WISE – MAX IV MINI-WORKSHOP

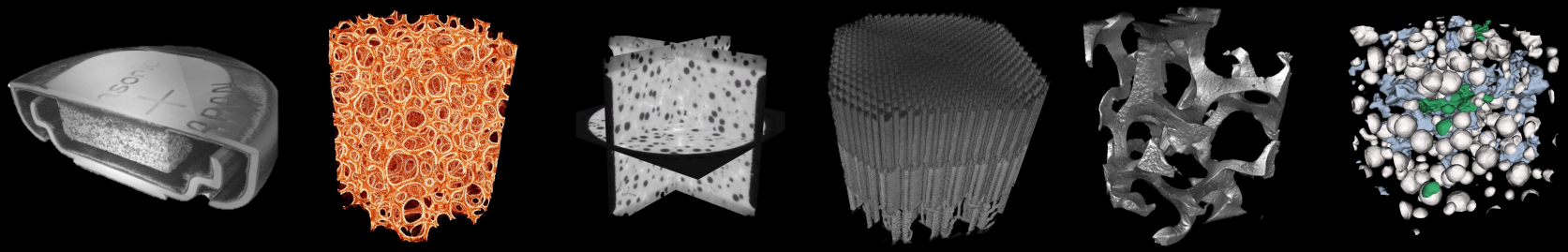
A NEW IMAGING BEAMLINE FOR MATERIALS SCIENCE @MAXIV

Wallenberg Initiative Materials Science for Sustainability

MAX IV

GTiMAX

General tomographic Imaging @ MAXIV



Stephen Hall, Division of Solid Mechanics, Lund University

Wallenberg Initiative Material Science for Sustainability

To achieve our climate and environmental goals, we need to reduce our environmental and climate footprints from the materials we use in our day-to-day lives and in industry. The aim of the Wallenberg Initiative Material Science for Sustainability is to create the conditions for a sustainable society by researching next generation of ecofriendly materials and manufacturing processes. This will also facilitate better technology for energy systems of the future, and to combat pollution and toxic emissions.

GTiMAX

General tomographic Imaging @ MAXIV

Background

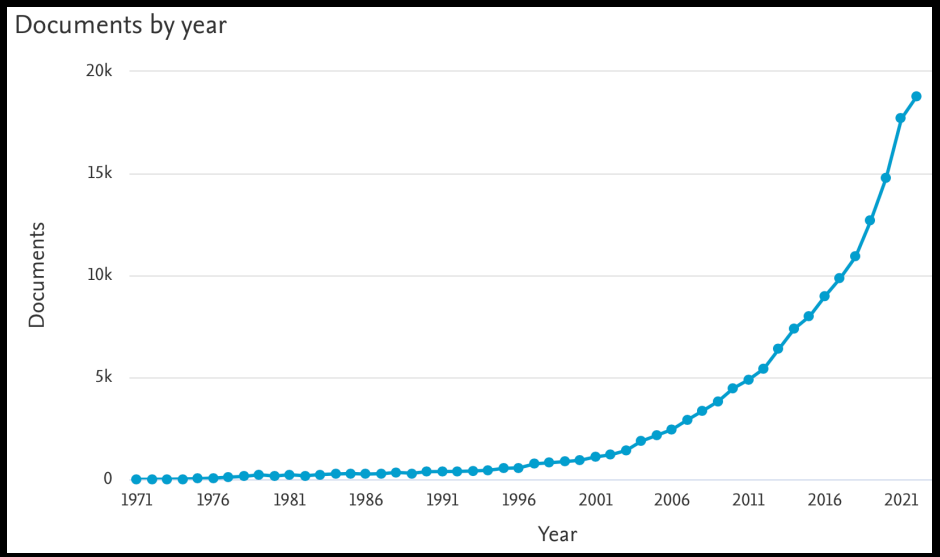
- *The GTiMAX beamline concept developed from the iMAX beamline concept.*
- *The iMAX concept started with a workshop in 2013 to discuss the science case/strategy for non-medical imaging at MAXIV.*
  - *The outcome was a clear recommendation to develop two complementary beamlines:*
    - *(i) NANO-MAX for imaging at the ultimate spatial resolution for small samples using nanobeam scanning and CXI/ptychography;*
    - *(ii) iMAX for studies of bulk materials with resolutions of 50 nm and up, with full-field, multi-modal and multi-scale imaging approaches.*

- *iMAX was presented at the 2013 MAX IV user meeting and the working group was invited by the MAX IV management to develop a CDR, which was submitted in November 2013 and accepted by the SAC in December 2013.*
- *iMAX was officially listed in the future beamlines in the MAXIV director's UM2014 presentation…*
- *In 2022 an expression of interest (EoI) for GTiMAX was submitted to the MAXIV strategy review*
- *In 2023 GTiMAX was supported by WISE for development of a Conceptual Design Report (CDR)*

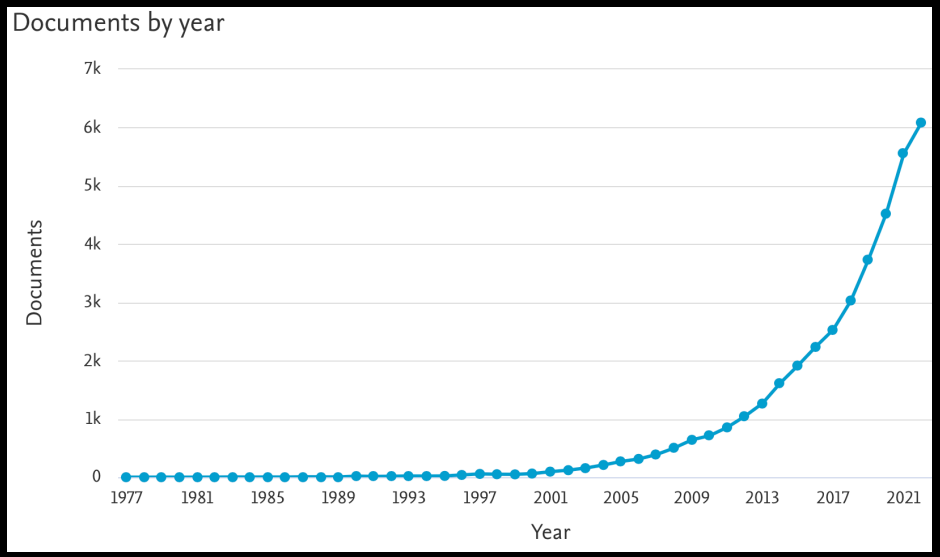
From the GTiMAX WISE proposal

X-ray tomography is one of the fastest growing synchrotron techniques and thus will be utilised by a wide range of science areas within WISE, as well as by a more extended research community covering a very broad scientific range. The brilliance of the MAXIV source will provide world-class 3D imaging, which, with the strong focus on in-situ/operando experiments, will provide a beamline capable of supporting excellent research in all the WISE focus areas.

