The Swedish Material Science Community's science cases for PETRA IV

Concept of Proposal 1

Bulk Hierarchical & Heterogeneous Materials and Processes in 4D

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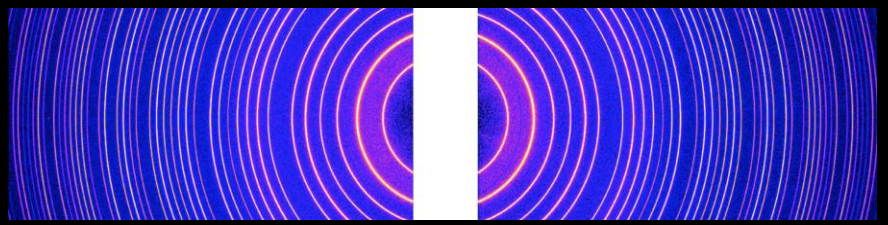

LUND INSTITUTE OF ADVANCED NEUTRON AND X-RAY SCIENCE LINXS

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Science case:

- **Structure:** Many natural and engineering materials have structures over a wide scale range from sub-nanometer crystal structures to porosity, precipitates and polycrystalline structures from the nanoscale up to microscales.

- **Processes** in these materials, including crystal phase changes precipitate evolution, intercalation, strain localisation and cracking or fracture, will also occur over the same wide scale range under the influence of external and internal loads, e.g., stress, temperature or chemistry.

- **Modelling** advances require details on the multi-scale structures, processes and coupling as well as understanding of inherent and evolving heterogeneity

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Science case:

- To understand the relationship between multi-scale material structures and their performance in engineering or natural situations requires:
  - Characterisation of material structures at different scales as well as the inter-relationships in pertinent sized samples
  - Understanding of how and in what order material structures evolve under loading
  - Connection of hierarchical/heterogeneous structures and processes with the performance/behaviour of the materials in their relevant environments/function
  - Understanding of heterogeneity in structures and processes at different scales
  - Connection between experimental evidence and insight with modelling and simulation

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Science areas:

- Material science (particularly metals)
  - Metals processing, metals in service, forming and heat treatment
- Functional materials
- Energy materials , including batteries
- Geotechnical engineering and natural hazards (rocks, soils, clays, cement/concrete)
- Granular materials
- Biomedical (e.g., bones, implants, scaffolds)
- High pressure science
- Geophysics – earth processes
- Archaeology and cultural heritage
- ….

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Requirements:

- Possibility to handle pertinent sample volumes
- Stability to enable micron scale spatial resolution
- In-situ environments for heat treatment, mechanical loading, chemical processes..
- Diffraction/WAXS, SAXS, tomography plus full-field 3DXRD/DCT
- Simultaneous measurements at different scales (or fast changing) to consider the same sample under the same conditions and reduce uncertainty of "sister tests with different methods
- Fast measurements
  - Rapid in-situ process simulation (bulk measurements)
  - Scanning for (micro-scale) spatial resolution with SAXS/WAXS
- Beam-size flexibility to enable full-field, bulk and scanning measurements
- High through-put
- Usability and user accessibility

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Initial concept outline:

- Building on existing P21.2 EH3 concept and set-up
- >38 keV
  - Penetration of bulk/dense materials and sample environments
  - Reduced chemical alteration
  - Q-range
- High stability set-up to enable micron-scale real-space resolution, including with scanning
- Fast measurements to enable sub-second temporal resolution for tomography and very fast scattering measurements for in-situ process monitoring / scanning tomography
- Micro-scale beam with low divergence from source for with beam-expander for full-field imaging/3DXRD

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Making use of Petra IV:

- High energy - penetration
- High flux - fast measurements and facilitation of e.g., **scanning-tomography** methods
- Small beam sizes – scanning

- **Scientific productivity** potential must be stressed
  - Wide user community
  - Multi-scale measurements for same sample under same conditions
  - Optimisation for integrated measurements and delivery of reduced data

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Modes:

- **Full-field with rotation**
  - Tomography with micron-scale spatial resolution and sub-second temporal resolution
  - 3DXRD/DCT coupled with tomography
- **High speed bulk measurements with complex/rapid in-situ experiments**
  - SAXS + WAXS
  - Coupled to tomography – simultaneous/rapid-change?
- **Scanning mode with pencil beam**
  - Spatially resolved WAXS (and SAXS?)
  - Intra-granular 3DXRD
  - Coupled to full-field tomography
- X-ray fluorescence tomography?

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Sample environment:

- Stable, dedicated mechanical loading system(s) with thermal control with rotation under load (e.g., RAMS)
  - Different set-ups for different load capacities / sample sizes?
- Furnace with tomography (full-field and scanning) possibility
- Induction heating with gases for rapid temperature cycling
- Dilatometer
- Beamline-Gleeble?
- Ease of integration of user environments

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Questions:

- What sample size / full-field beam size is required? 1, 5, 10 mm?
- What temporal resolutions are required for:
  - Process simulation and SAXS/WAXS
  - Tomography

- Sample environments?

- Simultaneous measurement or fast changing?

- Co-proposers (Swedish and international)?

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Reference Beamlines:

- ESRF- ID11
- APS – 1-ID

- CHESS – Structural Materials beamline (with RAMS)

- PetraIII - HEMS