Developing post-processing tools for in-situ diffraction studies of phase transformations in metallic materials

Understanding phase transformations and precipitation in metallic materials is of great importance, both for material producers – for example in the heat treatment of new alloys – and for end-users during welding or in service. The PETRA III synchrotron was used in-situ for an experiment observing the kinematics of phase transformations and precipitate formation in duplex stainless steels.

CHALLENGE

Heat treatment and welding are typically rapid processes in which the materials may undergo a 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 allows in-bulk structural information to be recorded during these processes.
Time-resolved in-situ experiments can be a great tool for understanding the behavior of materials under certain conditions. However, understanding, visualizing and post-processing large amounts of data is time-consuming and often requires some level of programming skills, in addition to competence regarding the scientific problem itself. This can be challenging for industry and is sometimes an obstacle for carrying out in-situ diffraction experiments. Currently available post-processing tools, such as MAUD or TOPAS, are generic fitting programs that require a crystallographic knowledge and the adjustment of parameters 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 specifically for metallic materials.

Heat treatment and welding (Credit: iStock / Kerkez)

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METHOD

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 at PETRA III, with a 10 Hz data acquisition frequency. The beamline P07 is operated by DESY's campus partner, Helmholtz-Zentrum hereon. The program was initially designed to analyze data measured during heating and cooling cycles of duplex stainless steel, but this data was also compared with in-house XRD and synchrotron radiation data measured during other experiments.

INSIGHTS & ANALYSIS

The study helped to successfully design and execute an experiment which allowed the kinetics of phase transformations in steel samples to be followed during relatively fast heating and cooling processes. Additionally, it was able to penetrate several millimeters into the sample of duplex stainless steel to observe in-depth changes. The project was also a great collaboration, promoting extensive discussions to ensure that the software has a user-friendly design and can provide relevant results in the production process as well as for the users of materials. The program can be used for similar experiments in the future, helping to create a simple routine for time-resolved diffraction experiments.

BENEFITS

This study was a success in terms of both software development and material studies. The high-energy beams at PETRA III and the results obtained through this collaborative study by numerous experts, such as SWERIM, Outukumpu and Alfa Laval, can be implemented directly by the manufacturers to minimize the formation of unwanted phases during the process. Not only was the hardware improved, but also the software in form of a post-processing tool for data analysis, which will be helpful in future studies. The case study was a good test for the software: both the setting and users belong to the target group for the final product.

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