Scopus: x-ray AND tomography AND Physical sciences



Scopus: x-ray AND tomography AND Physical sciences AND (4d OR in-situ OR operando)



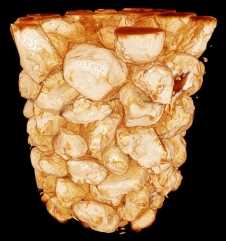
GTiMAX

General tomographic Imaging @ MAXIV

GTiMAX, will provide state-of-the-art 3D x-ray sub-micro to micro-resolution x-ray tomography to the material science community for the study of the internal 3D structures and processes of materials for advanced material understanding and development…

…with a strong focus on 4D imaging “in-situ” or “operando” experiments where materials can be studied in their relevant functional environments.

GTiMAX addresses all the components of the WISE matrix, as tomography gives access to the structure-property-performance relationships for a wide range of materials over a range of scales.



GTiMAX

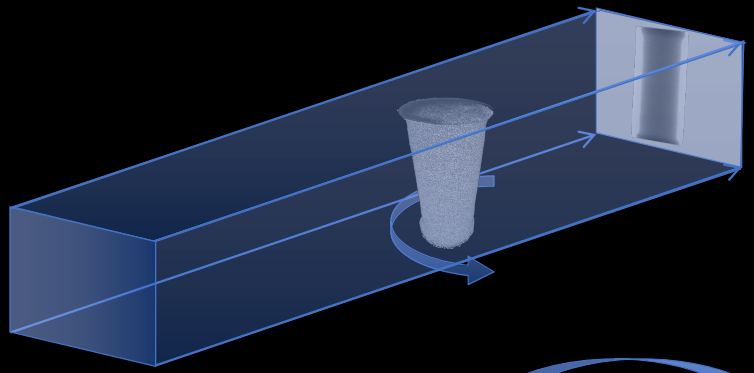
General tomographic Imaging @ MAXIV

- Absorption/phase contrast imaging in the 10-45+ keV range
- Medium sized (0.1 mm - 5 cm) samples.
- 3D spatial resolution in the range 100 nm – 5 µm
- Multi-scale
- High speed tomography for in-situ imaging of dynamic processes
- Focus on user-defined in-situ and operando experiments.
- Robust, user friendly operation
- Emphasis on high throughput and full service (including sample environments and 3D & 4D data processing/analysis tools)
- Support for users with little experience with synchrotron measurements and lack resources for data analysis

MAX IV

GTiMAX

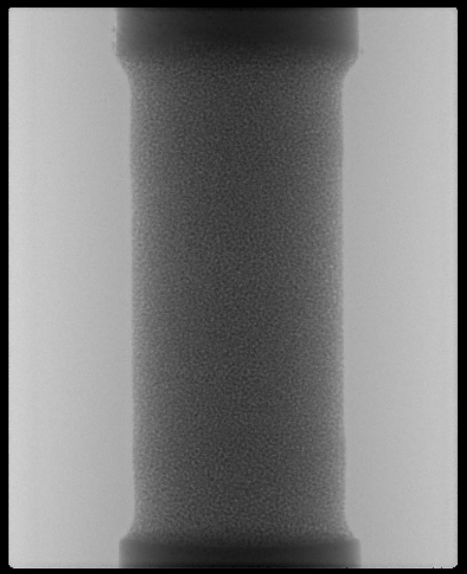
General tomographic Imaging @ MAXIV



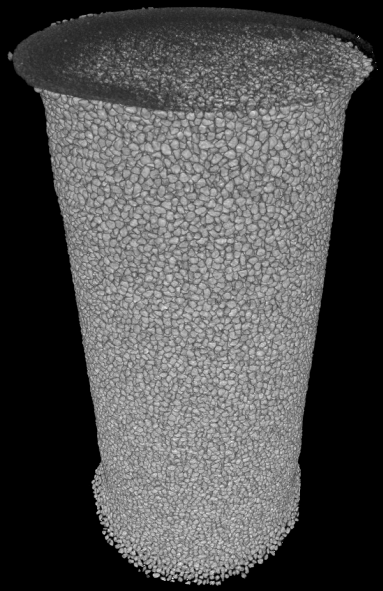
3D Imaging

Absorption & quantitative phase contrast imaging

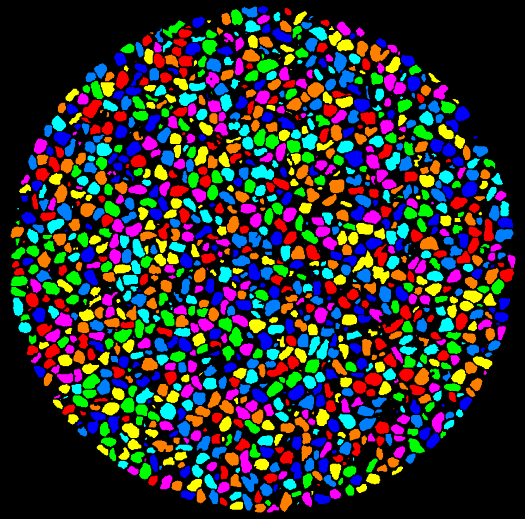
Radiographies



Reconstruction & Visualisation



Quantification & Analysis



GTiMAX

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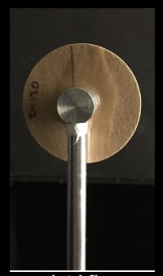
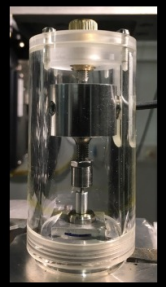
4D Imaging


