

NEXT Competence Centre | Associated project | Master thesis

Towards Automated Phase Identification of Synchrotron X-ray Diffraction Data for Sustainable Engineering Materials

Background

Sustainable materials and process research and development need to consider the effective use of resources and time to generate the desired novel solutions. Timely material and process analysis are thus important and tools such as synchrotron x-ray characterization can be highly beneficial due to the rapid analysis capability. High-throughput x-ray measurements has the potential to significantly enhance the pace of sustainable materials and process innovations. However, high-throughput large-scale synchrotron infrastructure measurements such as synchrotron x-ray diffraction (SXR) generate huge amounts of data and a key bottleneck in high-throughput SXR workflows is phase identification, which remains labor-intensive and expert-dependent. Automating this step, using e.g. machine learning, pattern recognition, and database-driven approaches, could dramatically increase throughput, reduce human bias, and support sustainable industrial development by enabling faster, more reliable decision-making.

Within this project, associated to the competence center [Neutron and X-ray science for industrial technology transitions \(NEXT\) | KTH](#), we aim to initiate development towards automating phase identification in SXR measurements on engineering materials such as advanced steels, nickel-based superalloys and cemented carbides. This Master thesis is the first step, and we foresee a follow-up project, formulated as a PhD project, to develop and deploy a complete solution for a novel semi-automated SXR phase identification workflow, with emphasis on transferability, throughput, and sustainable industry relevance.

Aims and objectives

This Master thesis aims to initiate the development of automated phase identification in synchrotron X-ray diffraction (SXR) measurements for engineering materials such as advanced steels, nickel-based superalloys, and cemented carbides. By exploring machine learning, pattern recognition, and database-driven approaches, the project seeks to reduce manual effort, improve throughput, and support sustainable industrial innovation. Conducted as an associated project to the NEXT competence center, the work will lay the foundation for a future PhD project focused on developing and deploying a semi-automated SXR workflow with strong emphasis on transferability, scalability, and industrial relevance.

Activities and project timeline

The project will begin with a review of current phase identification methods in SXR, including manual indexing, database matching, and emerging automated approaches. Selected engineering materials, such as advanced steels, nickel-based superalloys, and cemented carbides, will be selected together with NEXT industry partners and they will be measured

using SXR D to generate representative datasets. These datasets will be used to test and evaluate automated phase identification techniques, including machine learning and pattern recognition tools. The final phase will involve drafting recommendations for future integration of semi-automated phase identification into high-throughput SXR D workflows, with emphasis on sustainability, industrial relevance, and future deployment.

Activity	2025				
	Month 1	Month 2	Month 3	Month 4	Month 5
1. Literature survey and detailed plan					
2. Material selection and sample preparation					
3. X-ray measurements					
4. Testing of automated Phase ID approaches					
5. Reporting					

Starting date: January 2026 or as agreed.

Duration: 5 months

Collaborator: Scatterin AB

Location: KTH

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