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Operando chemical 4D imaging for advanced manufacturing and functional materials

09. August 2023

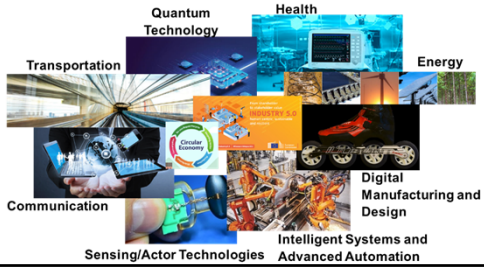
Topic/Motivation

Development and optimization of new functional materials requires in-depth understanding of their hierarchical structure, the dynamics of their properties and their reactivity

Understanding how materials properties develop

- During «production» (e.g. 3D printing, sample growth, mechanochemistry…)
- During function (e.g. battery, photovoltaic, new electronics …)

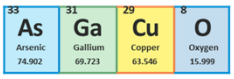
Complex studies requiring an whole experimental chain, not “just” one experiment

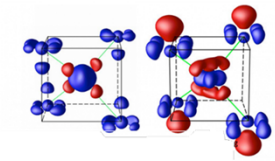


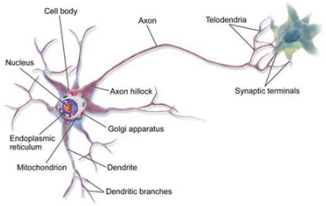
Topic/Motivation – synchrotron based

Understanding how materials properties develop

- During «production»
- During function







Elemental Composition	Electronic | Molecular Structure	Defects Interfaces Domains
X-Ray based Spectroscopies		Nano/Microscopies

CHEMICAL IMAGING

using the synchtron light source SLS

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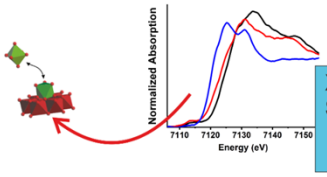
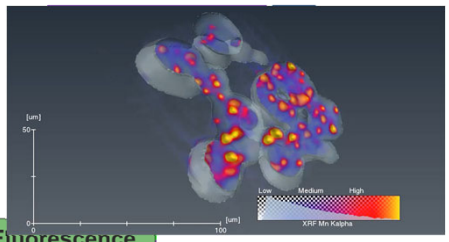
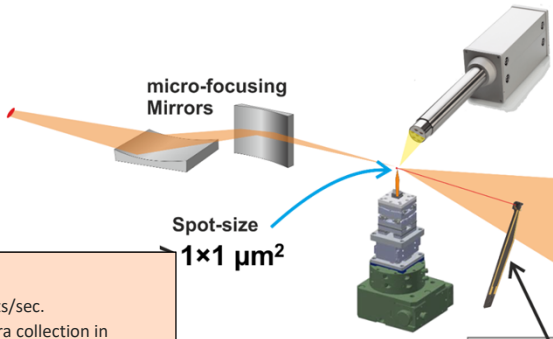
Chemical (and Physical) Imaging @microXAS

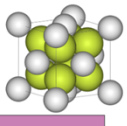


X-ray Absorption/Emission Spectrocopies
- Oxidation state
- Chemical speciation
- Local atomic coordination



X-ray Fluorescence
- Local element stoichiometry/composition



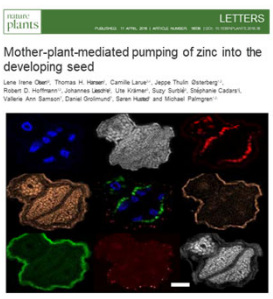


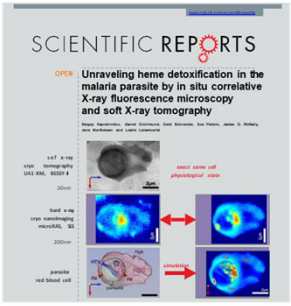
X-ray Diffraction
- Crystalline phase identification
- Chemical speciation
- Stress

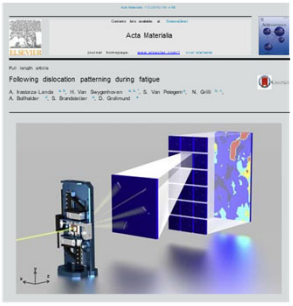
Transmission Signal (SiC diode)
- Absorption Contrast Imaging
- X-Ray Absorption Spectroscopy