Freezing


Fluid flow


Pressure


Compression


Tension


Adhesion

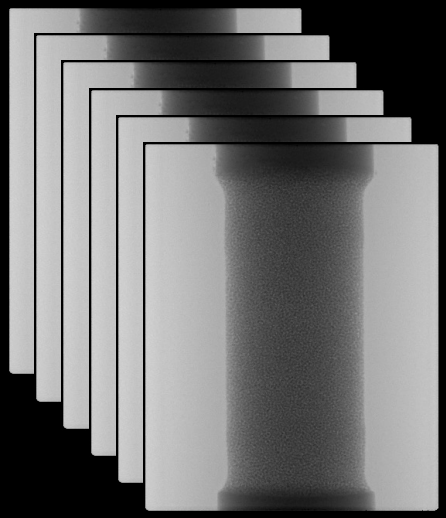

Vacuum

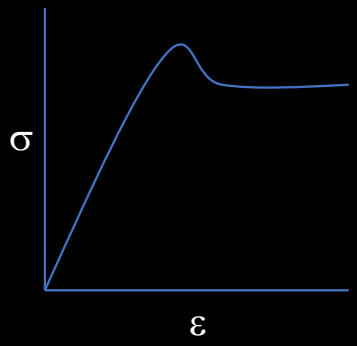

Humidity

Electrochemistry

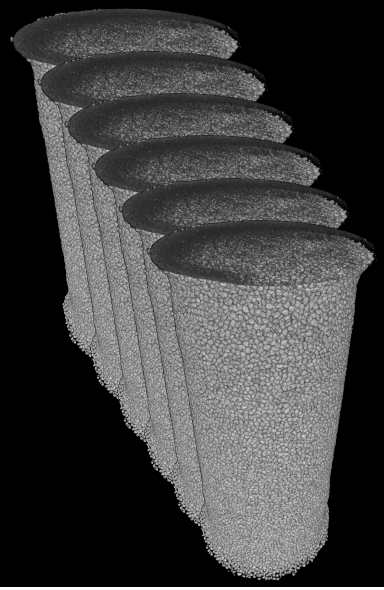
... and more

Radiographies

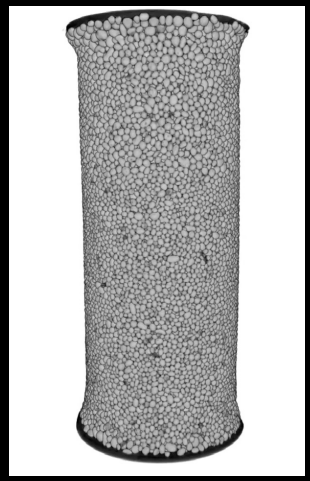




Reconstruction



4D Visualisation



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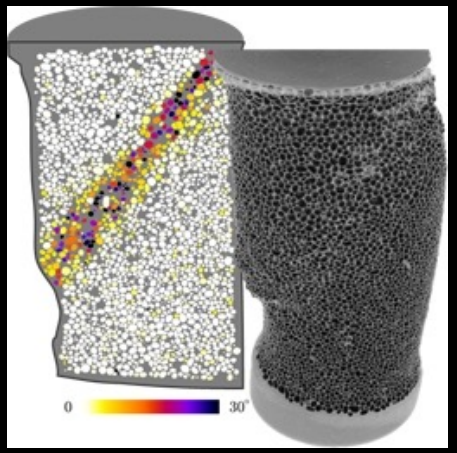
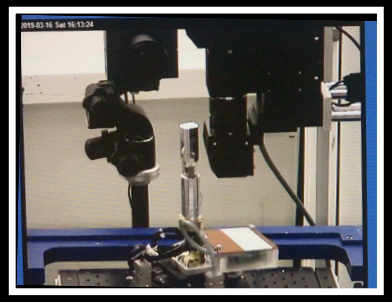


GTiMAX

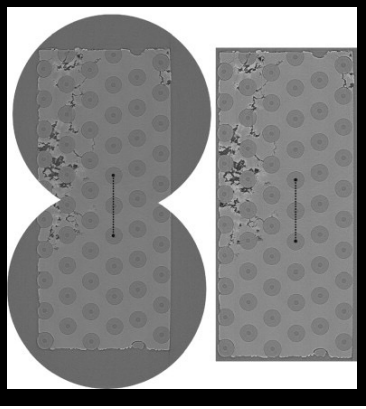
General tomographic Imaging @ MAXIV

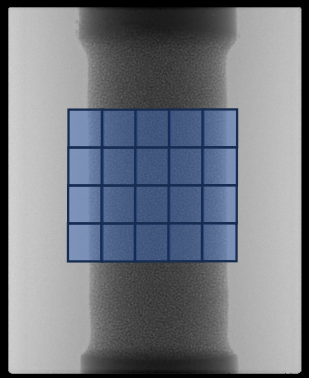
HIGH FLUX + FAST DETECTORS

CONTINUOUS IN-SITU /OPERANDO



Fast, extended field of view imaging
(stitch imaging)
& multiresolution





Kyrieleis et al., 2009

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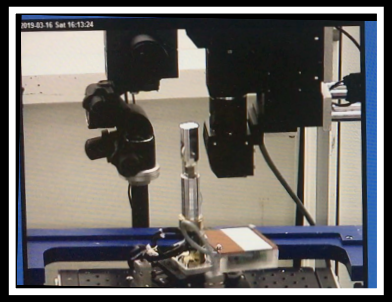

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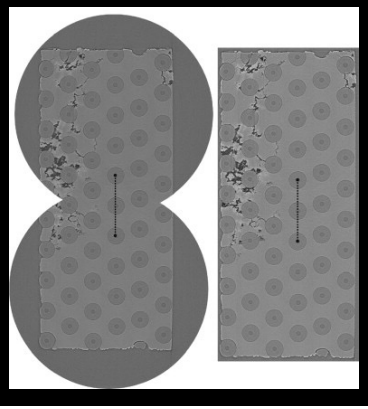
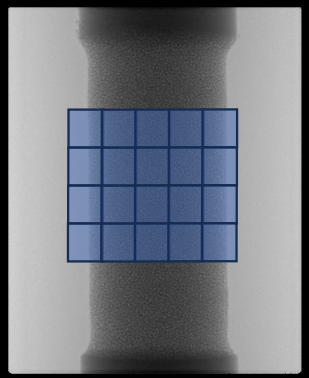
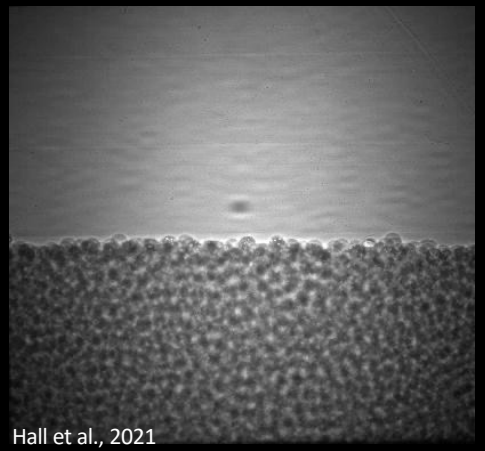


