}^N a_i = 1$

$(d_i * R)(x)$ possible components, smeared with instr. res.

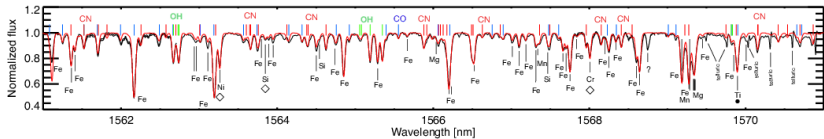
$B(x)$ background

determine \vec{a}

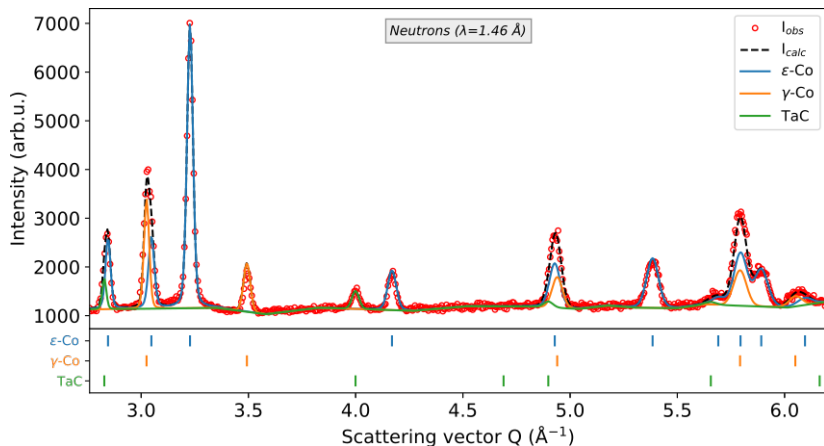
Nuclear Analytical Chemistry



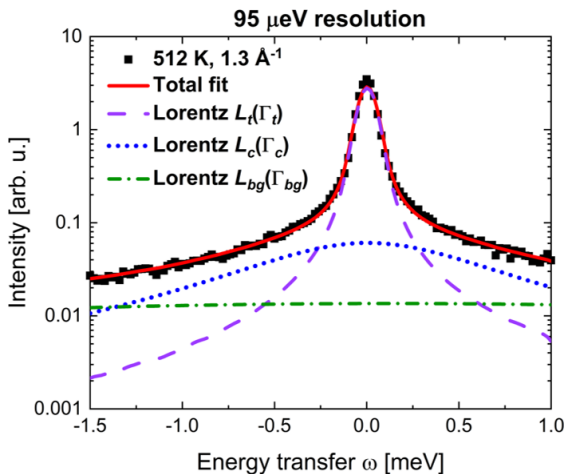
Astrospectroscopy



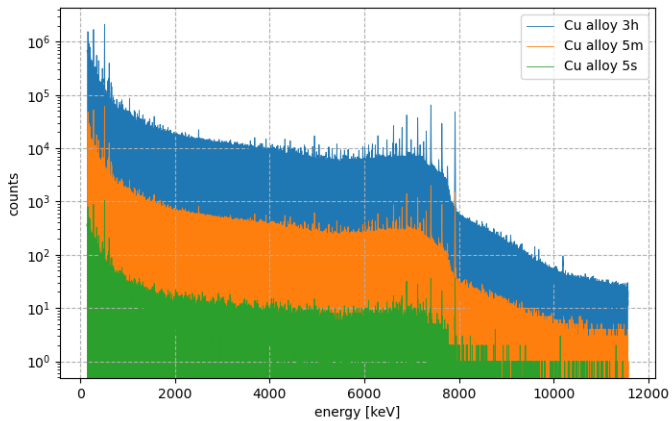
X-ray / Neutron diffraction



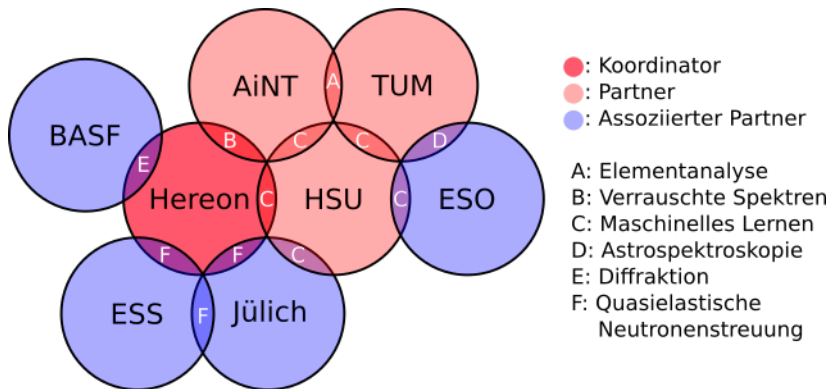
Quasielastic neutron scattering

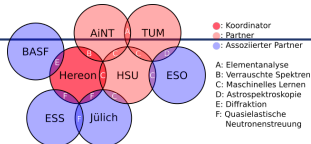


Noisy data



The collaboration

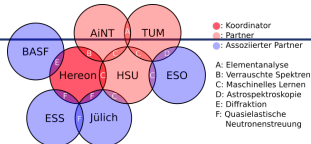




Lehrstuhl Informatik im Maschinenbau AI and ML for Cyber-Physical Systems Univ.-Prof. Dr. Oliver Niggemann

- deep learning timing analysis
- anomaly detection
- diagnostics and optimization of cyber-physical systems
- application focus: production plants and automation systems
- enabling neural networks to automatically learn the uncertainties of their results



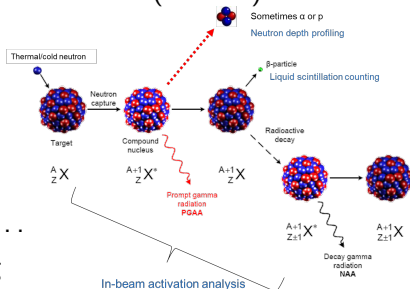


Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II)

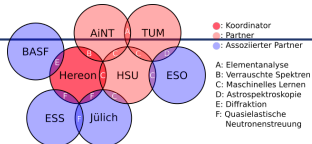
Elemental Analysis group

Dr. Christian Stieghorst

- user facility & in-house research
- nuclear phys., chemistry, archaeology, cond. mat. phys, ...
- data evaluation time-consuming
