In situ X-ray diffraction during heat treatments to guide machine learning modelling of phase transitions in steels

INDUSTRIAL PILOT PROJECT

THE INDUSTRIAL CHALLENGE

A recent development in steel modelling is machine learning (ML), a sub-branch of artificial intelligence (AI). ML is an important complement to physical based modelling methods, and some steel phenomena can only be modelled using a data-driven approach like ML. Ferritico develops ML models and software to predict phase transformations during heat treatments, so-called continuous cooling transformations (CCT), which is very difficult to predict accurately using any physical model. The modelling of CCT is critical input data for thermomechanical FEM simulations in process and product development, i.e. for case hardening and tool steels.

WHY USING A LARGE SCALE FACILITY

ML is a datadriven method and thus the CCT data must be of excellent quality. This can only be ensured through in situ measurements during real heat treatments. Traditionally this is performed indirectly by dilatometry, but the only viable measurement for direct in situ measurements is time-resolved synchrotron x-ray diffraction (SXRD). Such measurements would add key data for the modelling of CCT and provide excellent validation of the modelling.

HOW THE WORK WAS DONE

The experiments were conducted at the P07 beamline of Petra III, Hamburg. The samples were heated to austenitization temperatures, to fully transform the steel to the austenite phase, followed by continuous cooling at different rates and at different stages to investigate e.g. the effect of a rate change at low temperatures for the martensitic transformation. Considering the rapid heating and cooling applied, we needed to ensure time resolutions in the order of milli-seconds, about 50 ms, which means that the Pilatus detector was used. The evolution of the carbon diffusion was investigated by studying the peak shifts for the fcc and bcc phases. In addition, dislocation densities were possible to eliminate by the use of the Williamson-Hall and warren Averbach methods.

THE RESULTS AND EXPECTED IMPACT

The project successfully monitored and measured the volume fraction evolution of the ferrite, martensite as well as precipitate phases. The extremely precise in situ SXRD measurements provided high quality data to further refine the precision of the steel heat treatment simulation ML models. The data also enabled validation to calibrate the current version of the models and gave insights to where to focus future work of Ferritico ML model development.

Phase transformation temperatures

The aggregated average error for simulation of the temperatures on which transformation of the phases Ferrite, Pearlite, Bainite and Martensite are starting and finishing respectively. The benchmark is based on empirically measured CCT diagrams for 14 steel grades (some chemical compositions listed below) that are not included in the machine learning database and where benchmarking CCT data is available for 8-12 cooling rates. In the table, _s and _f refer to the start and finish temperature of the transformation of a phase, e.g. Fe_s being Ferrite start temperature.

	Ferritico error	Competitor error
Fe_s	34.9 °C	49.0 °C
Fe_f	45.7 °C	77.5 °C
P_s	28.4 °C	68.0 °C
P_f	55.2 °C	117.1 °C
B_s	53.6 °C	74.3 °C
B_f	40.1 °C	93.4 °C
M_s	39.6 °C	47.8 °C

The so far unprecedented model performance for CCT predictions has been confirmed with the high quality SXRD data that has been compared with the ML model simulation.

"The project and the generated SXRD data will have significant impact on steel simulation software performance and support industry transition from trial-and-error process and product development to a data-driven development process" ***/Claes Holmström, Ferritico***

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