Kyrieleis et al., 2009



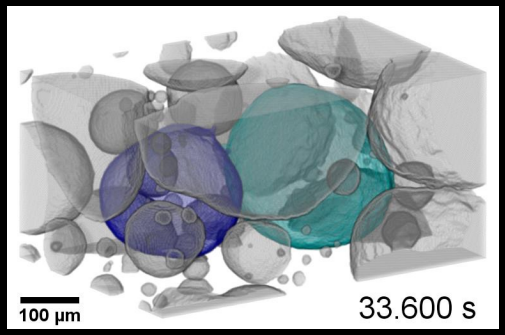
DYNAMIC IMAGING (100s kHz -> MHz)



Hall et al., 2021

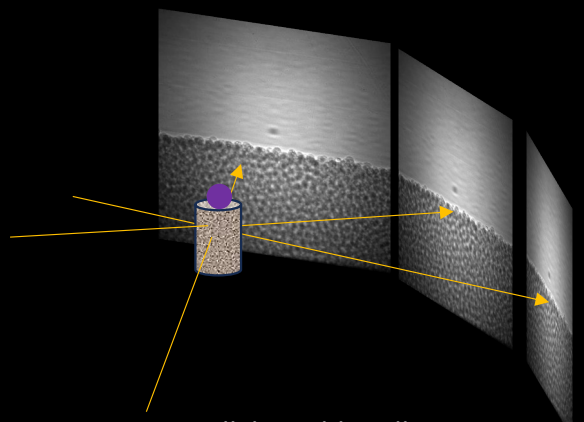
100 kHz radiography

HIGH SPEED TOMOGRAPHY



Aluminium foam development
Garcia-Moreno et al., 2021

DYNAMIC 3D IMAGING (100s kHz -> MHz)



See talk by Pablo Villanueva Perez

Results of the review of the call for Expressions of Interest (EoI) that was held in the end of May 2022

The review committee was comprised of the following individuals:

- Lars Börjesson (Chair), Professor, Chalmers University of Technology
- Massimo Altarelli, Senior Scientist, Max Planck Institute for the Structure and Dynamics of Matter
- Amina Taleb-Ibrahimi, Science Division Director, Synchrotron SOLEIL
- Anna Sandström, Director Science Policy and Relations Europe, AstraZeneca
- Axel Knop-Gericke, Professor, Max Planck Institute for Chemical Energy Conversion
- Jean Susini, Science Director or Life Sciences, Synchrotron SOLEIL
- Linda Young, Argonne Distinguished Fellow/Group Leader, Argonne National Labs
- Luca Artiglia, Staff Scientist, Paul Scherrer Institute
- Oscar Tjernberg, Professor, Royal Institute of Technology KTH1
- Marco Stampanoni, Group Leader, Paul Scherrer Institute
- Søren Pape Møller, Professor, Aarhus University
- Wah-Keat Lee, Program Manager, National Synchrotron Light Source II, BNL

Beamlines

1. S09 – GTiMAX: General Tomographic imaging beamline at MAX IV	A (clear pass)	This EoI is well developed and should be included in the roadmap with high priority.

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Short motivation

Tomographic imaging capabilities are almost a must-have to fully utilize the performance of MAX IV and a major gap in the current portfolio of facility. This proposal is of high quality and provides a solid science case which matches very well with the utilisation of the MAX IV source properties. The beamline proposed is of great relevance to the community in both its scope for capacity and quality of the science performed.

There is also a large size and variety of the potential community in comparison with other capabilities at MAX IV. Slightly more work needs to be done on the implementation strategy. It is also potentially a resource-hungry project from the data management and analysis point of view. There is no doubt whatsoever that such a beamline would be very productive.

Results of the review of the call for Expressions of Interest (EoI) that was held in the end of May 2022

Beamlines

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From the GTiMAX WISE proposal

> *The complementarity of GTiMAX with ForMAX and DanMAX, i.e., the dedicated focus on tomography at GTiMAX and the mixed modalities available at the other two beamlines, plus nano-imaging at NanoMAX, will provide a world-class suite of instruments for 3D materials characterization at MAXIV.*

Complementarity to other MAX IV beamlines

In the 10-35+ keV range, Nano-MAX, **GTiMAX,** ForMAX and DanMax will complement each other in a very natural way:

- *Nano-MAX*: scanning methods; ultimate spatial resolution; coherent x-ray imaging (CXI); monochromatic beam.
- DanMAX: Combined diffraction and imaging/diffraction-imaging beamline (limited time for tomography)
  - Development of GTiMAX would enable DanMAX to focus on developing diffraction-based imaging, which is of significant interest to the WISE materials community
- ForMAX: Combined SWAXS and imaging beamline (limited time for tomography and focus on forestry industry related science)

- Furthermore, a strong synergy is foreseen with the possibilities for materials science investigations
  - At higher energy ranges (40-200 keV) in the context of the Swedish collaboration at PETRA III
  - With imaging at the ESS
  - At laboratory x-ray tomography facilities, including Lund, Luleå, SU, SLU, Örebrö, DTU…