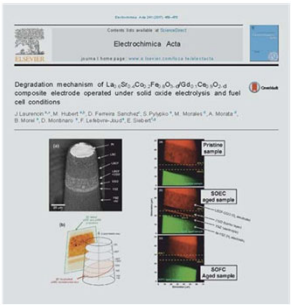
@microXAS
- **XRF**: ≈ 1M counts/sec. full spectra collection in "on-the-fly" mode
- **XRD**: 4M Eiger up to 700Hz / 500k and 1M PSI Eiger, **40kHz**

microXAS - multi-modal - multi-dimensional Chemical Imaging









health, biogenetics, energy (batteries, fuel cells), waste management, materials science, advanced manufacturing,

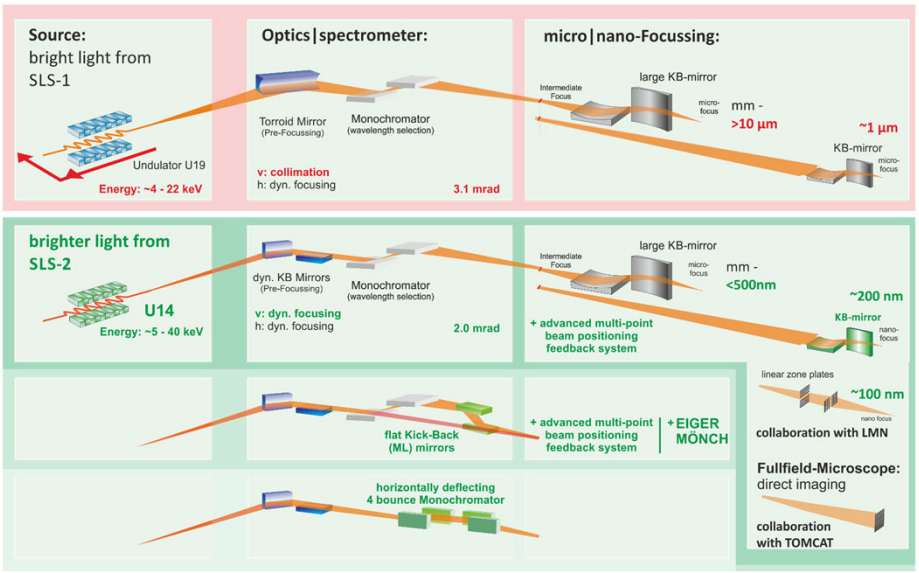
geology (geother-mal, CO2 storage, sustainable cement, pharma- ceutical, catalysis, nuclear science, environ-mental science, ...

Vision

- To develop a multifunctional characterization “center”
- Use the full potential of the upgraded SLS to develop a powerful beamline (based on microXAS) to study in-situ and operando the production and function of advanced materials
- To develop tailor made set-ups for different scientific topics
- To build an environment for the whole experimental chain (sample production, pre-characterization and complementary measurement, data analysis)
- To further strengthen the community which has been build up during SFA-AM (using the SLS)

Objectives: New microXAS

- Flexible focus
- Large working distance enabling installation of complex sample environments for operando studies
- Fast and easy switch between spectroscopy imaging and diffraction



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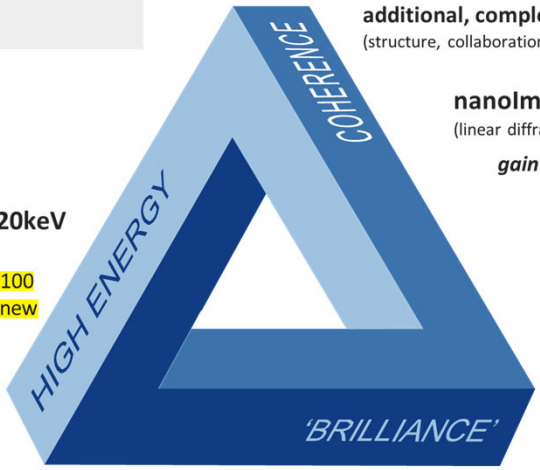
New microXAS – increased performance



additional, complementary imaging modes
(structure, collaboration cSAXS, TOMCAT, LMN)

nanoImaging
(linear diffractive optics, collaboration LMN)

gain factors:
spatial: >5
flux: >100

photon flux > 20keV
gain factors:
@ 20keV: >100
@ >20keV: new

spatial resolution
gain factor: >5

photon flux
gain factor: >100 (acceptance, ID)

