Active learning-based optimization of bainitic steels using probabilistic hybrid material models

Jürgen Spitaler[1], Natalia Bedoya[1], Bernd Schuscha[1], Christian Stecher[1], Manfred Mücke[1], Dominik Brandl[1], Daniel Scheiber[1], Han Tran[2], Heimo Gursch[2], Lorenz Romaner[3]
[1]Materials Center Leoben Forschung GmbH, Roseggerstrasse 12, 8700 Leoben, Austria
[2]Know-Center GmbH, Sandgasse 34, 8010 Graz, Austria
[3]Montanuniversität Leoben, Leoben, Austria

Juergen.spitaler@mcl.at

In materials development, creating new data points is often very costly due to the effort needed for materials synthesis, sample preparation and characterization. Therefore, all available knowledge in terms of data, physical models and expert knowledge should be exploited in the most efficient way, referred to as *optimal knowledge exploitation*. Moreover, the number of new samples/data points required in terms of synthesis and characterization of new materials should be kept at a minimum to save time and money, referred to as *sample efficiency*. We will present the methodology for the efficient optimization of bainitic steels as implemented in *ALPmat,* the MCL Active Learning Platform for accelerated materials development. For *optimal knowledge exploitation,* a hybrid approach is followed, where physical models and expert knowledge are combined with data from observations. The resulting hybrid models are part of an Active Learning Loop (ALL) addressing material design objectives in an iterative way via optimization of the material's chemistry and processing parameters, while also minimizing the number of new samples ensuring *sample efficiency.* We will present the details of the hybrid modeling approach for bainitic steels in terms of physical knowledge, data-driven models and combination thereof. Moreover, we will describe *ALPmat* with its hard- and software for the platform backbone, the FAIR database, the framework for running physical modeling and Bayesian optimization algorithms, and further integrated software services. Finally, we will show the results of the developed methodology as implemented in *ALPmat* for the improvement of bainitic steels. This use case covers a Bayesian multi-objective optimization of the uniform elongation and the yield strength as a function of chemical composition and processing parameters.