- information in spectra not yet completely exploited

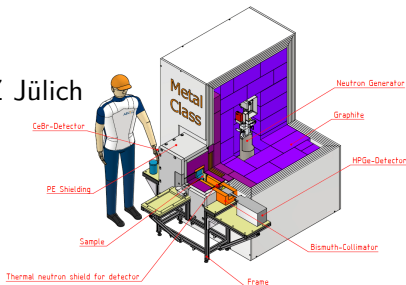


AiNT

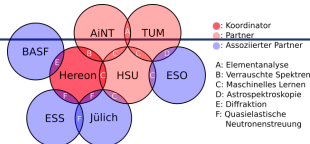


AiNT GmbH
Dr. Kai Krycki

- spin-off of RWTH Aachen & FZ Jülich
- nuclear simulation
- radiation protection
- measurement campaigns
- in-house lab neutron source
- fast measurements – analysis of metal scrap on conveyor belt

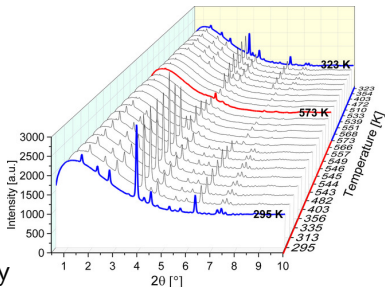


Hereon

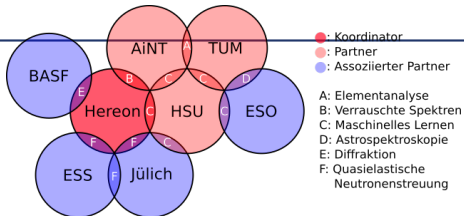


German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ)
Dr. Sebastian Busch

- user facility & in-house research
- outstation at DESY:
x-ray diffraction and tomography
- outstation at MLZ:
neutron diffraction and tomography
- also using QENS for in-house research
- human prior for model selection



Associated partners



- Dr. Gaspare Lo Curto, European Southern Observatory
- Dr. Bernd Hinrichsen, BASF SE
- Dr. Céline Durniak, The European Spallation Source
- Dr. Joachim Wuttke, Forschungszentrum Jülich

Pressing questions

- On which data do we train the models?
- Can we integrate mathematical or physical knowledge?
- Do we get realistic uncertainties / probability distributions?
- How can we get best performance for noisy data?

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