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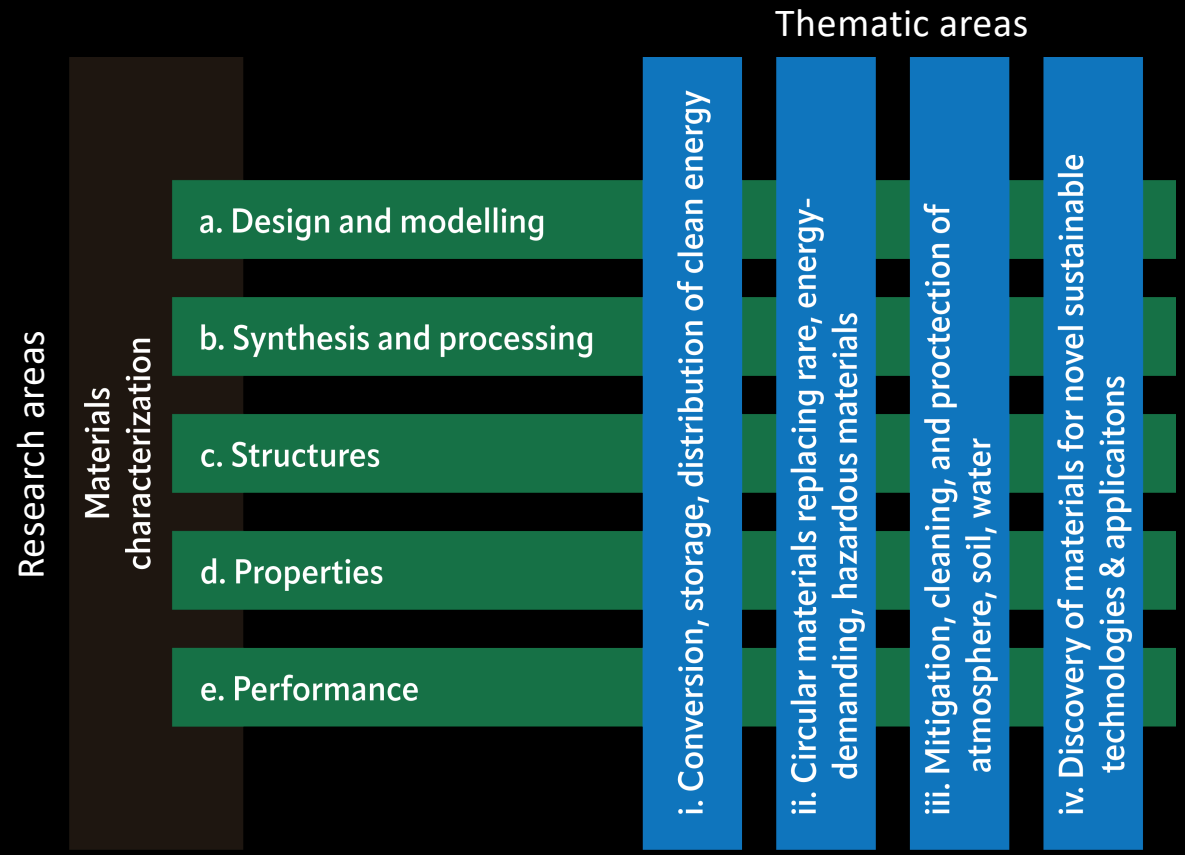


GTiMAX

General tomographic Imaging @ MAXIV

Research areas

Materials characterization

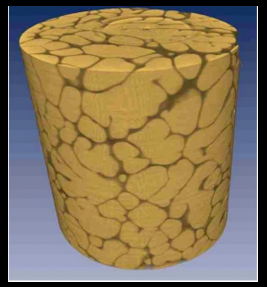
- a. Design and modelling
- b. Synthesis and processing
- c. Structures
- d. Properties
- e. Performance

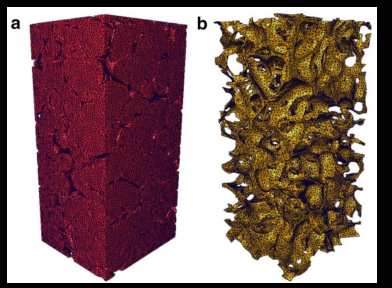
Thematic areas

- i. Conversion, storage, distribution of clean energy
- ii. Circular materials replacing rare, energy-demanding, hazardous materials
- iii. Mitigation, cleaning, and proctection of atmosphere, soil, water
- iv. Discovery of materials for novel sustainable technologies & applicaitons

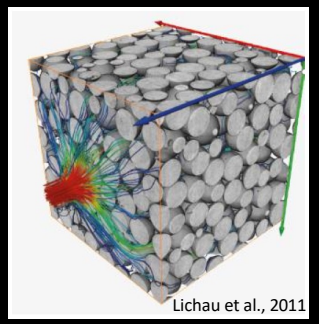
a) *Design and modelling*:

