TOOLS FOR ENHANCED DATA-ANALYSIS

Development of post-processing tools for in-situ diffraction studies of phase transformation in metallic materials

THE INDUSTRIAL CHALLENGE

Understanding phase transformations and precipitation in metallic materials is of great importance, both for material producers - for example during heat treatment of new alloys- and for the end-users during welding or in service.

WHY USING A LARGE-SCALE FACILITY?

Heat treatment and welding are typically rapid processes in which the materials may undergo phase transformation. Also, various types of precipitate may form. Understanding the thermodynamic and kinetic boundaries of these transformations is crucial in order to control and mitigate possible detrimental effects.

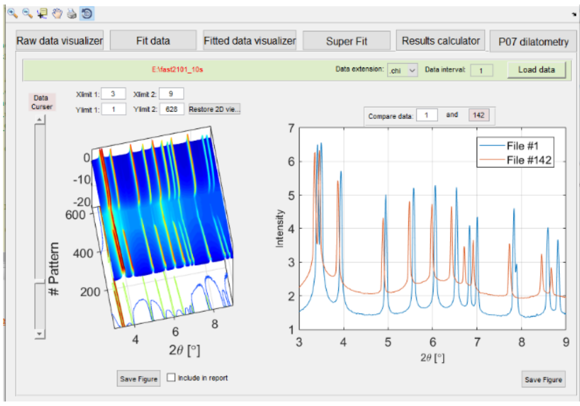
In-house experimental tools such as light/electron microscopy and X-ray diffraction can identify and provide quantitative information, but typically only for the final product and to a shallow depth. Using high energy and high flux synchrotron radiation enables recording in-bulk structural information during these processes.

NEED TO IMPROVE ANALYTICAL TOOL

Time-resolved in-situ experiments can provide a great tool to understand the behavior of materials under certain conditions. However, understanding, visualizing and post-processing large amounts of data is time-consuming and often require some level of programming skills besides competence of the scientific problem itself. This can be challenging for the industry and sometimes an obstacle for using in-situ diffraction experiments. Currently available post-processing tools such as MAUD or TOPAS are generic fitting programs that require crystallographic knowledge and parameters adjustment to model the data. In this project, the steel producer Outokumpu, end-user Alfa Laval and metal and steels research institute Swerim aimed to develop a simple and user-friendly tool specific for metallic materials. Diffraction patterns from duplex stainless steels undergoing different heating and cooling cycles had been collected during a Wide-Angle X-ray Scattering (WAXS) experiment at the P07 High Energy Materials Science (HEMS) beamline, PETRA III, with 10 Hz data acquisition frequency. The program was preliminary designed for analysing the measured data during heating and cooling cycles of duplex stainless-steel data but was further tested for in-house XRD and synchrotron radiation data measured during other experiments.

THE RESULTS AND EXPECTED IMPACT

The project was a great collaboration, promoting extensive discussions to ensure a program with user-friendly design and that can provide relevant results in the production process as well as for materials users.



The screenshot shows the first layer of the program that visualise measured data. Further layers allow fitting various peaks, checking the quality of the fit and performing crystallographic calculations. The program also allows the fitting of several experiments simultaneously. Besides being a simpler and more direct alternative to generic software it also has unique features such as synchronization of different input signals, as temperature. It also has a modular design so that more functionalities can be added in the future. The program can be used for future similar experiments helping to create a simple routine for time-resolved diffraction experiments.

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