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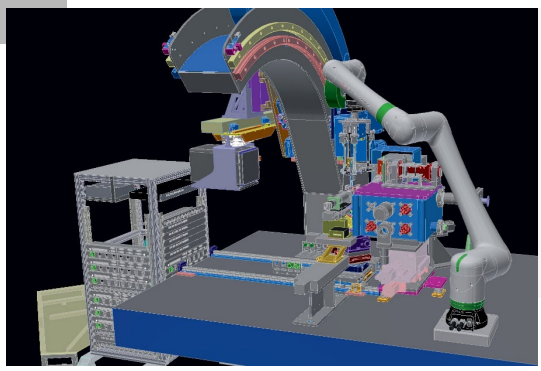
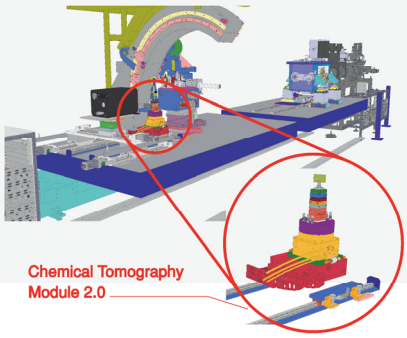
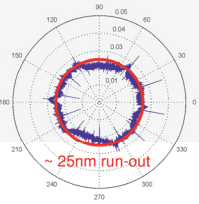
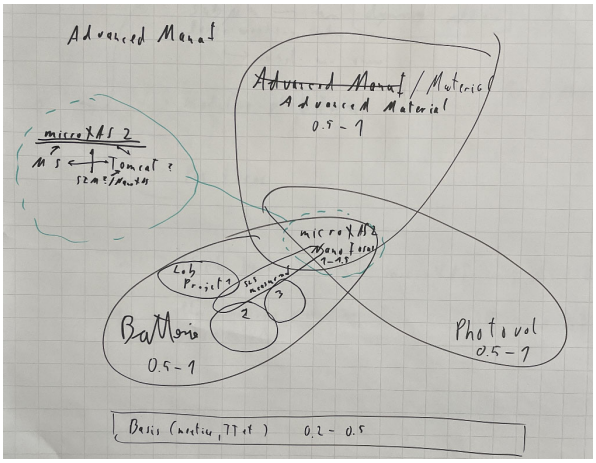
Flexible set up for endstations/sample environments







Approach



focus on selected science topics
or
focus on characterization platform
Or
mixture

Partner/Competences

We have

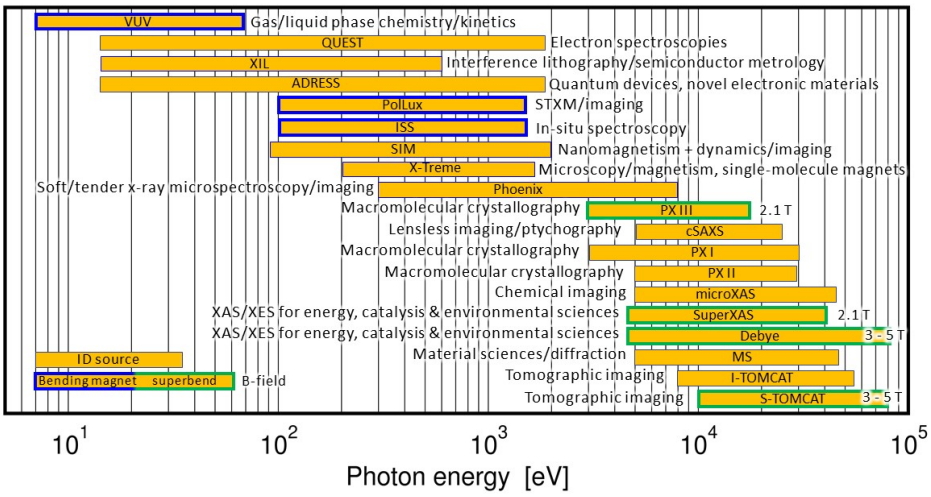
- Expertise in building, running and scientific use of beamlines (and we have an synchrotron source)
- Expertise in 3D in-situ/operando set-up (science and building), collaboration build up due to SFA-AM

We are looking for

- Groups to develop specific in-situ/operando set-ups (e.g. to be used at different experiments)
- Groups for complementary measurements (large scale e.g. other SLS, Neutron etc or lab based), pre-characterization
- Data Analysis (machine learning)
- Cobotics for the sample environment

We had first discussions with
Christian Leinenbach (Empa), Roland Loge (EPFL), Markus Bambach (ETHZ), Steven van Petegem (PSI), Yaroslav Romanyuk (EMPA)

Beamline activities and their accessed photon energies – SLS 2.0



The Swiss Light Source and SwissFEL at the Paul Scherrer Institute, Frithjof Nolting, Christoph Bostedt, Thomas Schietinger, and Hans Braun, European Physical Journal Plus, 138:126 (2023)