Image based modelling
+ digital twins

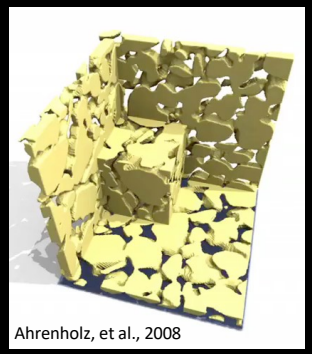




Madi et al., 2006

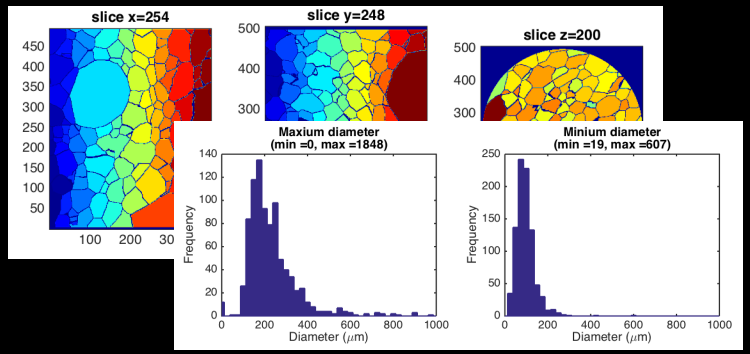


Lichau et al., 2011



Ahrenholz, et al., 2008

Morphological analysis and material statistics



Gordeyeva_etal_2016

Additive manufacturing +
topological optimisation

Wu et al.,2020

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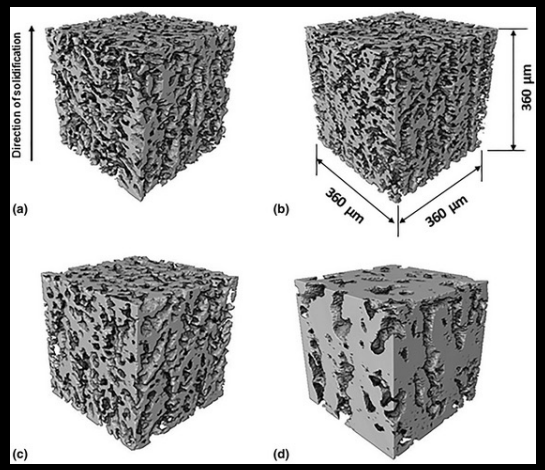
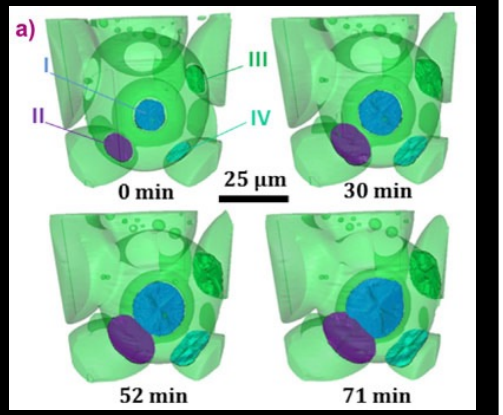
b) *Synthesis and processing*:

e.g., solidification



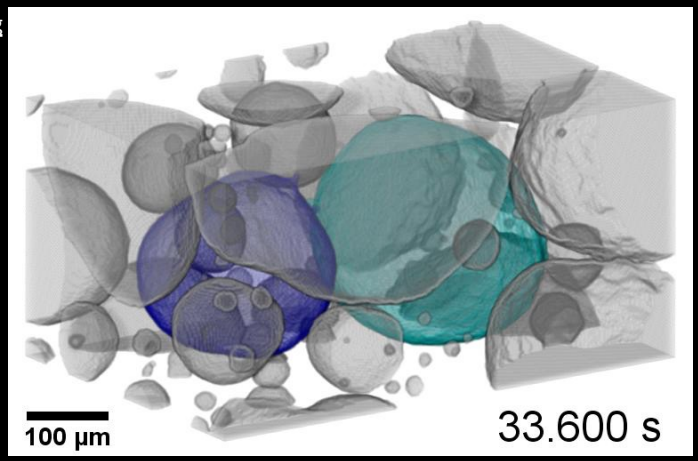
Lloreda-Jurado et al., 2020

e.g., sintering



Villanova et al., 2017

e.g., foaming



Aluminium foam development
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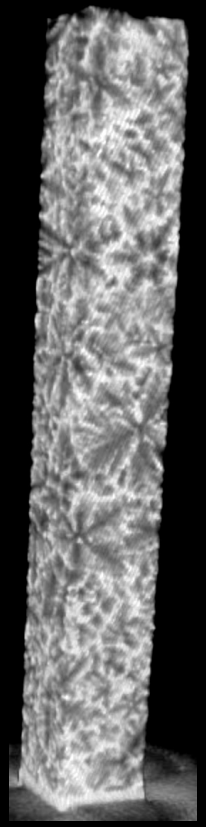
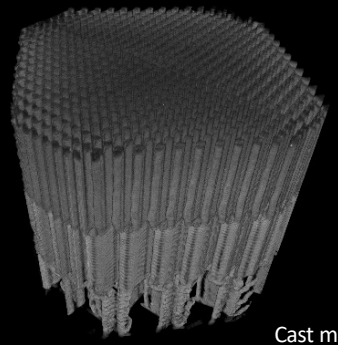
c) Structures:

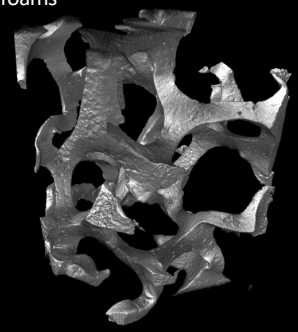


Magnesium alloy

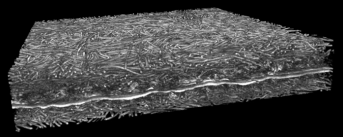
3D printed structures



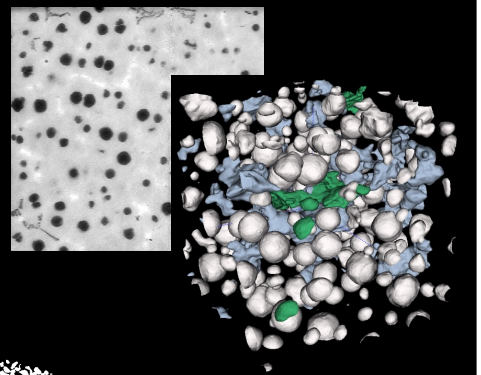
Metal foams



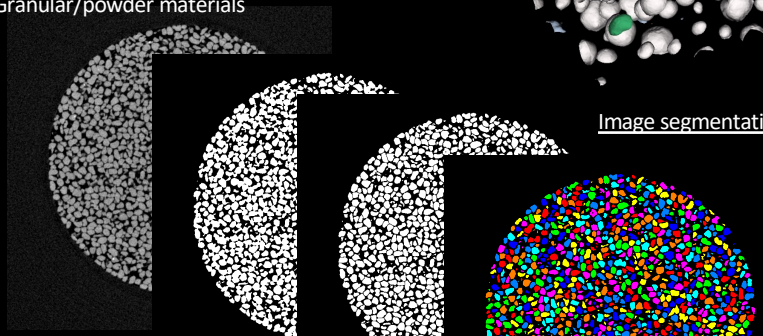
Fuel cell



Cast metal



Granular/powder materials



"Raw" image

Binarise

Watershed Segmentation

Image segmentation

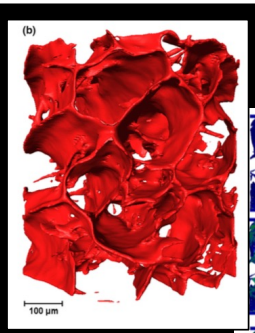
Label Individual Grains

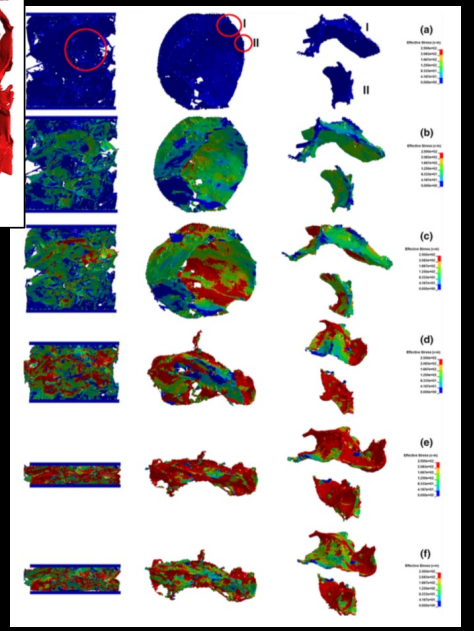
GTiMAX

General tomographic Imaging @ MAXIV

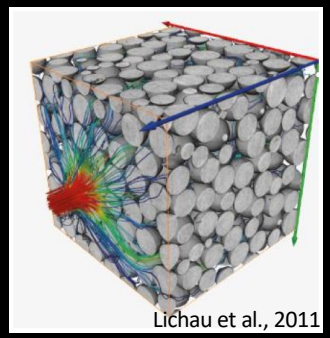
d) Properties:

"Digital twins"





Srinivasa, et al, 2017



Lichau et al., 2011

Thematic areas

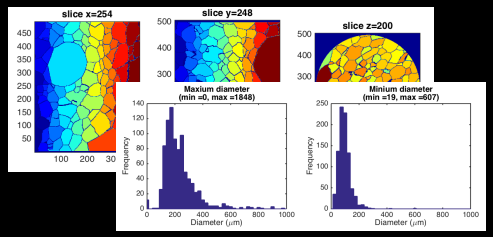
Research areas

Materials characterization

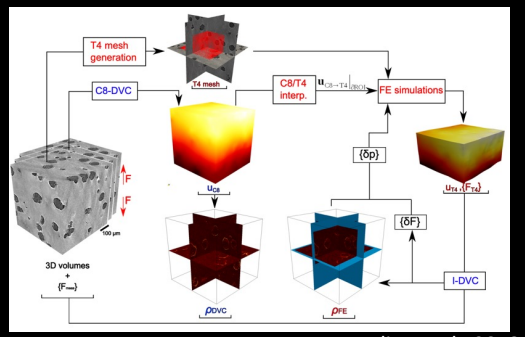
- a. Design and modelling
- b. Synthesis and processing
- c. Structures
- d. Properties
- e. Performance

- i. Conversion, storage, distribution of clean energy
- ii. Circular materials replacing rare, energy-demanding, hazardous materials
- iii. Mitigation, cleaning, and proctection of atmosphere, soil, water
- iv. Discovery of materials for novel sustainable technologies & applicaitons

Quantification



Parameter Identification



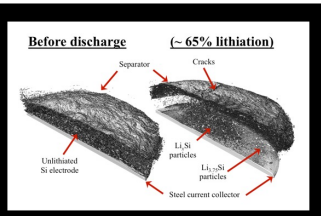
Buljac et al., 2018

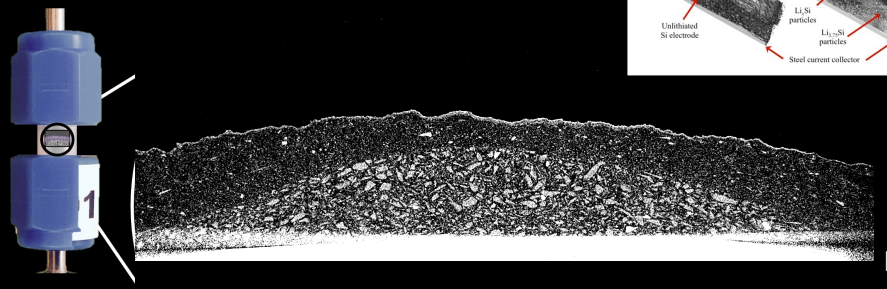
GTiMAX

General tomographic Imaging @ MAXIV

e) Performance:

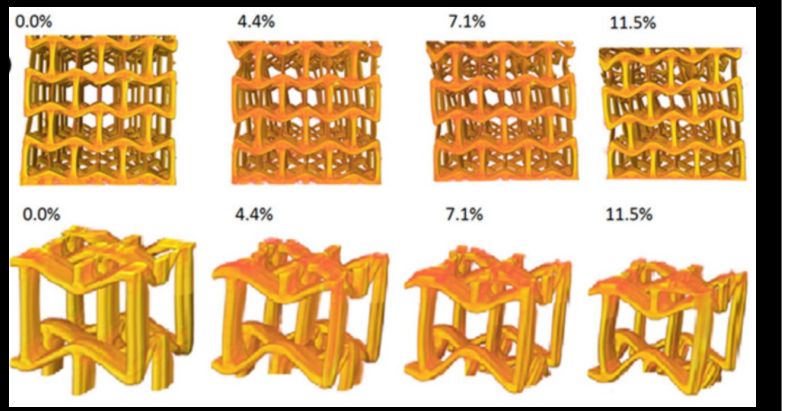
Battery mechanisms and failure processes





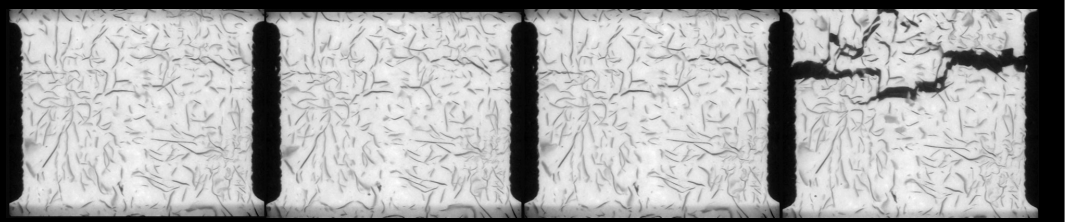
Paz et al.

