NEXT Competence Centre | ACC 4 | Project 4.1 | Master thesis No. 1

In situ high-throughput X-ray diffraction measurements conducted in both laboratory and large-scale facilities to advance thermodynamic database development for metal recycling, with emphasis on trace elements

Background

Against the broad background of industrial sustainability, steel production remains one of the most carbon-intensive sectors, accounting for approximately 7% of global CO_2 emissions. A significant portion of these emissions originates from traditional metal extraction processes, particularly the use of blast furnaces, which rely heavily on fossil fuels and virgin raw materials. In contrast, metal recycling offers a powerful pathway toward reducing environmental impact. By reusing existing metal resources, recycling dramatically lowers the demand for primary ore extraction and minimizes energy consumption. This not only reduces greenhouse gas emissions but also conserves natural resources.

For structural materials derived from recycled sources, the presence of impurity elements plays a critical role in determining performance and reliability. The presence of trace elements such as tin (Sn) and antimony (Sb) introduces complex phase behavior and transformation pathways that must be accurately captured to ensure reliable performance. Computational materials design (CMD) approaches based on CALPHAD databases are well established for accelerating the development of structural materials and their associated processes. To enhance the predictive power of CMD for recycled metals, it is essential to develop and refine the databases of trace elements. In-situ high-throughput experiments offer unique capabilities to probe phase transformation and microstructural evolution with high efficiency under elevated temperatures.

Within the competence center Neutron and X-ray science for industrial technology transitions (NEXT) | KTH, we are aiming to develop a streamlined in situ high-throughput research framework that holistically addresses specimen synthesis, sample environments, data acquisition, analysis, thermodynamic database development, and model validation. In this master thesis project, we aim to develop such a framework specifically for the study of recycled structural metals containing trace elements. Our focus will be on generating experimental data for the development and refinement of thermodynamic descriptions of phase equilibria, involving Sn, Sb, and other relevant impurities.

Aims and objectives

This Master thesis project aims at mapping the phase equilibria for different metal recycling alloy systems using in situ high-throughput XRD methods at both laboratory and large-scale synchrotron facilities. The experimental data will be used for development of thermodynamic databases for metal recycling, through collaboration with the Thermo-Calc software AB. This development will directly contribute to the industrial sustainable transitions.

Activities and project timeline

The following activities will be included in the project:

Activity	2026				
	Month 1	Month 2	Month 3	Month 4	Month 5
1. Literature survey and detailed plan					
2. Planning of beamtimes					
3. Sample preparation					
4. X-ray measurements					
5. Analysis					
6. Reporting					

Starting date: January 2026 or as agreed.

Duration: 5 months

Location: KTH

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