Topologically optimised 3D printed structres for tuned peformance/propoerties



Wu et al.,2020, Materials & Design

Material fracture and failure



In-situ tensile test on lamella graphite cast iron

Research areas

Materials characterization

- a. Design and modelling
- b. Synthesis and processing
- c. Structures
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Thematic areas

- i. Conversion, storage, distribution of clean energy
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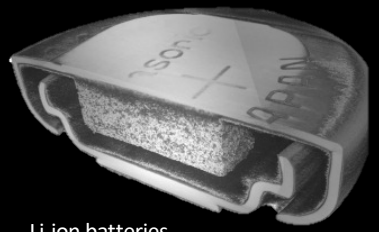
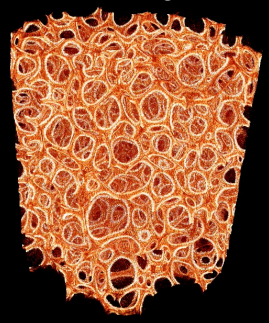
GTiMAX

General tomographic Imaging @ MAXIV

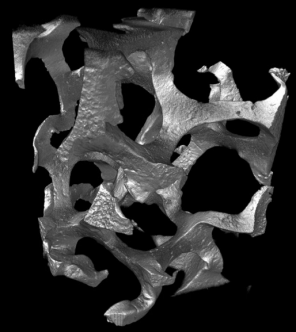
Thematic areas



Li-ion batteries



Foam for district heating



Aluminium foam for light weight construction

Thematic areas

Research areas

Materials characterization

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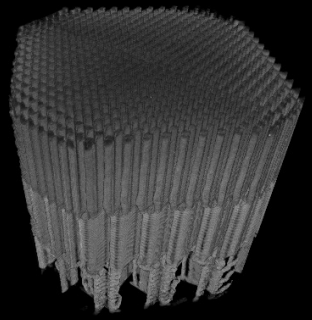
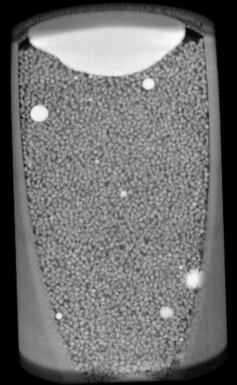
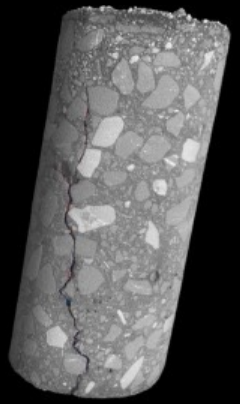


3D printed water filter

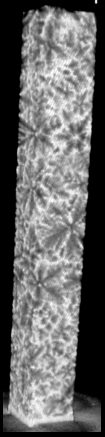


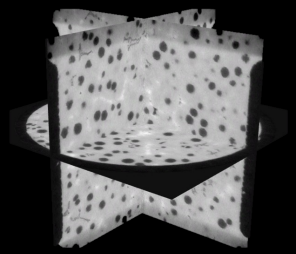
NAPL polluted Sand

Concrete → green concrete

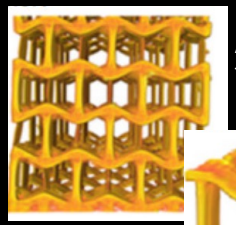


Magnesium alloys for dissolvable implants

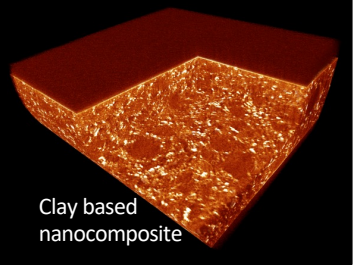




Cast iron – reduce carbon



Additive manufacturing + topological optimisation



Clay based nanocomposite

And many more…

GTiMAX

General tomographic Imaging @ MAXIV

- Absorption/phase contrast imaging in the 10-45+ keV range
- Medium sized (0.1 mm - 5 cm) samples.
- 3D spatial resolution in the range 100 nm – 5 µm
- Multi-scale
- High speed tomography for in-situ imaging of dynamic processes
- Focus on user-defined in-situ and operando experiments.
- Robust, user friendly operation
- Emphasis on high throughput and full service (including sample environments and 3D & 4D data processing/analysis tools)
- Support for users with little experience with synchrotron measurements and lack resources for data analysis

MAX IV

GTiMAX

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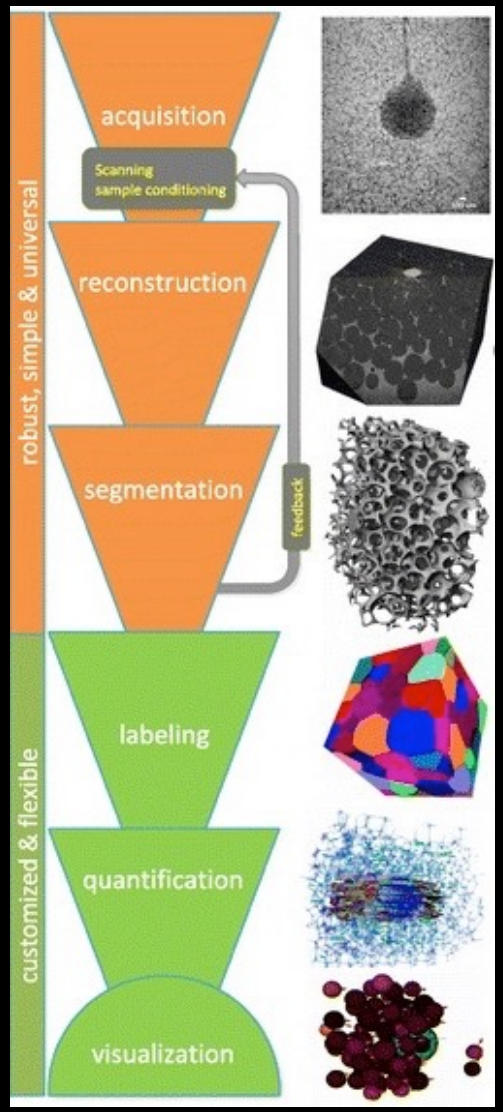

(Matej et al., 2017)

Excerpts from the extended review comments of the review of the MAXIV Expressions of Interest (EoI) (May 2022)

Tomography is THE tool to study structural and functional features of materials

The argument of the proposal for securing MAX IV's role at the international forefront is judged to be outstanding overall. X-ray tomographic imaging is rapidly becoming increasingly important for many areas of materials science (both fundamental and applied).

very obviously offers outstanding opportunities for a very wide range of research that has high potential long-term societal impact

It has also a large potential to be an important asset for industrial use

This project would complete the portfolio of imaging beamlines currently available at MAXIV, and the proposed beamline would clearly put MAX IV at the international forefront of x-ray tomographic imaging.

A multiscale X-ray tomography platform should be seen as a priority and has the potential to be a flagship beamline for MAX IV.